

Supplement of Atmos. Chem. Phys., 19, 4075–4091, 2019
<https://doi.org/10.5194/acp-19-4075-2019-supplement>
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Atmospheric
Chemistry
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Supplement of

Mechanistic and kinetics investigations of oligomer formation from Criegee intermediate reactions with hydroxyalkyl hydroperoxides

Long Chen et al.

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Contents:

Table S1 Y/X (Y = M06-2X, CCSD(T), X = 6-311+G(2df,2p), def2-TZVP) calculated energy barrier($\Delta E_a^\#$, $\Delta G_a^\#$) for the addition reactions of carbonyl oxides with HHPs based on the M06-2X/6-311+G(2df,2p) optimized geometries (kcal·mol⁻¹)

Table S2 The partition function of every vibrational mode involved in the complex IM1a

Table S3 The partition function of every vibrational mode involved in the complex IM2a

Table S4 AIM properties at the bond critical points for the forming bonds B1-B4

Table S5 Rate coefficients (cm³ molecule⁻¹ s⁻¹) of CH₂OO reactions with P1a, P1b, P1c and P1d computed at different temperatures

Table S6 Rate coefficients (cm³ molecule⁻¹ s⁻¹) of *anti*-CH₃CHOO reactions with P3a, P3b, P3c and P3d computed at different temperatures

Table S7 Rate coefficients (cm³ molecule⁻¹ s⁻¹) of *syn*-CH₃CHOO reactions with P5a, P5b, P5c and P5d computed at different temperatures

Table S8 Rate coefficients (cm³ molecule⁻¹ s⁻¹) of (CH₃)₂CHOO reactions with P7a, P7b, P7c and P7d computed at different temperatures

Table S9 Rate coefficients (cm³ molecule⁻¹ s⁻¹) of elementary reactions R1a and R9

Figure S1. PES (ΔG and ΔE (*italic*)) for the reaction of CH₂OO with HO-CH₂OO-H (Pb₁) calculated at the M06-2X/def2-TZVP//M06-2X/6-311+G(2df,2p) level of theory

Figure S2 PES (ΔG and ΔE (*italic*)) for the reaction of HO-C(CH₃)HOO-H with *anti*-(a) and *syn*-CH₃CHOO(b) calculated at the M06-2X/def2-TZVP//M06-2X/6-311+G(2df,2p) level of theory

Figure S3 PES (ΔG and ΔE (*italic*)) for the reaction of (CH₃)₂COO with HO-C(CH₃)₂OO-H (Pb₃) calculated at the M06-2X/def2-TZVP//M06-2X/6-311+G(2df,2p) level of theory

Figure S4. Optimized geometries, z-matrices and vibrational frequencies of all stationary points in the reaction of 2CH₂OO with HO-CH₂OO-H at the M06-2X/6-311+G(2df,2p) level of theory

Figure S5. PES (ΔG and ΔE (*italic*)) for the reaction of HO-CH₂OO-H (Pa₁) with OH computed at the M06-2X/def2-TZVP//M06-2X/6-311+G(2df,2p) level of theory

Figure S6. Optimized geometries, z-matrices and vibrational frequencies of all stationary points in the reaction of 2*anti*-CH₃CHOO with HO-CH(CH₃)OO-H(Pa₂ and Pb₂) at the M06-2X/6-311+G(2df,2p) level of theory

Figure S7. Optimized geometries, z-matrices and vibrational frequencies of all stationary points in the reaction of 2*syn*-CH₃CHOO with HO-CH(CH₃)OO-H(Pa_{2'} and Pb_{2'}) at the M06-2X/6-311+G(2df,2p) level of theory

Figure S8. Optimized geometries, z-matrices and vibrational frequencies of all stationary points in the reaction of (CH₃)₂COO with HO-C(CH₃)₂OO-H at the M06-2X/6-311+G(2df,2p) level of theory

Figure S9. PES (ΔG and ΔE (*italic*)) of distinct SCI reactions with HO-CH(CH₃)OO-H(Pa₂) calculated at the M06-2X/def2-TZVP//M06-2X/6-311+G(2df,2p) level of theory

Figure S10. PES (ΔG and ΔE (*italic*)) of distinct SCI reactions with HO-CH(CH₃)OO-H(Pa₂) calculated at the M06-2X/def2-TZVP//M06-2X/6-311+G(2df,2p) level of theory

Figure S11. PES (ΔG and ΔE (*italic*)) of distinct SCI reactions with HO-C(CH₃)₂OO-H(Pa₃) calculated at the M06-2X/def2-TZVP//M06-2X/6-311+G(2df,2p) level of theory

Table S1 Y/X (Y = M06-2X, CCSD(T), X = 6-311+G(2df,2p), def2-TZVP) calculated energy barrier($\Delta E_a^\#$, $\Delta G_a^\#$) for the addition reactions of carbonyl oxides with HHPs based on the M06-2X/6-311+G(2df,2p) optimized geometries (kcal·mol⁻¹)

| Reactions | CCSD(T)/6-311+G(2df,2p) | | M06-2X/def2-TZVP | |
|-----------|---------------------------------------|---------------------------------------|---------------------------------------|---------------------------------------|
| | $\Delta E_a^\#$ | $\Delta G_a^\#$ | $\Delta E_a^\#$ | $\Delta G_a^\#$ |
| R1a | 9.4 ^a ; 7.9 ^b | 10.1 ^a ; 8.6 ^b | 8.0 ^a ; 7.6 ^b | 8.8 ^a ; 8.4 ^b |
| R1b | 13.0 ^a ; 11.6 ^b | 13.3 ^a ; 11.9 ^b | 11.9 ^a ; 11.4 ^b | 12.2 ^a ; 11.7 ^b |
| R1c | 8.1 ^a ; 6.7 ^b | 9.2 ^a ; 7.8 ^b | 6.9 ^a ; 6.4 ^b | 7.9 ^a ; 7.4 ^b |
| R1d | 8.6 ^a ; 7.6 ^b | 10.2 ^a ; 9.2 ^b | 7.0 ^a ; 6.7 ^b | 8.7 ^a ; 8.4 ^b |
| R3a | 6.6 ^a ; 4.9 ^b | 7.1 ^a ; 5.4 ^b | 5.8 ^a ; 4.4 ^b | 6.2 ^a ; 5.8 ^b |
| R3b | 8.4 ^a ; 7.3 ^b | 9.7 ^a ; 8.6 ^b | 7.3 ^a ; 6.8 ^b | 8.8 ^a ; 8.3 ^b |
| R3c | 6.5 ^a ; 4.8 ^b | 7.3 ^a ; 5.6 ^b | 5.8 ^a ; 5.4 ^b | 6.6 ^a ; 6.2 ^b |
| R3d | 8.4 ^a ; 6.8 ^b | 9.7 ^a ; 8.1 ^b | 7.3 ^a ; 6.8 ^b | 8.6 ^a ; 8.1 ^b |
| R5a | 12.3 ^a ; 10.9 ^b | 13.2 ^a ; 11.8 ^b | 11.5 ^a ; 11.1 ^b | 12.5 ^a ; 12.1 ^b |
| R5b | 11.0 ^a ; 9.4 ^b | 12.4 ^a ; 10.8 ^b | 10.6 ^a ; 10.1 ^b | 12.0 ^a ; 11.5 ^b |
| R5c | 12.0 ^a ; 10.6 ^b | 13.3 ^a ; 11.9 ^b | 11.3 ^a ; 10.9 ^b | 12.5 ^a ; 12.1 ^b |
| R5d | 12.2 ^a ; 11.0 ^b | 13.8 ^a ; 12.6 ^b | 11.4 ^a ; 11.0 ^b | 13.0 ^a ; 12.6 ^b |

a and b represent without and with considering the BSSE correction

According to the principle of statistical thermodynamics, the entropy can be described as eqn

(1)

$$S = \frac{H - G}{T} \quad (1)$$

where H is the enthalpy; G is the free energy; T is the temperature in Kelvin. The relationship between the entropy and the partition function can be written as eqn (2)

$$S = k \ln \frac{q^N}{N!} + NkT \left(\frac{\partial \ln q}{\partial T} \right)_{V,N} \quad (2)$$

where k is the Boltzmann constant; q is the partition function, it mainly includes translation (q_{trans}), vibration (q_{vib}), external rotation (q_{rot}), electronic (q_{ele}) and torsional (q_{tor}) partition functions ($q = q_{trans}q_{vib}q_{rot}q_{ele}q_{tor}$) (Mendes, et al., 2014). Among these partition functions, the q_{vib} plays an important role in determining the entropic factors. Thus, the q_{vib} is used to evaluate the contribution of vibrational mode to the entropic factor. The q_{vib} can be described as eqn (3)

$$q_{vib} = \exp\left(-\frac{1}{2} \frac{hv}{kT}\right) \times \left(\frac{1}{1 - e^{-hv/kT}}\right) \quad (3)$$

Table S2 The partition function of every vibrational mode involved in the complex IM1a

| N | ν | q_{vib} | percent(%) |
|----|---------|------------------|------------|
| 1 | 51.49 | 4.03 | 30.43 |
| 2 | 123.66 | 1.66 | 12.52 |
| 3 | 149.16 | 1.37 | 10.31 |
| 4 | 158.76 | 1.28 | 9.66 |
| 5 | 199.39 | 1.00 | 7.58 |
| 6 | 242.53 | 0.81 | 6.12 |
| 7 | 257.19 | 0.76 | 5.74 |
| 8 | 422.78 | 0.42 | 3.15 |
| 9 | 501.75 | 0.33 | 2.48 |
| 10 | 538.04 | 0.30 | 2.24 |
| 11 | 642.00 | 0.22 | 1.69 |
| 12 | 723.92 | 0.18 | 1.37 |
| 13 | 858.58 | 0.13 | 0.97 |
| 14 | 896.89 | 0.12 | 0.89 |
| 15 | 958.09 | 0.10 | 0.76 |
| 16 | 1070.70 | 0.08 | 0.58 |
| 17 | 1093.27 | 0.07 | 0.55 |
| 18 | 1112.93 | 0.07 | 0.52 |
| 19 | 1134.12 | 0.07 | 0.50 |
| 20 | 1270.31 | 0.05 | 0.36 |
| 21 | 1300.08 | 0.04 | 0.33 |
| 22 | 1397.45 | 0.03 | 0.26 |
| 23 | 1429.61 | 0.03 | 0.24 |
| 24 | 1456.77 | 0.03 | 0.23 |
| 25 | 1506.87 | 0.03 | 0.20 |
| 26 | 1588.46 | 0.02 | 0.17 |
| 27 | 1674.72 | 0.02 | 0.13 |
| 28 | 3088.99 | 0.00 | 0.00 |
| 29 | 3148.98 | 0.00 | 0.00 |
| 30 | 3162.08 | 0.00 | 0.00 |
| 31 | 3162.65 | 0.00 | 0.00 |
| 32 | 3305.08 | 0.00 | 0.00 |
| 33 | 3868.49 | 0.00 | 0.00 |

Table S3 The partition function of every vibrational mode involved in the complex IM2a

| N | ν | q_{vib} | percent(%) |
|----|---------|------------------|------------|
| 1 | 45.57 | 4.56 | 19.74 |
| 2 | 66.77 | 3.10 | 13.44 |
| 3 | 93.88 | 2.20 | 9.52 |
| 4 | 102.82 | 2.00 | 8.68 |
| 5 | 122.46 | 1.67 | 7.25 |
| 6 | 144.25 | 1.41 | 6.12 |
| 7 | 151.51 | 1.34 | 5.82 |
| 8 | 186.88 | 1.08 | 4.66 |
| 9 | 236.15 | 0.84 | 3.62 |
| 10 | 242.41 | 0.81 | 3.52 |
| 11 | 324.58 | 0.58 | 2.51 |
| 12 | 383.38 | 0.47 | 2.05 |
| 13 | 460.65 | 0.37 | 1.61 |
| 14 | 475.56 | 0.35 | 1.54 |
| 15 | 546.86 | 0.29 | 1.25 |
| 16 | 589.00 | 0.26 | 1.12 |
| 17 | 676.46 | 0.20 | 0.89 |
| 18 | 704.48 | 0.19 | 0.82 |
| 19 | 751.93 | 0.17 | 0.73 |
| 20 | 889.93 | 0.12 | 0.52 |
| 21 | 904.59 | 0.12 | 0.50 |
| 22 | 957.33 | 0.10 | 0.44 |
| 23 | 1053.66 | 0.08 | 0.35 |
| 24 | 1082.87 | 0.07 | 0.33 |
| 25 | 1103.67 | 0.07 | 0.31 |
| 26 | 1123.39 | 0.07 | 0.29 |
| 27 | 1129.87 | 0.07 | 0.29 |
| 28 | 1139.95 | 0.06 | 0.28 |
| 29 | 1188.07 | 0.06 | 0.25 |
| 30 | 1271.30 | 0.05 | 0.20 |
| 31 | 1306.97 | 0.04 | 0.19 |
| 32 | 1353.81 | 0.04 | 0.17 |
| 33 | 1383.99 | 0.04 | 0.16 |
| 34 | 1415.10 | 0.03 | 0.14 |
| 35 | 1438.67 | 0.03 | 0.14 |
| 36 | 1455.62 | 0.03 | 0.13 |
| 37 | 1457.70 | 0.03 | 0.13 |
| 38 | 1501.08 | 0.03 | 0.12 |
| 39 | 1569.37 | 0.02 | 0.10 |
| 40 | 1663.59 | 0.02 | 0.08 |
| 41 | 3104.57 | 0.00 | 0.00 |
| 42 | 3113.88 | 0.00 | 0.00 |

| | | | |
|----|---------|------|------|
| 43 | 3140.47 | 0.00 | 0.00 |
| 44 | 3173.49 | 0.00 | 0.00 |
| 45 | 3187.95 | 0.00 | 0.00 |
| 46 | 3286.9 | 0.00 | 0.00 |
| 47 | 3436.06 | 0.00 | 0.00 |
| 48 | 3910.66 | 0.00 | 0.00 |

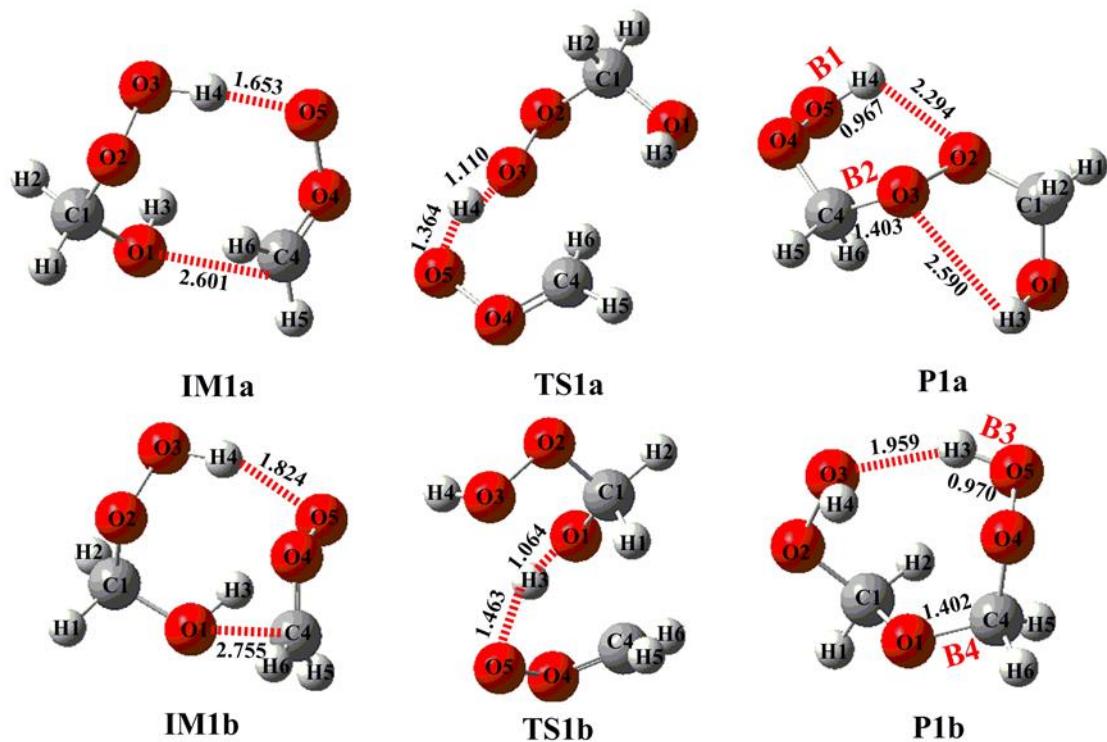


Table S4 AIM properties at the bond critical points for the forming bonds B1-B4

| Bond | ρ (e/ \AA^3) | ∇^2 (e/ \AA^3) | Eigenvalue 1 | Eigenvalue 2 | Eigenvalue 3 |
|-----------|-----------------------------|---------------------------------|--------------|--------------|--------------|
| B1(O5-H4) | 0.370 | -2.776 | -1.9316 | -1.8598 | 1.0148 |
| B2(O3-C4) | 0.271 | -0.559 | -0.5734 | -0.5112 | 0.5258 |
| B3(O5-H3) | 0.364 | -2.760 | -1.945 | -1.8743 | 1.0588 |
| B4(O1-C4) | 0.269 | -0.565 | -0.5734 | -0.5054 | 0.5139 |

Table S5 Rate coefficients ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) of CH_2OO reactions with P1a, P1b, P1c and P1d computed at different temperatures

| T/K | $k_{(\text{CH}_2\text{OO} + \text{P1a})}$ | $k_{(\text{CH}_2\text{OO} + \text{P1b})}$ | $k_{(\text{CH}_2\text{OO} + \text{P1c})}$ | $k_{(\text{CH}_2\text{OO} + \text{P1d})}$ |
|-----|---|---|---|---|
| 273 | 5.1×10^{-12} | 3.5×10^{-12} | 8.2×10^{-13} | 4.8×10^{-11} |
| 280 | 4.0×10^{-12} | 2.9×10^{-12} | 7.1×10^{-13} | 3.7×10^{-11} |
| 298 | 2.3×10^{-12} | 1.9×10^{-12} | 5.2×10^{-13} | 1.9×10^{-11} |
| 300 | 2.2×10^{-12} | 1.8×10^{-12} | 5.0×10^{-13} | 1.8×10^{-11} |
| 320 | 1.3×10^{-12} | 1.2×10^{-12} | 3.7×10^{-13} | 1.0×10^{-11} |
| 340 | 8.3×10^{-13} | 8.5×10^{-13} | 2.8×10^{-13} | 5.9×10^{-12} |
| 360 | 5.6×10^{-13} | 6.3×10^{-13} | 2.3×10^{-13} | 3.8×10^{-12} |
| 380 | 4.0×10^{-13} | 4.9×10^{-13} | 1.9×10^{-13} | 2.5×10^{-12} |
| 400 | 3.0×10^{-13} | 3.9×10^{-13} | 1.6×10^{-13} | 1.8×10^{-12} |

Table S6 Rate coefficients ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) of *anti*-CH₃CHO reactions with P3a, P3b, P3c and P3d computed at different temperatures

| T/K | $k_{(\text{anti+P3a})}$ | $k_{(\text{anti+P3b})}$ | $k_{(\text{anti+P3c})}$ | $k_{(\text{anti+P3d})}$ |
|-----|-------------------------|-------------------------|-------------------------|-------------------------|
| 273 | 3.5×10^{-9} | 2.3×10^{-9} | 1.7×10^{-7} | 2.1×10^{-9} |
| 280 | 2.3×10^{-9} | 1.4×10^{-9} | 1.0×10^{-7} | 1.4×10^{-9} |
| 298 | 8.8×10^{-10} | 5.8×10^{-10} | 2.9×10^{-8} | 5.9×10^{-10} |
| 300 | 8.0×10^{-10} | 5.3×10^{-10} | 2.6×10^{-8} | 5.4×10^{-10} |
| 320 | 3.2×10^{-10} | 2.3×10^{-10} | 7.9×10^{-9} | 2.3×10^{-10} |
| 340 | 1.4×10^{-10} | 1.1×10^{-10} | 2.8×10^{-9} | 1.1×10^{-10} |
| 360 | 7.1×10^{-11} | 5.8×10^{-11} | 1.1×10^{-9} | 5.9×10^{-11} |
| 380 | 3.8×10^{-11} | 3.3×10^{-11} | 4.9×10^{-10} | 3.4×10^{-11} |
| 400 | 2.2×10^{-11} | 2.0×10^{-11} | 2.4×10^{-10} | 2.0×10^{-11} |

Table S7 Rate coefficients ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) of *syn*-CH₃CHO reactions with P5a, P5b, P5c and P5d computed at different temperatures

| T/K | $k_{(\text{syn+P5a})}$ | $k_{(\text{syn+P5b})}$ | $k_{(\text{syn+P5c})}$ | $k_{(\text{syn+P5d})}$ |
|-----|------------------------|------------------------|------------------------|------------------------|
| 273 | 2.1×10^{-11} | 1.7×10^{-13} | 2.1×10^{-11} | 2.4×10^{-13} |
| 280 | 1.5×10^{-11} | 1.4×10^{-13} | 1.5×10^{-11} | 2.0×10^{-13} |
| 298 | 7.5×10^{-12} | 1.0×10^{-13} | 7.6×10^{-12} | 1.4×10^{-13} |
| 300 | 6.9×10^{-12} | 9.7×10^{-14} | 7.0×10^{-12} | 1.4×10^{-13} |
| 320 | 3.5×10^{-12} | 6.9×10^{-14} | 3.6×10^{-12} | 9.6×10^{-14} |
| 340 | 1.9×10^{-12} | 5.2×10^{-14} | 2.0×10^{-12} | 7.1×10^{-14} |
| 360 | 1.1×10^{-12} | 4.0×10^{-14} | 1.2×10^{-12} | 5.5×10^{-14} |
| 380 | 7.1×10^{-13} | 3.0×10^{-14} | 7.3×10^{-13} | 4.4×10^{-14} |
| 400 | 4.7×10^{-13} | 2.6×10^{-14} | 4.9×10^{-13} | 3.6×10^{-14} |

Table S8 Rate coefficients ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) of $(\text{CH}_3)_2\text{CHOO}$ reactions with P7a, P7b, P7c and P7d computed at different temperatures

| T/K | $k_{((\text{CH}_3)_2\text{CHOO} + \text{P7a})}$ | $k_{((\text{CH}_3)_2\text{CHOO} + \text{P7b})}$ | $k_{((\text{CH}_3)_2\text{CHOO} + \text{P7c})}$ | $k_{((\text{CH}_3)_2\text{CHOO} + \text{P7d})}$ |
|-----|---|---|---|---|
| 273 | 7.8×10^{-14} | 9.1×10^{-14} | 1.8×10^{-12} | 4.5×10^{-13} |
| 280 | 6.8×10^{-14} | 8.2×10^{-14} | 1.5×10^{-12} | 3.9×10^{-13} |
| 298 | 5.0×10^{-14} | 6.6×10^{-14} | 1.0×10^{-12} | 2.8×10^{-13} |
| 300 | 4.8×10^{-14} | 6.5×10^{-14} | 9.9×10^{-13} | 2.7×10^{-13} |
| 320 | 3.6×10^{-14} | 5.3×10^{-14} | 6.9×10^{-13} | 1.9×10^{-13} |
| 340 | 2.8×10^{-14} | 4.5×10^{-14} | 5.1×10^{-13} | 1.5×10^{-13} |
| 360 | 2.2×10^{-14} | 3.9×10^{-14} | 3.9×10^{-13} | 1.2×10^{-13} |
| 380 | 1.9×10^{-14} | 3.5×10^{-14} | 3.1×10^{-13} | 9.6×10^{-14} |
| 400 | 1.6×10^{-14} | 3.1×10^{-14} | 2.5×10^{-13} | 8.0×10^{-14} |

Table S9 Rate coefficients ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$) of elementary reactions R1a and R9

| T | $k_{\text{TST(R1a)}}$ | $k_{\text{CVTST(R1a)}}$ | $k_{\text{TST(R9)}}$ | $k_{\text{CVTST(R9)}}$ |
|-----|-----------------------|-------------------------|-----------------------|------------------------|
| 273 | 1.2×10^{-11} | 3.5×10^{-11} | 5.5×10^{-9} | 1.3×10^{-8} |
| 280 | 9.4×10^{-12} | 2.6×10^{-11} | 3.7×10^{-9} | 8.5×10^{-9} |
| 298 | 5.4×10^{-12} | 1.4×10^{-11} | 1.5×10^{-9} | 3.2×10^{-9} |
| 300 | 5.1×10^{-12} | 1.3×10^{-11} | 1.3×10^{-9} | 2.9×10^{-9} |
| 320 | 3.0×10^{-12} | 7.2×10^{-12} | 5.5×10^{-10} | 1.1×10^{-9} |
| 340 | 1.9×10^{-12} | 4.2×10^{-12} | 2.6×10^{-10} | 5.0×10^{-10} |
| 360 | 1.2×10^{-12} | 2.7×10^{-12} | 1.4×10^{-10} | 2.4×10^{-10} |
| 380 | 8.6×10^{-13} | 1.8×10^{-12} | 7.1×10^{-11} | 1.3×10^{-10} |
| 400 | 6.3×10^{-13} | 1.2×10^{-12} | 4.1×10^{-11} | 7.3×10^{-11} |

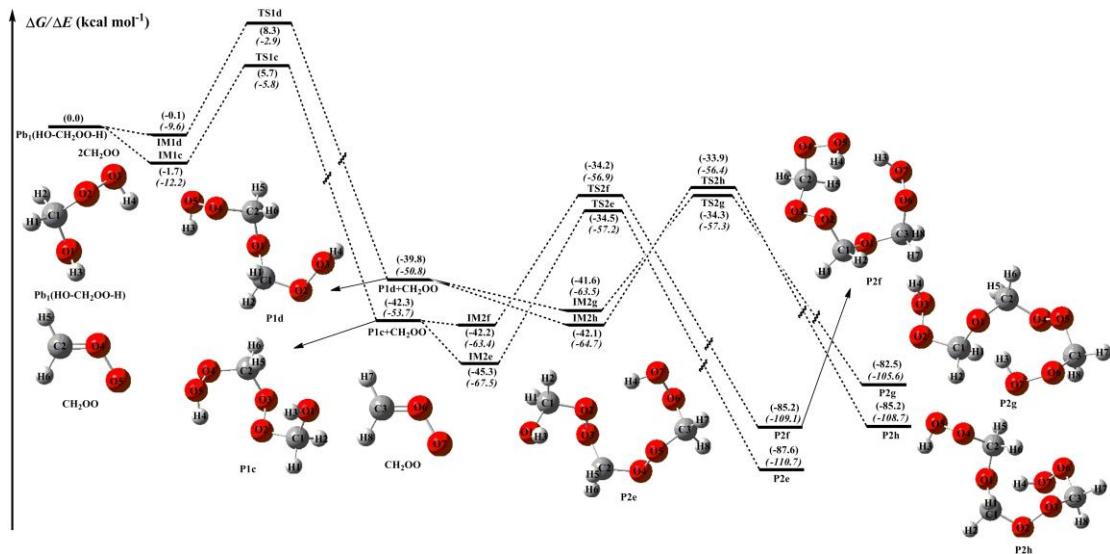


Figure S1. PES (ΔG and ΔE (*italic*)) for the reaction of CH_2OO with $\text{HO}-\text{CH}_2\text{OO}-\text{H}$ (Pb_1) calculated at the M06-2X/def2-TZVP//M06-2X/6-311+G(2df,2p) level of theory

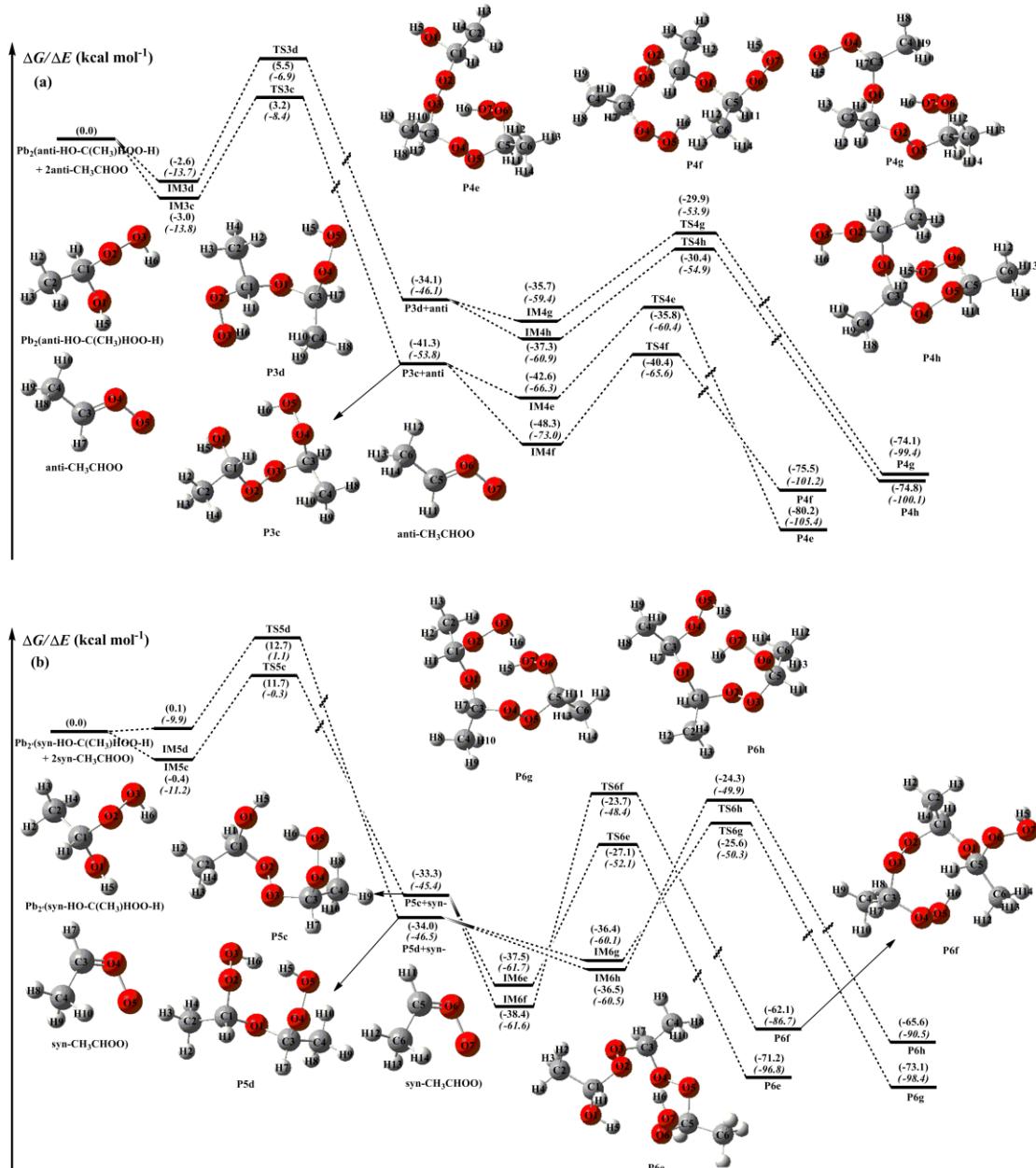


Figure S2 PES (ΔG and ΔE (*italic*)) for the reaction of HO-C(CH₃)HOO-H with *anti*-(a) and *syn*-CH₃CHOO(b) calculated at the M06-2X/def2-TZVP//M06-2X/6-311+G(2df,2p) level of theory

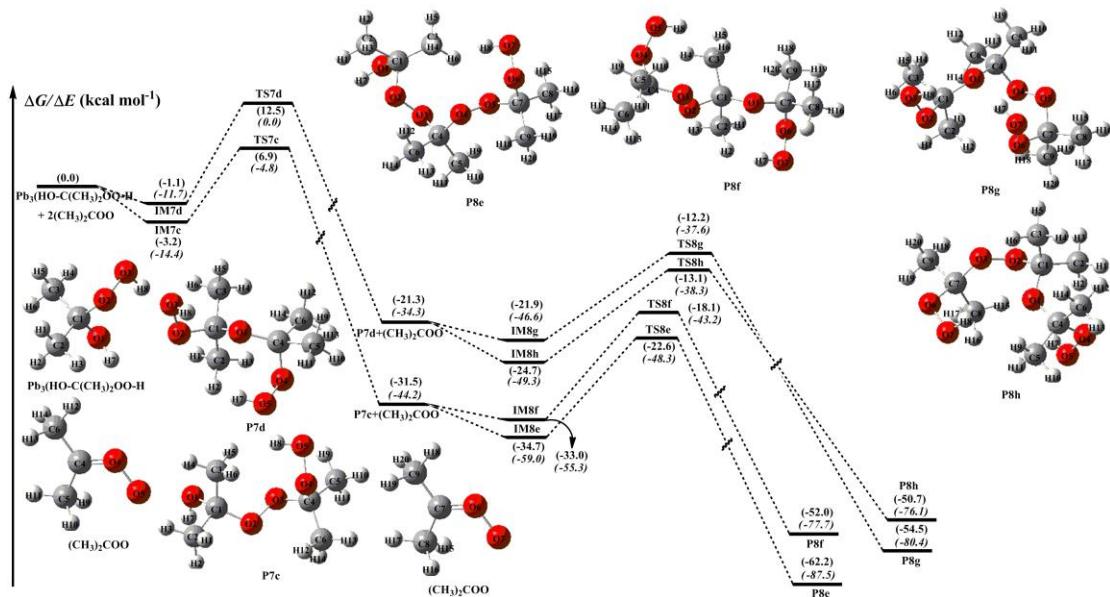


Figure S3 PES (ΔG and ΔE (italic)) for the reaction of $(\text{CH}_3)_2\text{COO}$ with $\text{HO-C(CH}_3)_2\text{OO-H}$ (Pb_3) calculated at the M06-2X/def2-TZVP//M06-2X/6-311+G(2df,2p) level of theory

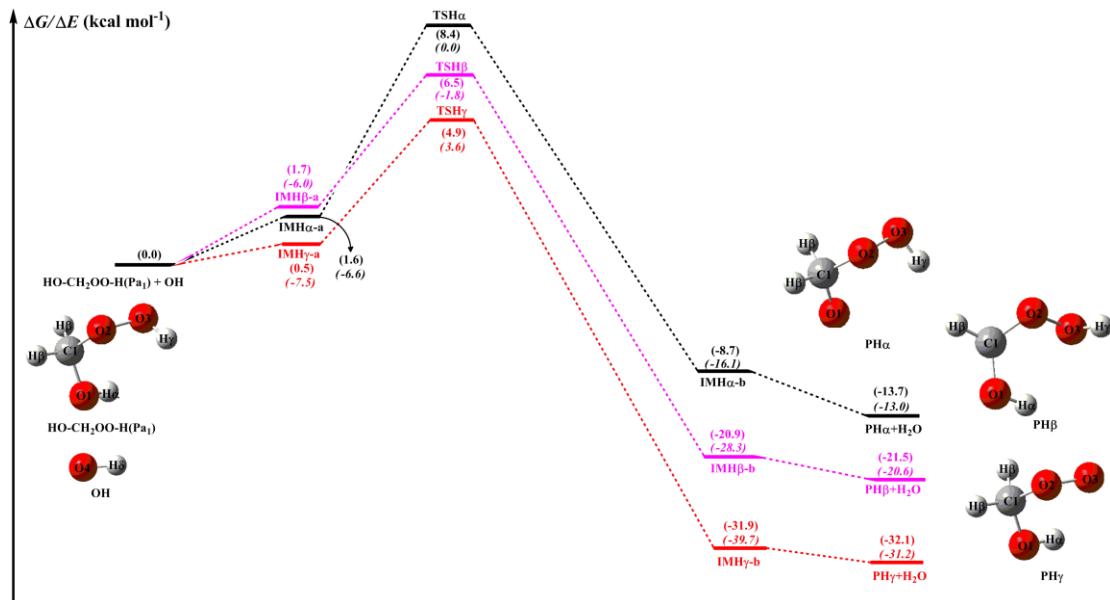


Figure S5. PES (ΔG and ΔE (*italic*)) for the reaction of HO-CH₂OO-H (Pa₁) with OH computed at the M06-2X/def2-TZVP//M06-2X/6-311+G(2df,2p) level of theory

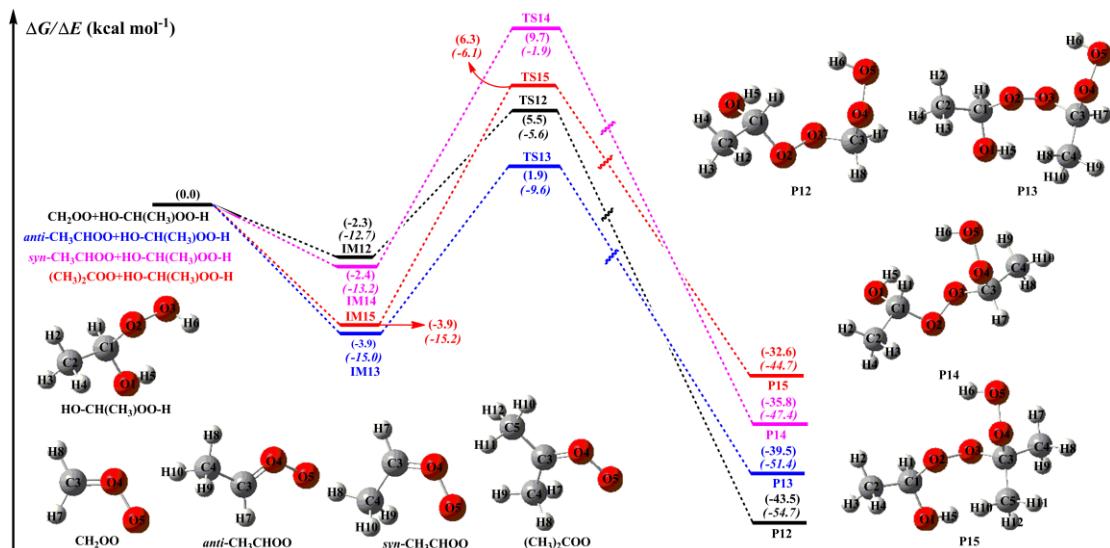


Figure S9. PES (ΔG and ΔE (*italic*)) of distinct SCI reactions with $\text{HO-CH}(\text{CH}_3)\text{OO-H}$ (Pa₂) calculated at the M06-2X/def2-TZVP//M06-2X/6-311+G(2df,2p) level of theory

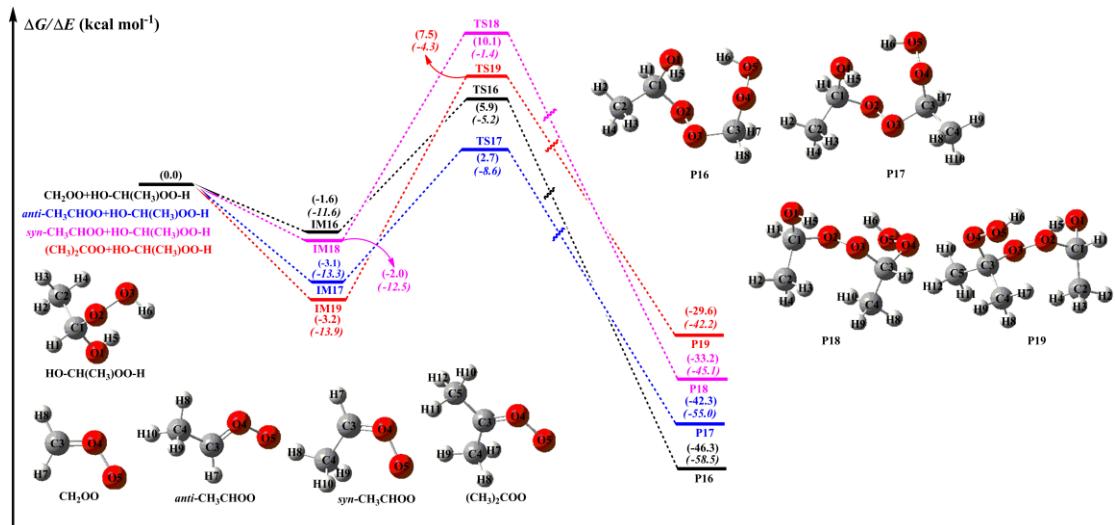


Figure S10. PES (ΔG and ΔE (*italic*)) of distinct SCI reactions with $\text{HO-CH}(\text{CH}_3)\text{OO-H}$ (Pa₂) calculated at the M06-2X/def2-TZVP//M06-2X/6-311+G(2df,2p) level of theory

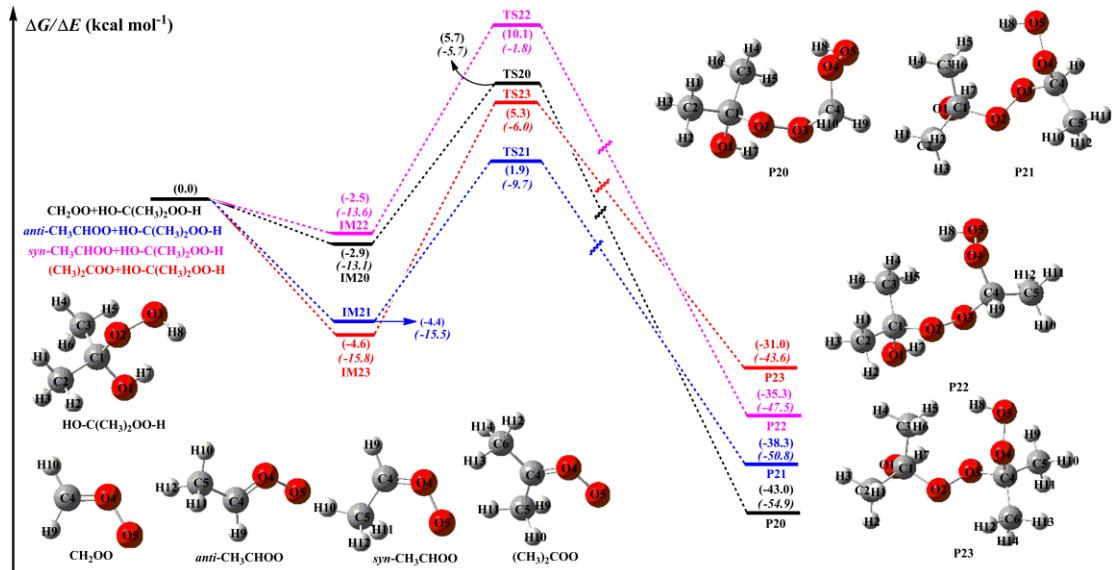
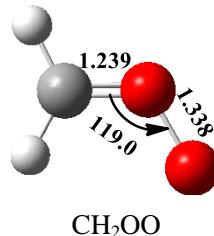


Figure S11. PES (ΔG and ΔE (*italic*)) of distinct SCI reactions with $\text{HO-C(CH}_3)_2\text{OO-H}$ (Pa₃) calculated at the M06-2X/def2-TZVP//M06-2X/6-311+G(2df,2p) level of theory

Figure S4. Optimized geometries, z-matrices and vibrational frequencies of all stationary points in the reaction of 2CH₂OO with HO-CH₂OO-H at the M06-2X/6-311+G(2df,2p) level of theory



| | | | | | | | |
|---|---|----|---|----|---|----|---|
| C | | | | | | | |
| O | 1 | B1 | | | | | |
| O | 2 | B2 | 1 | A1 | | | |
| H | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| H | 1 | B4 | 2 | A3 | 3 | D2 | 0 |

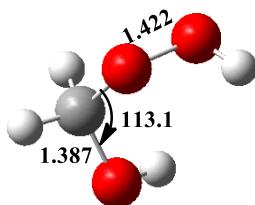
Variables:

| | |
|----|--------------|
| B1 | 1.23895372 |
| B2 | 1.33773725 |
| B3 | 1.08411000 |
| B4 | 1.08104852 |
| A1 | 119.01084624 |
| A2 | 118.71143342 |
| A3 | 115.75496765 |
| D1 | 0.00000000 |
| D2 | 180.00000000 |

Harmonic Vibrational Frequencies (cm⁻¹):

547.22 712.25 944.77 1021.21 1264.15 1434.06 1628.10 3142.26 3296.00

Rotational constants (B/GHZ): 81.8651497 12.6910280 10.9876788



Pa₁(HO-CH₂OO-H)

| | | | | | | | |
|---|---|----|---|----|---|----|---|
| C | | | | | | | |
| O | 1 | B1 | | | | | |
| O | 2 | B2 | 1 | A1 | | | |
| H | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| H | 1 | B4 | 2 | A3 | 3 | D2 | 0 |
| O | 1 | B5 | 2 | A4 | 3 | D3 | 0 |
| H | 3 | B6 | 2 | A5 | 1 | D4 | 0 |
| H | 6 | B7 | 1 | A6 | 2 | D5 | 0 |

Variables:

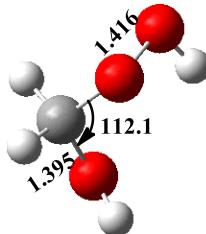
| | |
|----|------------|
| B1 | 1.40359950 |
| B2 | 1.42184472 |

| | |
|----|---------------|
| B3 | 1.08832012 |
| B4 | 1.09298865 |
| B5 | 1.38702567 |
| B6 | 0.96387803 |
| B7 | 0.95983640 |
| A1 | 106.22681004 |
| A2 | 103.84544465 |
| A3 | 108.76259188 |
| A4 | 113.09492724 |
| A5 | 101.24544362 |
| A6 | 108.59940983 |
| D1 | -174.17439700 |
| D2 | -55.77995767 |
| D3 | 68.78269175 |
| D4 | -116.34697036 |
| D5 | -78.72946929 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 187.55 | 261.78 | 396.49 | 476.16 | 636.54 | 947.37 | 1066.60 | 1100.18 | 1138.48 | 1294.22 |
| 1395.95 | 1421.31 | 1430.83 | 1501.76 | 3073.24 | 3162.27 | 3850.45 | 3903.89 | | |

Rotational constants (B/GHZ): 17.3837324 6.0872099 5.0358587



Pb₁(HO-CH₂OO-H)

| | | | | | | | |
|---|---|----|---|----|---|----|---|
| C | | | | | | | |
| O | 1 | B1 | | | | | |
| O | 2 | B2 | 1 | A1 | | | |
| H | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| H | 1 | B4 | 2 | A3 | 3 | D2 | 0 |
| O | 1 | B5 | 2 | A4 | 3 | D3 | 0 |
| H | 3 | B6 | 2 | A5 | 1 | D4 | 0 |
| H | 6 | B7 | 1 | A6 | 2 | D5 | 0 |

Variables:

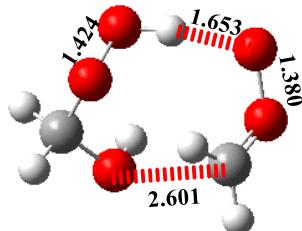
| | |
|----|--------------|
| B1 | 1.39846990 |
| B2 | 1.41549630 |
| B3 | 1.09221672 |
| B4 | 1.08851868 |
| B5 | 1.39462498 |
| B6 | 0.96568050 |
| B7 | 0.96059450 |
| A1 | 107.51359566 |

| | |
|----|---------------|
| A2 | 103.96617277 |
| A3 | 110.05328386 |
| A4 | 112.05221718 |
| A5 | 102.42638690 |
| A6 | 109.14726274 |
| D1 | -168.56099031 |
| D2 | -49.08547865 |
| D3 | 69.49009664 |
| D4 | -75.33464713 |
| D5 | 70.40550778 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 185.98 | 350.68 | 427.05 | 458.09 | 649.20 | 961.31 | 1059.11 | 1114.93 | 1125.96 | 1292.58 |
| 1382.71 | 1430.87 | 1444.34 | 1504.42 | 3085.79 | 3154.05 | 3828.21 | 3893.48 | | |

Rotational constants (B/GHZ): 17.7484920 5.9989349 5.0693236



IM1a

| C | | | | | | | |
|---|----|-----|---|-----|---|-----|---|
| H | 1 | B1 | | | | | |
| H | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 | 0 |
| O | 1 | B4 | 4 | A3 | 2 | D2 | 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 | 0 |
| C | 5 | B6 | 1 | A5 | 4 | D4 | 0 |
| H | 7 | B7 | 5 | A6 | 1 | D5 | 0 |
| H | 7 | B8 | 5 | A7 | 1 | D6 | 0 |
| O | 7 | B9 | 5 | A8 | 1 | D7 | 0 |
| O | 7 | B10 | 5 | A9 | 1 | D8 | 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 | 0 |
| H | 12 | B12 | 1 | A11 | 5 | D10 | 0 |

Variables:

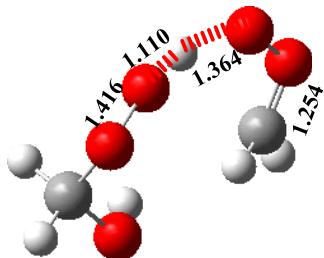
| | |
|----|------------|
| B1 | 1.09193463 |
| B2 | 1.08849176 |
| B3 | 2.24430673 |
| B4 | 1.39051082 |
| B5 | 0.99633873 |
| B6 | 3.06560927 |
| B7 | 1.08259664 |
| B8 | 1.08495294 |
| B9 | 2.22859774 |

| | |
|-----|---------------|
| B10 | 1.23265549 |
| B11 | 1.40521222 |
| B12 | 0.96272306 |
| A1 | 111.28650697 |
| A2 | 142.88476256 |
| A3 | 37.63600756 |
| A4 | 114.28220506 |
| A5 | 87.19146587 |
| A6 | 128.81480221 |
| A7 | 44.14002611 |
| A8 | 71.65730745 |
| A9 | 97.34905266 |
| A10 | 112.10771126 |
| A11 | 107.25214062 |
| D1 | 113.20365830 |
| D2 | -129.89551688 |
| D3 | 75.73345389 |
| D4 | -89.79001655 |
| D5 | -17.33812910 |
| D6 | -120.38255440 |
| D7 | 136.53226895 |
| D8 | 114.73764822 |
| D9 | 68.63114204 |
| D10 | -75.96210566 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 51.49 | 123.65 | 149.15 | 158.76 | 199.39 | 242.52 | 257.19 | 422.77 | 501.74 | 538.03 |
| 641.99 | 723.92 | 858.57 | 896.89 | 958.08 | 1070.70 | 1093.26 | 1112.92 | 1134.11 | 1270.31 |
| 1300.07 | 1397.45 | 1429.61 | 1456.76 | 1506.87 | 1588.45 | 1674.71 | 3088.99 | 3148.97 | |
| 3162.07 | 3162.64 | 3305.07 | 3868.49 | | | | | | |

Rotational constants (B/GHZ): 3.7514986 1.8833579 1.4348672



TS1a

| C | | | | | | | |
|---|---|--|----|---|----|---|------|
| H | 1 | | B1 | | | | |
| H | 1 | | B2 | 2 | A1 | | |
| O | 1 | | B3 | 3 | A2 | 2 | D1 0 |
| O | 1 | | B4 | 4 | A3 | 2 | D2 0 |
| H | 4 | | B5 | 1 | A4 | 5 | D3 0 |

| | | | | | | | |
|---|----|-----|---|-----|---|-----|---|
| C | 4 | B6 | 1 | A5 | 5 | D4 | 0 |
| H | 7 | B7 | 4 | A6 | 1 | D5 | 0 |
| H | 7 | B8 | 4 | A7 | 1 | D6 | 0 |
| O | 7 | B9 | 4 | A8 | 1 | D7 | 0 |
| O | 7 | B10 | 4 | A9 | 1 | D8 | 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 | 0 |
| H | 12 | B12 | 1 | A11 | 5 | D10 | 0 |

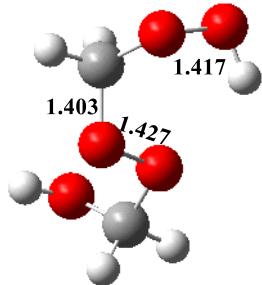
Variables:

| | |
|-----|---------------|
| B1 | 1.09236135 |
| B2 | 1.08804886 |
| B3 | 2.24424874 |
| B4 | 1.39811878 |
| B5 | 1.10965849 |
| B6 | 2.11376185 |
| B7 | 1.08564528 |
| B8 | 1.08422517 |
| B9 | 2.17270169 |
| B10 | 1.25371695 |
| B11 | 1.39546227 |
| B12 | 0.95934668 |
| A1 | 111.33252841 |
| A2 | 141.56828263 |
| A3 | 37.39819679 |
| A4 | 138.86224365 |
| A5 | 106.32634151 |
| A6 | 112.74521149 |
| A7 | 79.64310141 |
| A8 | 68.13881085 |
| A9 | 91.69184623 |
| A10 | 112.30561165 |
| A11 | 108.39573179 |
| D1 | 116.64933959 |
| D2 | -125.38714617 |
| D3 | 5.28588587 |
| D4 | 86.71869259 |
| D5 | 70.46269736 |
| D6 | -49.76277905 |
| D7 | -140.38093414 |
| D8 | -171.03190235 |
| D9 | 64.04282937 |
| D10 | -88.61169385 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|-----------------|--------|--------|--------|---------|---------|---------|---------|---------|---------|
| 590.85 <i>i</i> | 61.86 | 109.90 | 155.04 | 258.66 | 330.27 | 385.33 | 433.96 | 466.27 | 556.61 |
| 651.70 | 842.43 | 908.64 | 957.59 | 1057.32 | 1094.16 | 1115.57 | 1135.39 | 1210.01 | 1259.37 |

1312.34 1401.35 1436.84 1444.56 1504.18 1522.86 1634.53 1893.64 3081.68
 3142.96 3162.29 3278.38 3919.52
 Rotational constants (B/GHZ): 5.7500143 1.4940110 1.2740921



P1a

C

| | | | | | | | |
|---|----|-----|---|-----|---|-----|---|
| H | 1 | B1 | | | | | |
| H | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 | 0 |
| O | 1 | B4 | 4 | A3 | 2 | D2 | 0 |
| H | 5 | B5 | 1 | A4 | 4 | D3 | 0 |
| C | 4 | B6 | 1 | A5 | 5 | D4 | 0 |
| H | 7 | B7 | 4 | A6 | 1 | D5 | 0 |
| H | 7 | B8 | 4 | A7 | 1 | D6 | 0 |
| O | 7 | B9 | 4 | A8 | 1 | D7 | 0 |
| O | 7 | B10 | 4 | A9 | 1 | D8 | 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 | 0 |
| H | 12 | B12 | 1 | A11 | 5 | D10 | 0 |

Variables:

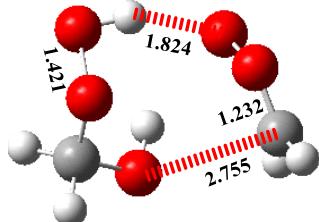
| | |
|-----|--------------|
| B1 | 1.09278103 |
| B2 | 1.08804767 |
| B3 | 2.26024320 |
| B4 | 1.40633987 |
| B5 | 2.29368981 |
| B6 | 1.40291402 |
| B7 | 1.09010644 |
| B8 | 1.09036134 |
| B9 | 2.28349823 |
| B10 | 1.38766992 |
| B11 | 1.38454575 |
| B12 | 0.96001864 |
| A1 | 111.03580539 |
| A2 | 140.99983857 |
| A3 | 37.41311012 |
| A4 | 159.52170894 |
| A5 | 128.73347664 |
| A6 | 104.06981016 |

| | |
|-----|---------------|
| A7 | 110.34401285 |
| A8 | 106.81981294 |
| A9 | 112.99544627 |
| A10 | 112.90571768 |
| A11 | 108.81709236 |
| D1 | 110.30671017 |
| D2 | -128.62298419 |
| D3 | -163.71292412 |
| D4 | 64.16608871 |
| D5 | 136.46268868 |
| D6 | 14.81755872 |
| D7 | -71.43436757 |
| D8 | -109.16769572 |
| D9 | 69.36407861 |
| D10 | -78.57478123 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 30.18 | 72.61 | 157.09 | 181.77 | 305.50 | 376.67 | 418.82 | 421.71 | 490.98 | 610.56 | 680.47 |
| 892.84 | 966.13 | 1053.48 | 1067.22 | 1116.56 | 1140.12 | 1142.95 | 1185.22 | 1305.98 | | |
| 1339.30 | 1398.02 | 1410.36 | 1432.97 | 1457.82 | 1458.26 | 1504.03 | 3083.47 | 3102.60 | | |
| 3160.70 | 3174.77 | 3802.76 | 3909.20 | | | | | | | |

Rotational constants (B/GHZ): 5.9322654 1.4514673 1.3429018



IM1b

| | | | | | | | |
|---|---|-----|---|-----|----|-----|---|
| C | | | | | | | |
| O | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| C | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| O | 5 | B7 | 2 | A6 | 1 | D5 | 0 |
| O | 5 | B8 | 2 | A7 | 1 | D6 | 0 |
| H | 1 | B9 | 2 | A8 | 5 | D7 | 0 |
| H | 1 | B10 | 2 | A9 | 5 | D8 | 0 |
| O | 1 | B11 | 2 | A10 | 5 | D9 | 0 |
| H | 4 | B12 | 1 | A11 | 12 | D10 | 0 |

Variables:

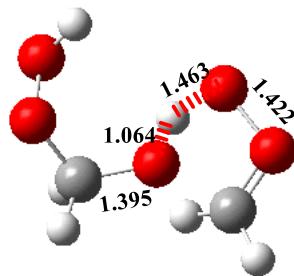
| | |
|----|------------|
| B1 | 1.40080832 |
| B2 | 0.96726628 |

| | |
|-----|--------------|
| B3 | 2.26933462 |
| B4 | 2.75470408 |
| B5 | 1.08334781 |
| B6 | 1.08276277 |
| B7 | 2.22141378 |
| B8 | 1.23165769 |
| B9 | 1.08880954 |
| B10 | 1.09185771 |
| B11 | 1.39521073 |
| B12 | 0.97956338 |
| A1 | 108.07810054 |
| A2 | 101.44725504 |
| A3 | 116.14951018 |
| A4 | 121.41226346 |
| A5 | 63.56643339 |
| A6 | 68.95898494 |
| A7 | 87.04598340 |
| A8 | 107.15652046 |
| A9 | 111.17484923 |
| A10 | 112.63307909 |
| A11 | 101.66754461 |
| D1 | -22.98049505 |
| D2 | 65.04627094 |
| D3 | 59.89222066 |
| D4 | 176.04280736 |
| D5 | -87.05510272 |
| D6 | -58.36146674 |
| D7 | -87.09989462 |
| D8 | 151.03444773 |
| D9 | 28.36800286 |
| D10 | 94.81429795 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 72.04 | 86.72 | 139.83 | 162.23 | 177.47 | 249.40 | 270.96 | 438.36 | 528.28 | 549.83 | 627.73 |
| 698.19 | 718.23 | 906.21 | 946.33 | 1090.21 | 1099.12 | 1110.60 | 1133.31 | 1263.78 | 1302.17 | |
| 1394.48 | 1439.43 | 1457.30 | 1502.53 | 1542.61 | 1681.85 | 3079.78 | 3152.18 | 3153.95 | | |
| 3299.66 | 3522.35 | 3791.16 | | | | | | | | |

Rotational constants (B/GHZ): 3.6364140 1.9053619 1.5431218



TS1b

| | | | | | | |
|---|---|-----|---|-----|----|-------|
| C | | | | | | |
| O | 1 | B1 | | | | |
| H | 2 | B2 | 1 | A1 | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 0 |
| C | 2 | B4 | 1 | A3 | 4 | D2 0 |
| H | 5 | B5 | 2 | A4 | 1 | D3 0 |
| H | 5 | B6 | 2 | A5 | 1 | D4 0 |
| O | 5 | B7 | 2 | A6 | 1 | D5 0 |
| O | 5 | B8 | 2 | A7 | 1 | D6 0 |
| H | 1 | B9 | 2 | A8 | 5 | D7 0 |
| H | 1 | B10 | 2 | A9 | 5 | D8 0 |
| O | 1 | B11 | 2 | A10 | 5 | D9 0 |
| H | 4 | B12 | 1 | A11 | 12 | D10 0 |

Variables:

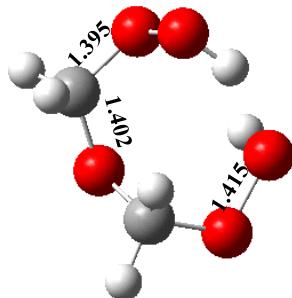
| | |
|-----|---------------|
| B1 | 1.39505172 |
| B2 | 1.06436688 |
| B3 | 2.25738999 |
| B4 | 2.02056504 |
| B5 | 1.08479080 |
| B6 | 1.08427018 |
| B7 | 2.16375976 |
| B8 | 1.25550533 |
| B9 | 1.08948659 |
| B10 | 1.09600897 |
| B11 | 1.39429682 |
| B12 | 0.96524204 |
| A1 | 109.89749303 |
| A2 | 96.63285190 |
| A3 | 119.36262780 |
| A4 | 106.95259056 |
| A5 | 87.46712512 |
| A6 | 71.09182158 |
| A7 | 92.70873641 |
| A8 | 109.15338965 |
| A9 | 111.01751086 |
| A10 | 111.65375567 |
| A11 | 108.13664266 |
| D1 | -33.80470151 |
| D2 | -117.52849662 |
| D3 | -100.45382300 |
| D4 | 22.17662678 |
| D5 | 108.65489249 |
| D6 | 141.36310093 |

D7 92.44996439
 D8 -30.73008333
 D9 -152.57144045
 D10 85.99718652

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 415.22 <i>i</i> | 40.20 | 99.91 | 148.49 | 205.00 | 314.15 | 349.23 | 431.37 | 437.34 | 543.07 | 653.19 |
| 860.79 | 906.53 | 964.29 | 1081.17 | 1109.99 | 1138.65 | 1204.54 | 1237.56 | 1252.56 | | |
| 1345.51 | 1423.49 | 1427.10 | 1438.53 | 1497.31 | 1537.87 | 1648.60 | 2188.55 | 3048.32 | | |
| 3150.56 | 3154.89 | 3280.64 | 3823.52 | | | | | | | |

Rotational constants (B/GHZ): 5.2607094 1.4842848 1.2265723



P1b

| C | | B1 | | | | | |
|---|---|-----|---|-----|---|-----|---|
| O | 1 | | | | | | |
| H | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| C | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| O | 5 | B7 | 2 | A6 | 1 | D5 | 0 |
| O | 5 | B8 | 2 | A7 | 1 | D6 | 0 |
| H | 1 | B9 | 2 | A8 | 5 | D7 | 0 |
| H | 1 | B10 | 2 | A9 | 5 | D8 | 0 |
| O | 1 | B11 | 2 | A10 | 5 | D9 | 0 |
| H | 4 | B12 | 1 | A11 | 2 | D10 | 0 |

Variables:

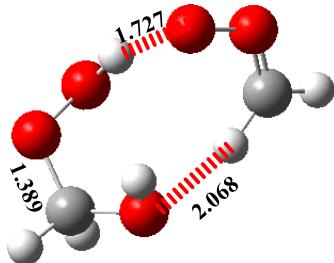
| | |
|-----|------------|
| B1 | 1.39646466 |
| B2 | 2.81289310 |
| B3 | 2.28646347 |
| B4 | 1.40195246 |
| B5 | 1.08773954 |
| B6 | 1.09184508 |
| B7 | 2.29107602 |
| B8 | 1.39505286 |
| B9 | 1.09030466 |
| B10 | 1.09296995 |
| B11 | 1.39952417 |

| | |
|-----|---------------|
| B12 | 0.96841304 |
| A1 | 84.04500359 |
| A2 | 93.33213382 |
| A3 | 117.88717196 |
| A4 | 105.66638951 |
| A5 | 111.18657932 |
| A6 | 108.78967345 |
| A7 | 114.09161968 |
| A8 | 109.64046157 |
| A9 | 111.00065620 |
| A10 | 110.84454877 |
| A11 | 95.79808701 |
| D1 | -42.74310231 |
| D2 | -83.79203073 |
| D3 | -168.60139383 |
| D4 | -47.40725336 |
| D5 | 38.07853217 |
| D6 | 76.32887374 |
| D7 | 131.10525667 |
| D8 | 7.65714895 |
| D9 | -116.00092950 |
| D10 | -18.80481243 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 135.00 | 145.58 | 202.53 | 213.91 | 346.24 | 421.73 | 442.75 | 481.31 | 592.03 | 611.01 |
| 640.47 | 947.94 | 955.88 | 1007.76 | 1102.38 | 1118.74 | 1131.21 | 1192.18 | 1221.83 | |
| 1326.90 | 1342.21 | 1419.16 | 1434.41 | 1445.01 | 1482.50 | 1487.94 | 1522.29 | 3081.27 | |
| 3094.55 | 3146.10 | 3170.45 | 3727.57 | 3794.55 | | | | | |

Rotational constants (B/GHZ): 3.89771194 2.2929822 1.6941060



IM1c

| C | | | | | | | |
|---|---|----|----|----|---|----|---|
| H | 1 | | B1 | | | | |
| H | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| O | 1 | B4 | 4 | A3 | 2 | D2 | 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 | 0 |
| C | 4 | B6 | 1 | A5 | 5 | D4 | 0 |
| H | 7 | B7 | 4 | A6 | 1 | D5 | 0 |

| | | | | | | | |
|---|----|-----|---|-----|---|-----|---|
| H | 7 | B8 | 4 | A7 | 1 | D6 | 0 |
| O | 7 | B9 | 4 | A8 | 1 | D7 | 0 |
| O | 7 | B10 | 4 | A9 | 1 | D8 | 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 | 0 |
| H | 12 | B12 | 1 | A11 | 5 | D10 | 0 |

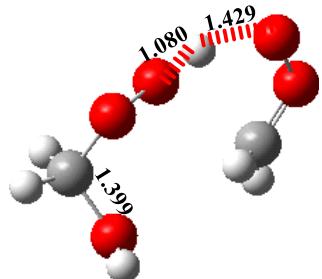
Variables:

| | |
|-----|---------------|
| B1 | 1.09046364 |
| B2 | 1.09261770 |
| B3 | 2.27498814 |
| B4 | 1.38916094 |
| B5 | 0.98761059 |
| B6 | 3.04672330 |
| B7 | 1.08393484 |
| B8 | 1.08944632 |
| B9 | 2.23124355 |
| B10 | 1.23599820 |
| B11 | 1.40212287 |
| B12 | 0.96429357 |
| A1 | 111.05797735 |
| A2 | 87.45762310 |
| A3 | 36.32914297 |
| A4 | 104.58806432 |
| A5 | 91.90056559 |
| A6 | 133.50361129 |
| A7 | 59.98514632 |
| A8 | 58.71049427 |
| A9 | 79.87433376 |
| A10 | 112.68359912 |
| A11 | 108.27238062 |
| D1 | -143.15021687 |
| D2 | -131.88141217 |
| D3 | 88.16754998 |
| D4 | 143.38332110 |
| D5 | 117.96489328 |
| D6 | 5.28488483 |
| D7 | -100.38932397 |
| D8 | -127.52170069 |
| D9 | 66.46706035 |
| D10 | 44.27403697 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 77.37 | 87.29 | 118.68 | 143.76 | 174.83 | 226.15 | 270.08 | 412.86 | 446.90 | 551.99 | 631.82 |
| 703.53 | 770.05 | 899.27 | 963.03 | 1075.11 | 1125.66 | 1127.41 | 1138.57 | 1290.24 | 1292.41 | |
| 1368.81 | 1445.95 | 1465.16 | 1514.58 | 1592.94 | 1656.63 | 3078.32 | 3106.21 | 3137.37 | | |
| 3262.65 | 3333.76 | 3847.00 | | | | | | | | |

Rotational constants (B/GHZ): 4.1249905 1.5380280 1.3541956



TS1c

| C | | | | | | | |
|---|----|-----|---|-----|---|-----|---|
| H | 1 | B1 | | | | | |
| H | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| O | 1 | B4 | 4 | A3 | 2 | D2 | 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 | 0 |
| C | 4 | B6 | 1 | A5 | 5 | D4 | 0 |
| H | 7 | B7 | 4 | A6 | 1 | D5 | 0 |
| H | 7 | B8 | 4 | A7 | 1 | D6 | 0 |
| O | 7 | B9 | 4 | A8 | 1 | D7 | 0 |
| O | 7 | B10 | 4 | A9 | 1 | D8 | 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 | 0 |
| H | 12 | B12 | 1 | A11 | 5 | D10 | 0 |

Variables:

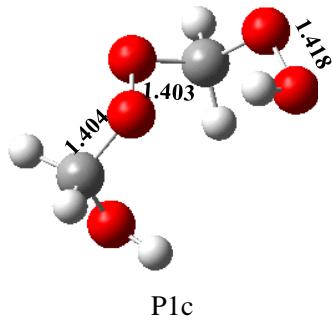
| | |
|-----|--------------|
| B1 | 1.08834267 |
| B2 | 1.09098647 |
| B3 | 2.24850821 |
| B4 | 1.39542161 |
| B5 | 1.07990772 |
| B6 | 2.10510054 |
| B7 | 1.08477369 |
| B8 | 1.08304653 |
| B9 | 2.17191319 |
| B10 | 1.25228579 |
| B11 | 1.39940584 |
| B12 | 0.96008114 |
| A1 | 111.34228110 |
| A2 | 82.25871571 |
| A3 | 37.18494329 |
| A4 | 137.39356271 |
| A5 | 102.38445807 |
| A6 | 110.23472364 |
| A7 | 81.62634578 |
| A8 | 69.10655673 |

| | |
|-----|---------------|
| A9 | 91.25481400 |
| A10 | 112.69680826 |
| A11 | 109.11408821 |
| D1 | -140.35342444 |
| D2 | -137.77810136 |
| D3 | 23.43473810 |
| D4 | 102.14409738 |
| D5 | 69.08255577 |
| D6 | -51.96070192 |
| D7 | -140.37025526 |
| D8 | -172.14953376 |
| D9 | 73.90957895 |
| D10 | 78.04491034 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 444.43 <i>i</i> | 85.01 | 121.97 | 150.19 | 224.38 | 316.38 | 391.24 | 412.83 | 473.35 | 561.73 |
| 640.54 | 837.64 | 902.44 | 964.66 | 1056.78 | 1104.75 | 1122.39 | 1144.23 | 1230.55 | 1261.66 |
| 1313.57 | 1388.98 | 1435.68 | 1442.39 | 1502.48 | 1545.25 | 1648.19 | 2075.05 | 3100.75 | |
| 3150.53 | 3172.59 | 3284.86 | 3900.85 | | | | | | |

Rotational constants (B/GHZ): 5.4134777 1.5210588 1.2867685



P1c

| C | | B1 | | | | | |
|---|----|-----|---|-----|---|-----|---|
| H | 1 | | | | | | |
| H | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| O | 1 | B4 | 4 | A3 | 2 | D2 | 0 |
| H | 5 | B5 | 1 | A4 | 4 | D3 | 0 |
| C | 4 | B6 | 1 | A5 | 5 | D4 | 0 |
| H | 7 | B7 | 4 | A6 | 1 | D5 | 0 |
| H | 7 | B8 | 4 | A7 | 1 | D6 | 0 |
| O | 7 | B9 | 4 | A8 | 1 | D7 | 0 |
| O | 7 | B10 | 4 | A9 | 1 | D8 | 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 | 0 |
| H | 12 | B12 | 1 | A11 | 5 | D10 | 0 |

Variables:

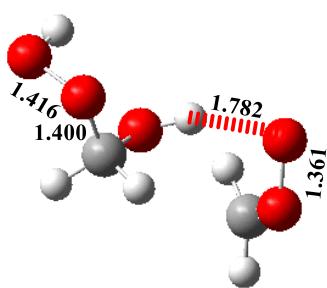
| | |
|----|------------|
| B1 | 1.08799697 |
| B2 | 1.09266730 |
| B3 | 2.28275845 |

| | |
|-----|---------------|
| B4 | 1.40439172 |
| B5 | 2.30963075 |
| B6 | 1.40301252 |
| B7 | 1.08999704 |
| B8 | 1.08884085 |
| B9 | 2.28389831 |
| B10 | 1.38942698 |
| B11 | 1.38890401 |
| B12 | 0.96086739 |
| A1 | 111.14188870 |
| A2 | 83.33957356 |
| A3 | 36.42924134 |
| A4 | 142.55329882 |
| A5 | 116.44916198 |
| A6 | 103.75434043 |
| A7 | 110.81234223 |
| A8 | 106.60253194 |
| A9 | 113.29761144 |
| A10 | 113.18409069 |
| A11 | 109.34093879 |
| D1 | -139.20137611 |
| D2 | -136.55054616 |
| D3 | -123.05508909 |
| D4 | 85.73972105 |
| D5 | 135.82759445 |
| D6 | 14.74523235 |
| D7 | -72.22722885 |
| D8 | -109.92615292 |
| D9 | 72.80077979 |
| D10 | 67.55024409 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 52.34 | 122.81 | 165.98 | 193.47 | 360.42 | 393.57 | 413.65 | 461.69 | 494.73 | 637.42 |
| 669.12 | 895.05 | 962.81 | 1055.36 | 1071.58 | 1112.53 | 1132.52 | 1139.34 | 1187.24 | |
| 1304.97 | 1329.91 | 1386.94 | 1406.08 | 1443.87 | 1458.11 | 1468.76 | 1511.42 | 3084.92 | |
| 3113.13 | 3176.99 | 3185.22 | 3806.52 | 3893.02 | | | | | |

Rotational constants (B/GHZ): 4.8837919 1.6280646 1.5251948



IM1d

| | | | | | | | |
|---|---|-----|---|-----|---|-----|---|
| C | | | | | | | |
| O | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| C | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| O | 5 | B7 | 2 | A6 | 1 | D5 | 0 |
| O | 5 | B8 | 2 | A7 | 1 | D6 | 0 |
| H | 1 | B9 | 2 | A8 | 8 | D7 | 0 |
| H | 1 | B10 | 2 | A9 | 8 | D8 | 0 |
| O | 1 | B11 | 2 | A10 | 8 | D9 | 0 |
| H | 4 | B12 | 1 | A11 | 2 | D10 | 0 |

Variables:

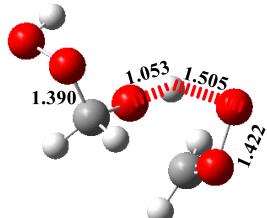
| | |
|-----|---------------|
| B1 | 1.39184722 |
| B2 | 0.97951118 |
| B3 | 2.26831849 |
| B4 | 2.84383962 |
| B5 | 1.08289919 |
| B6 | 1.08392000 |
| B7 | 2.22421909 |
| B8 | 1.23490771 |
| B9 | 1.08994860 |
| B10 | 1.09316960 |
| B11 | 1.39949743 |
| B12 | 0.96615439 |
| A1 | 108.66118511 |
| A2 | 95.15492618 |
| A3 | 121.49458385 |
| A4 | 128.59537979 |
| A5 | 61.57653409 |
| A6 | 62.57822124 |
| A7 | 82.22777023 |
| A8 | 107.72780280 |
| A9 | 112.18565229 |
| A10 | 112.03065997 |
| A11 | 91.43188118 |
| D1 | 112.04097538 |
| D2 | -176.68359091 |
| D3 | 53.99856023 |
| D4 | 167.57297018 |
| D5 | -90.32950518 |
| D6 | -62.59597667 |
| D7 | -141.59020116 |

D8 -18.33374995
D9 97.82144144
D10 -11.86208360

Harmonic Vibrational Frequencies (cm⁻¹):

34.20 59.12 96.11 105.16 176.74 202.51 263.42 349.72 443.45 545.48 640.52
697.12 843.16 915.62 960.73 1079.52 1109.59 1116.80 1136.09 1266.48 1323.65
1429.27 1440.47 1446.10 1473.38 1502.30 1656.34 3082.10 3146.58 3147.18
3293.83 3467.77 3809.79

Rotational constants (B/GHZ): 6.7624473 0.9811448 0.9394169



TS1d

| | | | | | | | |
|---|---|-----|---|-----|----|-----|---|
| C | | | | | | | |
| O | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| C | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| O | 5 | B7 | 2 | A6 | 1 | D5 | 0 |
| O | 5 | B8 | 2 | A7 | 1 | D6 | 0 |
| H | 1 | B9 | 2 | A8 | 5 | D7 | 0 |
| H | 1 | B10 | 2 | A9 | 5 | D8 | 0 |
| O | 1 | B11 | 2 | A10 | 5 | D9 | 0 |
| H | 4 | B12 | 1 | A11 | 12 | D10 | 0 |

Variables:

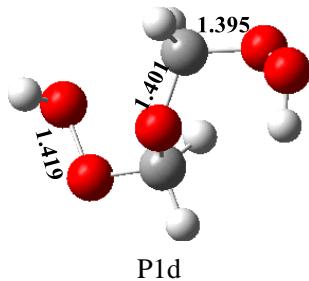
| | |
|-----|--------------|
| B1 | 1.40541536 |
| B2 | 1.05306931 |
| B3 | 2.26335509 |
| B4 | 2.01062737 |
| B5 | 1.08597113 |
| B6 | 1.08260109 |
| B7 | 2.16703780 |
| B8 | 1.25738886 |
| B9 | 1.09046133 |
| B10 | 1.09313474 |
| B11 | 1.38997707 |
| B12 | 0.96551861 |
| A1 | 108.04626998 |
| A2 | 95.81237725 |

| | |
|-----|---------------|
| A3 | 112.24458528 |
| A4 | 108.32341448 |
| A5 | 84.09262558 |
| A6 | 71.82185776 |
| A7 | 94.93969707 |
| A8 | 107.98183471 |
| A9 | 111.10058481 |
| A10 | 111.01747364 |
| A11 | 97.83507199 |
| D1 | 112.85465019 |
| D2 | -165.16194270 |
| D3 | 52.12346906 |
| D4 | 173.29716560 |
| D5 | -98.63749406 |
| D6 | -67.23448226 |
| D7 | -78.65069600 |
| D8 | 44.70191553 |
| D9 | 160.43655525 |
| D10 | 100.07184294 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 399.95 <i>i</i> | 59.34 | 109.49 | 147.50 | 178.17 | 314.92 | 328.67 | 443.02 | 468.18 | 563.14 | 647.07 |
| 857.27 | 913.34 | 970.10 | 1055.70 | 1132.49 | 1139.96 | 1208.96 | 1233.28 | 1281.29 | | |
| 1342.36 | 1417.61 | 1432.86 | 1447.95 | 1500.20 | 1534.71 | 1607.27 | 2318.31 | 3084.38 | | |
| 3148.33 | 3151.10 | 3278.92 | 3822.07 | | | | | | | |

Rotational constants (B/GHZ): 6.6335969 1.2418419 1.1818513



| C | | B1 | | A1 | | D1 | 0 |
|---|---|-----|---|-----|---|----|---|
| O | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| C | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| O | 5 | B7 | 2 | A6 | 1 | D5 | 0 |
| O | 5 | B8 | 2 | A7 | 1 | D6 | 0 |
| H | 1 | B9 | 2 | A8 | 5 | D7 | 0 |
| H | 1 | B10 | 2 | A9 | 5 | D8 | 0 |
| O | 1 | B11 | 2 | A10 | 5 | D9 | 0 |

H 4 B12 1 A11 12 D10 0

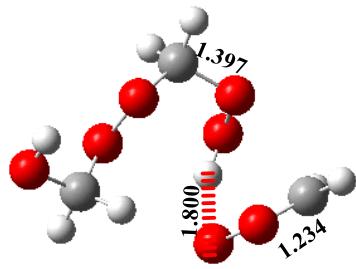
Variables:

B1 1.39808457
B2 2.54839991
B3 2.26299013
B4 1.40109812
B5 1.09123452
B6 1.08860231
B7 2.26939151
B8 1.39496620
B9 1.09343679
B10 1.08931684
B11 1.39426065
B12 0.96455873
A1 113.57827446
A2 95.52695437
A3 115.45423948
A4 111.58410450
A5 106.67705262
A6 96.40200195
A7 111.61911985
A8 110.67125046
A9 109.22685294
A10 111.73566404
A11 109.24375150
D1 -155.35127738
D2 -73.26293472
D3 37.27111681
D4 160.21236150
D5 -113.62518114
D6 -79.30908289
D7 15.81484525
D8 138.46564495
D9 -107.44667061
D10 83.13692692

Harmonic Vibrational Frequencies (cm⁻¹):

72.32 90.50 151.25 174.41 256.79 285.48 355.68 389.15 517.23 590.13 689.58
956.84 965.21 1004.65 1099.11 1119.14 1123.52 1189.23 1223.38 1324.31
1351.15 1418.16 1421.08 1436.79 1449.17 1491.02 1517.53 3080.86 3106.85
3152.31 3174.86 3820.99 3842.82

Rotational constants (B/GHZ): 7.5821035 1.2816526 1.1924133



IM2a

| C | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 1 | B1 | | | | | |
| H | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| O | 1 | B4 | 4 | A3 | 2 | D2 | 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 | 0 |
| C | 5 | B6 | 1 | A5 | 4 | D4 | 0 |
| H | 7 | B7 | 5 | A6 | 1 | D5 | 0 |
| H | 7 | B8 | 5 | A7 | 1 | D6 | 0 |
| O | 7 | B9 | 5 | A8 | 1 | D7 | 0 |
| O | 7 | B10 | 5 | A9 | 1 | D8 | 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 | 0 |
| O | 12 | B12 | 1 | A11 | 5 | D10 | 0 |
| C | 13 | B13 | 12 | A12 | 1 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 12 | D12 | 0 |
| H | 14 | B15 | 13 | A14 | 12 | D13 | 0 |
| O | 14 | B16 | 13 | A15 | 12 | D14 | 0 |
| H | 17 | B17 | 14 | A16 | 13 | D15 | 0 |

Variables:

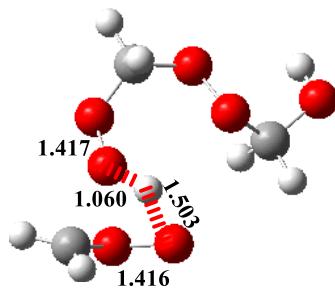
| | |
|-----|------------|
| B1 | 1.08988363 |
| B2 | 1.08990783 |
| B3 | 2.30167009 |
| B4 | 1.39674415 |
| B5 | 0.98469338 |
| B6 | 2.70891340 |
| B7 | 1.08284091 |
| B8 | 1.08512776 |
| B9 | 2.22979926 |
| B10 | 1.23359936 |
| B11 | 1.39017378 |
| B12 | 1.43268519 |
| B13 | 1.40341318 |
| B14 | 1.08778468 |
| B15 | 1.09010598 |
| B16 | 1.38936274 |
| B17 | 0.96003195 |

| | |
|-----|---------------|
| A1 | 112.56515164 |
| A2 | 80.07049835 |
| A3 | 35.55734957 |
| A4 | 98.64788909 |
| A5 | 137.48661170 |
| A6 | 111.68529288 |
| A7 | 68.55344125 |
| A8 | 76.93420325 |
| A9 | 90.54297570 |
| A10 | 113.76157523 |
| A11 | 106.63788571 |
| A12 | 105.35826636 |
| A13 | 103.89028096 |
| A14 | 108.71124010 |
| A15 | 112.73237897 |
| A16 | 108.74926881 |
| D1 | -137.47081525 |
| D2 | -145.80060400 |
| D3 | 97.56904113 |
| D4 | -107.63461386 |
| D5 | -83.38171650 |
| D6 | 156.31654248 |
| D7 | 64.37397360 |
| D8 | 34.37027424 |
| D9 | 88.30041855 |
| D10 | -80.05073945 |
| D11 | 161.56374166 |
| D12 | -170.05631440 |
| D13 | -52.25066845 |
| D14 | 73.23464199 |
| D15 | -72.71154424 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 45.57 | 66.77 | 93.87 | 102.81 | 122.46 | 144.25 | 151.50 | 186.87 | 236.15 | 242.40 | 324.57 |
| 383.37 | 460.65 | 475.55 | 546.85 | 588.99 | 676.46 | 704.47 | 751.92 | 889.93 | 904.59 | |
| 957.32 | 1053.65 | 1082.87 | 1103.67 | 1123.38 | 1129.87 | 1139.95 | 1188.07 | 1271.30 | | |
| 1306.97 | 1353.81 | 1383.99 | 1415.10 | 1438.66 | 1455.62 | 1457.70 | 1501.07 | 1569.37 | | |
| 1663.59 | 3104.56 | 3113.87 | 3140.47 | 3173.48 | 3187.95 | 3286.92 | 3436.05 | 3910.66 | | |

Rotational constants (B/GHZ): 1.6892434 0.9067425 0.7015963



TS2a

C

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 1 | B1 | | | | | |
| H | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 | 0 |
| O | 1 | B4 | 4 | A3 | 2 | D2 | 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 | 0 |
| C | 4 | B6 | 1 | A5 | 5 | D4 | 0 |
| H | 7 | B7 | 4 | A6 | 1 | D5 | 0 |
| H | 7 | B8 | 4 | A7 | 1 | D6 | 0 |
| O | 7 | B9 | 4 | A8 | 1 | D7 | 0 |
| O | 7 | B10 | 4 | A9 | 1 | D8 | 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 | 0 |
| O | 12 | B12 | 1 | A11 | 5 | D10 | 0 |
| C | 13 | B13 | 12 | A12 | 1 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 12 | D12 | 0 |
| H | 14 | B15 | 13 | A14 | 12 | D13 | 0 |
| O | 14 | B16 | 13 | A15 | 12 | D14 | 0 |
| H | 17 | B17 | 14 | A16 | 13 | D15 | 0 |

Variables:

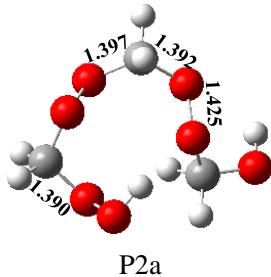
| | |
|-----|------------|
| B1 | 1.09048353 |
| B2 | 1.08946064 |
| B3 | 2.29390121 |
| B4 | 1.40053475 |
| B5 | 1.05987870 |
| B6 | 2.03446157 |
| B7 | 1.08499052 |
| B8 | 1.08348969 |
| B9 | 2.16595257 |
| B10 | 1.25473572 |
| B11 | 1.38695811 |
| B12 | 1.43058879 |
| B13 | 1.40977475 |
| B14 | 1.08774904 |
| B15 | 1.08984162 |
| B16 | 1.38682739 |

| | |
|-----|---------------|
| B17 | 0.96001843 |
| A1 | 112.45099433 |
| A2 | 137.04083125 |
| A3 | 35.74938867 |
| A4 | 97.18922543 |
| A5 | 136.15498864 |
| A6 | 107.47965602 |
| A7 | 83.65696172 |
| A8 | 71.50085949 |
| A9 | 94.31535569 |
| A10 | 113.63871609 |
| A11 | 106.45848008 |
| A12 | 105.59804582 |
| A13 | 103.75707173 |
| A14 | 108.66367202 |
| A15 | 112.40634252 |
| A16 | 108.85458353 |
| D1 | 99.12083365 |
| D2 | -146.59130157 |
| D3 | 104.09980232 |
| D4 | 26.29211804 |
| D5 | -66.74191041 |
| D6 | 171.57560754 |
| D7 | 83.52045154 |
| D8 | 52.15373696 |
| D9 | 89.49960538 |
| D10 | -74.85799528 |
| D11 | 147.67673854 |
| D12 | -170.95609238 |
| D13 | -53.29097995 |
| D14 | 72.26569892 |
| D15 | -74.65608515 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 422.04 <i>i</i> | 45.71 | 79.71 | 99.69 | 105.97 | 140.19 | 165.91 | 176.37 | 321.38 | 337.62 | 374.91 |
| 442.37 | 466.90 | 480.64 | 579.15 | 606.29 | 680.92 | 842.96 | 891.11 | 913.74 | 965.11 | |
| 1053.02 | 1068.77 | 1102.60 | 1135.64 | 1142.15 | 1172.02 | 1190.47 | 1239.94 | 1264.83 | | |
| 1307.38 | 1347.52 | 1393.62 | 1410.33 | 1433.68 | 1443.30 | 1458.72 | 1491.80 | 1574.24 | | |
| 1616.94 | 2254.04 | 3107.48 | 3113.55 | 3166.94 | 3176.08 | 3188.73 | 3297.14 | 3905.15 | | |

Rotational constants (B/GHZ): 1.9471020 0.8831406 0.6636227



P2a

C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| H | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| O | 1 | B4 | 4 | A3 | 2 | D2 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 0 |
| C | 4 | B6 | 1 | A5 | 5 | D4 0 |
| H | 7 | B7 | 4 | A6 | 1 | D5 0 |
| H | 7 | B8 | 4 | A7 | 1 | D6 0 |
| O | 7 | B9 | 4 | A8 | 1 | D7 0 |
| O | 7 | B10 | 4 | A9 | 1 | D8 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 0 |
| O | 12 | B12 | 1 | A11 | 5 | D10 0 |
| C | 13 | B13 | 12 | A12 | 1 | D11 0 |
| H | 14 | B14 | 13 | A13 | 12 | D12 0 |
| H | 14 | B15 | 13 | A14 | 12 | D13 0 |
| O | 14 | B16 | 13 | A15 | 12 | D14 0 |
| H | 17 | B17 | 14 | A16 | 13 | D15 0 |

Variables:

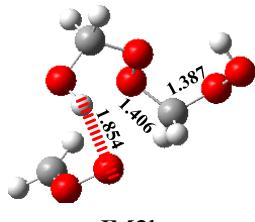
| | |
|-----|--------------|
| B1 | 1.08996953 |
| B2 | 1.08989693 |
| B3 | 2.29105378 |
| B4 | 1.39705916 |
| B5 | 2.53724197 |
| B6 | 1.39570642 |
| B7 | 1.08997228 |
| B8 | 1.09061376 |
| B9 | 2.26051329 |
| B10 | 1.38984608 |
| B11 | 1.39157329 |
| B12 | 1.42458804 |
| B13 | 1.41623303 |
| B14 | 1.08836733 |
| B15 | 1.09049357 |
| B16 | 1.38234993 |
| B17 | 0.96044175 |
| A1 | 111.81227637 |

| | |
|-----|---------------|
| A2 | 132.26587240 |
| A3 | 36.26474406 |
| A4 | 85.91659127 |
| A5 | 130.53995581 |
| A6 | 111.06955137 |
| A7 | 103.92225613 |
| A8 | 95.25773354 |
| A9 | 113.06503292 |
| A10 | 113.67872899 |
| A11 | 108.24810586 |
| A12 | 105.48195397 |
| A13 | 104.09420845 |
| A14 | 108.10670957 |
| A15 | 112.31296775 |
| A16 | 109.03401662 |
| D1 | 89.07606744 |
| D2 | -161.48051552 |
| D3 | 124.26494635 |
| D4 | 59.52514124 |
| D5 | -74.12610961 |
| D6 | 164.48719366 |
| D7 | 77.48674924 |
| D8 | 44.19866703 |
| D9 | 105.98976860 |
| D10 | -72.88027127 |
| D11 | 135.66147153 |
| D12 | -171.39482513 |
| D13 | -53.42255826 |
| D14 | 71.65226008 |
| D15 | -73.31751266 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 52.27 | 103.09 | 116.62 | 130.12 | 150.15 | 179.87 | 239.09 | 306.22 | 331.34 | 379.91 |
| 448.91 | 471.18 | 504.65 | 570.38 | 586.23 | 670.49 | 688.97 | 877.65 | 916.74 | 966.44 |
| 1040.31 | 1067.87 | 1082.97 | 1123.09 | 1128.37 | 1131.04 | 1152.39 | 1168.89 | 1210.57 | |
| 1309.15 | 1331.05 | 1347.03 | 1401.90 | 1404.85 | 1423.70 | 1451.59 | 1465.45 | 1466.75 | |
| 1471.54 | 1505.44 | 3097.16 | 3101.46 | 3106.91 | 3166.86 | 3169.16 | 3179.32 | 3736.17 | |
| 3904.14 | | | | | | | | | |

Rotational constants (B/GHZ): 1.7837111 1.0548781 0.7459496



IM2b

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | | | | | | | |
| O | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| C | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| O | 5 | B7 | 2 | A6 | 1 | D5 | 0 |
| O | 5 | B8 | 2 | A7 | 1 | D6 | 0 |
| H | 1 | B9 | 2 | A8 | 8 | D7 | 0 |
| H | 1 | B10 | 2 | A9 | 8 | D8 | 0 |
| O | 1 | B11 | 2 | A10 | 8 | D9 | 0 |
| C | 4 | B12 | 1 | A11 | 2 | D10 | 0 |
| H | 13 | B13 | 4 | A12 | 1 | D11 | 0 |
| H | 13 | B14 | 4 | A13 | 1 | D12 | 0 |
| O | 13 | B15 | 4 | A14 | 1 | D13 | 0 |
| O | 16 | B16 | 13 | A15 | 4 | D14 | 0 |
| H | 17 | B17 | 16 | A16 | 13 | D15 | 0 |

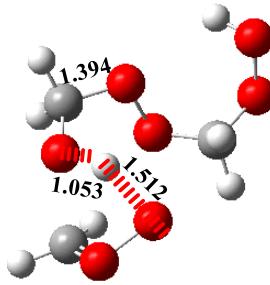
Variables:

| | |
|-----|--------------|
| B1 | 1.38110497 |
| B2 | 0.97806555 |
| B3 | 2.28717162 |
| B4 | 2.78408003 |
| B5 | 1.08347963 |
| B6 | 1.08586218 |
| B7 | 2.22647943 |
| B8 | 1.23496196 |
| B9 | 1.09420375 |
| B10 | 1.09089084 |
| B11 | 1.40561815 |
| B12 | 1.40632027 |
| B13 | 1.09093937 |
| B14 | 1.09061095 |
| B15 | 1.38743459 |
| B16 | 1.41689926 |
| B17 | 0.96679943 |
| A1 | 108.87790588 |
| A2 | 95.07927923 |
| A3 | 127.87407982 |
| A4 | 126.66948896 |
| A5 | 61.21356138 |
| A6 | 64.36724709 |
| A7 | 83.59146399 |
| A8 | 112.88898577 |

| | |
|-----|---------------|
| A9 | 107.99969684 |
| A10 | 113.03863037 |
| A11 | 136.61980845 |
| A12 | 103.98919999 |
| A13 | 109.97048831 |
| A14 | 112.74021862 |
| A15 | 109.14749481 |
| A16 | 102.46600373 |
| D1 | 71.61729278 |
| D2 | -8.18908864 |
| D3 | -121.73394953 |
| D4 | -7.34620069 |
| D5 | 93.51373958 |
| D6 | 121.57231875 |
| D7 | -100.67987837 |
| D8 | 136.65223571 |
| D9 | 14.50151620 |
| D10 | -83.50487238 |
| D11 | 149.52685355 |
| D12 | 28.42751256 |
| D13 | -96.41461274 |
| D14 | 88.46210761 |
| D15 | -77.34408045 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-------------------------------|---------|---------|---------|---------|-----------|-----------|-----------|---------|--------|--------|
| 46.25 | 62.77 | 73.49 | 87.97 | 118.74 | 136.50 | 165.84 | 207.30 | 216.23 | 256.96 | 305.38 |
| 383.78 | 413.49 | 491.96 | 541.09 | 567.04 | 647.87 | 692.05 | 723.66 | 894.73 | 896.94 | |
| 968.53 | 1056.97 | 1103.99 | 1108.56 | 1131.19 | 1139.30 | 1162.92 | 1200.91 | 1273.34 | | |
| 1301.87 | 1333.93 | 1394.56 | 1409.87 | 1453.41 | 1461.98 | 1464.77 | 1474.07 | 1519.24 | | |
| 1660.30 | 3073.86 | 3100.07 | 3131.77 | 3134.30 | 3176.76 | 3279.41 | 3531.30 | 3799.98 | | |
| Rotational constants (B/GHZ): | | | | | 1.7916930 | 0.7734349 | 0.6442762 | | | |



TS2b

| | | | | | | | |
|---|---|--|----|---|----|---|------|
| C | | | | | | | |
| O | 1 | | B1 | | | | |
| H | 2 | | B2 | 1 | A1 | | |
| O | 1 | | B3 | 2 | A2 | 3 | D1 0 |
| C | 2 | | B4 | 1 | A3 | 4 | D2 0 |
| H | 5 | | B5 | 2 | A4 | 1 | D3 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| O | 5 | B7 | 2 | A6 | 1 | D5 | 0 |
| O | 5 | B8 | 2 | A7 | 1 | D6 | 0 |
| H | 1 | B9 | 2 | A8 | 5 | D7 | 0 |
| H | 1 | B10 | 2 | A9 | 5 | D8 | 0 |
| O | 1 | B11 | 2 | A10 | 5 | D9 | 0 |
| C | 4 | B12 | 1 | A11 | 12 | D10 | 0 |
| H | 13 | B13 | 4 | A12 | 1 | D11 | 0 |
| H | 13 | B14 | 4 | A13 | 1 | D12 | 0 |
| O | 13 | B15 | 4 | A14 | 1 | D13 | 0 |
| O | 16 | B16 | 13 | A15 | 4 | D14 | 0 |
| H | 17 | B17 | 16 | A16 | 13 | D15 | 0 |

Variables:

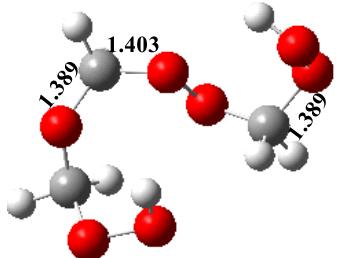
| | |
|-----|--------------|
| B1 | 1.39502528 |
| B2 | 1.05260297 |
| B3 | 2.26047176 |
| B4 | 2.02403623 |
| B5 | 1.08523997 |
| B6 | 1.08433626 |
| B7 | 2.17140994 |
| B8 | 1.25568657 |
| B9 | 1.09110598 |
| B10 | 1.09445435 |
| B11 | 1.39416675 |
| B12 | 1.40833772 |
| B13 | 1.08909028 |
| B14 | 1.08795784 |
| B15 | 1.38725212 |
| B16 | 1.41708408 |
| B17 | 0.96615157 |
| A1 | 111.61493178 |
| A2 | 98.01644964 |
| A3 | 120.02520637 |
| A4 | 107.27681762 |
| A5 | 86.34704641 |
| A6 | 71.51306729 |
| A7 | 92.61939092 |
| A8 | 109.79557098 |
| A9 | 109.58878956 |
| A10 | 113.02497097 |
| A11 | 133.75223406 |
| A12 | 104.63837476 |
| A13 | 110.14185079 |
| A14 | 112.32775449 |

| | |
|-----|---------------|
| A15 | 108.59744787 |
| A16 | 102.58741540 |
| D1 | 38.00190645 |
| D2 | -49.25705322 |
| D3 | -99.28023230 |
| D4 | 23.43900737 |
| D5 | 110.64015518 |
| D6 | 143.17008711 |
| D7 | 159.17335504 |
| D8 | 37.63768563 |
| D9 | -85.02396625 |
| D10 | 53.65158443 |
| D11 | 132.50697958 |
| D12 | 11.82954061 |
| D13 | -112.95957016 |
| D14 | 83.05278903 |
| D15 | -82.68278521 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 406.95 <i>i</i> | 55.00 | 60.59 | 89.20 | 136.11 | 142.34 | 169.06 | 196.89 | 274.70 | 313.18 | 361.41 |
| 429.25 | 439.30 | 484.52 | 545.20 | 613.54 | 686.26 | 859.81 | 890.21 | 911.14 | 963.21 | |
| 1031.81 | 1064.85 | 1115.81 | 1129.07 | 1134.76 | 1163.12 | 1193.48 | 1214.41 | 1247.77 | | |
| 1312.87 | 1340.34 | 1405.96 | 1421.04 | 1434.67 | 1444.79 | 1449.77 | 1483.22 | 1513.70 | | |
| 1625.15 | 2336.79 | 3068.43 | 3116.20 | 3135.60 | 3142.64 | 3188.30 | 3271.80 | 3813.88 | | |

Rotational constants (B/GHZ): 2.2651765 0.7597666 0.6430710



P2b

| | | | | | | | |
|---|---|--|-----|---|-----|---|------|
| C | | | | | | | |
| O | 1 | | B1 | | | | |
| H | 2 | | B2 | 1 | A1 | | |
| O | 1 | | B3 | 2 | A2 | 3 | D1 0 |
| C | 2 | | B4 | 1 | A3 | 4 | D2 0 |
| H | 5 | | B5 | 2 | A4 | 1 | D3 0 |
| H | 5 | | B6 | 2 | A5 | 1 | D4 0 |
| O | 5 | | B7 | 2 | A6 | 1 | D5 0 |
| O | 5 | | B8 | 2 | A7 | 1 | D6 0 |
| H | 1 | | B9 | 2 | A8 | 5 | D7 0 |
| H | 1 | | B10 | 2 | A9 | 5 | D8 0 |
| O | 1 | | B11 | 2 | A10 | 5 | D9 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 4 | B12 | 1 | A11 | 2 | D10 | 0 |
| H | 13 | B13 | 4 | A12 | 1 | D11 | 0 |
| H | 13 | B14 | 4 | A13 | 1 | D12 | 0 |
| O | 13 | B15 | 4 | A14 | 1 | D13 | 0 |
| O | 16 | B16 | 13 | A15 | 4 | D14 | 0 |
| H | 17 | B17 | 16 | A16 | 13 | D15 | 0 |

Variables:

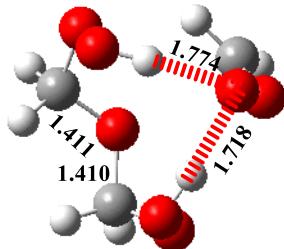
| | |
|-----|---------------|
| B1 | 1.38923007 |
| B2 | 2.47710069 |
| B3 | 2.27535158 |
| B4 | 1.40812992 |
| B5 | 1.09024509 |
| B6 | 1.09152910 |
| B7 | 2.26689874 |
| B8 | 1.38976120 |
| B9 | 1.08773067 |
| B10 | 1.09222482 |
| B11 | 1.40308826 |
| B12 | 1.39938622 |
| B13 | 1.08943437 |
| B14 | 1.08897042 |
| B15 | 1.38947138 |
| B16 | 1.41735556 |
| B17 | 0.96627625 |
| A1 | 100.74337231 |
| A2 | 109.37831232 |
| A3 | 118.07175381 |
| A4 | 109.29106202 |
| A5 | 110.59965632 |
| A6 | 93.87139699 |
| A7 | 109.94625415 |
| A8 | 106.21614541 |
| A9 | 112.00249249 |
| A10 | 114.00410880 |
| A11 | 141.02106713 |
| A12 | 103.73756378 |
| A13 | 110.84141369 |
| A14 | 113.02432109 |
| A15 | 108.86687448 |
| A16 | 102.36095130 |
| D1 | 40.71739136 |
| D2 | -38.28209208 |
| D3 | -123.98237274 |
| D4 | -0.09671928 |

| | |
|-----|--------------|
| D5 | 89.21285794 |
| D6 | 122.74711748 |
| D7 | 166.79996842 |
| D8 | 45.32337066 |
| D9 | -78.12030609 |
| D10 | -77.69334427 |
| D11 | 156.21249938 |
| D12 | 35.52046663 |
| D13 | -88.93935348 |
| D14 | 88.20021650 |
| D15 | -81.57055734 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 49.63 | 85.41 | 100.29 | 114.16 | 143.49 | 170.55 | 196.92 | 300.77 | 339.79 | 373.56 | 385.00 |
| 422.92 | 430.48 | 491.87 | 577.64 | 620.92 | 683.71 | 886.83 | 964.30 | 967.28 | 994.18 | |
| 1071.88 | 1111.61 | 1118.78 | 1135.66 | 1138.19 | 1171.59 | 1203.77 | 1226.50 | 1324.92 | | |
| 1335.18 | 1354.65 | 1399.72 | 1429.53 | 1444.13 | 1447.95 | 1454.31 | 1459.82 | 1485.46 | | |
| 1505.45 | 3096.88 | 3104.02 | 3115.79 | 3167.24 | 3172.80 | 3184.82 | 3802.56 | 3804.43 | | |

Rotational constants (B/GHZ): 2.3684565 0.7647451 0.6638408



IM2c

| C | | B1 | | A1 | | D1 | 0 |
|---|----|-----|----|-----|----|-----|---|
| H | 1 | | | | | | |
| H | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| O | 1 | B4 | 4 | A3 | 3 | D2 | 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 | 0 |
| C | 5 | B6 | 1 | A5 | 4 | D4 | 0 |
| H | 7 | B7 | 5 | A6 | 1 | D5 | 0 |
| H | 7 | B8 | 5 | A7 | 1 | D6 | 0 |
| O | 7 | B9 | 5 | A8 | 1 | D7 | 0 |
| O | 7 | B10 | 5 | A9 | 1 | D8 | 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 | 0 |
| C | 12 | B12 | 1 | A11 | 5 | D10 | 0 |
| H | 13 | B13 | 12 | A12 | 1 | D11 | 0 |
| H | 13 | B14 | 12 | A13 | 1 | D12 | 0 |
| O | 13 | B15 | 12 | A14 | 1 | D13 | 0 |
| O | 16 | B16 | 13 | A15 | 12 | D14 | 0 |
| H | 17 | B17 | 16 | A16 | 13 | D15 | 0 |

Variables:

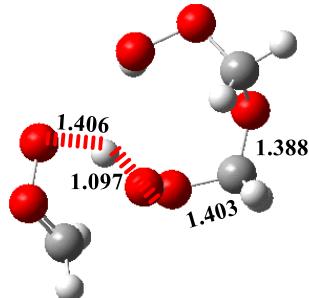
| | |
|-----|---------------|
| B1 | 1.09173357 |
| B2 | 1.09176734 |
| B3 | 2.27577887 |
| B4 | 1.38540952 |
| B5 | 0.98225148 |
| B6 | 3.15396968 |
| B7 | 1.08351633 |
| B8 | 1.08593208 |
| B9 | 2.22471154 |
| B10 | 1.23092006 |
| B11 | 1.41043256 |
| B12 | 1.41127256 |
| B13 | 1.09272220 |
| B14 | 1.09064191 |
| B15 | 1.38086711 |
| B16 | 1.41872472 |
| B17 | 0.97937323 |
| A1 | 111.75486058 |
| A2 | 138.05627343 |
| A3 | 36.17564227 |
| A4 | 100.35720007 |
| A5 | 89.14156252 |
| A6 | 130.84903723 |
| A7 | 30.92016001 |
| A8 | 75.05781953 |
| A9 | 104.97079052 |
| A10 | 110.13473721 |
| A11 | 118.80943987 |
| A12 | 109.99615222 |
| A13 | 108.88105126 |
| A14 | 111.48489040 |
| A15 | 107.93570473 |
| A16 | 101.34831941 |
| D1 | -102.98030066 |
| D2 | 141.56318281 |
| D3 | -97.21480171 |
| D4 | 92.81035561 |
| D5 | 54.77784378 |
| D6 | 145.67746133 |
| D7 | -105.07658079 |
| D8 | -89.91177852 |
| D9 | -81.03102241 |
| D10 | 137.28754439 |

D11 -3.10865002
 D12 119.26575569
 D13 -125.94687678
 D14 78.42619470
 D15 -103.17900909

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 58.24 | 74.27 | 98.25 | 124.05 | 144.64 | 150.67 | 186.06 | 198.66 | 257.24 | 274.00 | 356.48 |
| 431.97 | 446.67 | 551.94 | 555.92 | 574.44 | 651.59 | 724.28 | 756.86 | 908.71 | 956.01 | |
| 964.84 | 1009.82 | 1094.74 | 1130.53 | 1149.53 | 1154.97 | 1182.88 | 1217.23 | 1271.00 | | |
| 1326.64 | 1347.04 | 1423.57 | 1459.49 | 1465.41 | 1490.68 | 1515.50 | 1550.13 | 1598.10 | | |
| 1692.66 | 3074.86 | 3083.55 | 3140.80 | 3149.45 | 3149.98 | 3295.73 | 3449.88 | 3522.12 | | |

Rotational constants (B/GHZ): 1.3332535 1.2296427 0.9436559



TS2c

| C | | | B1 | | | | |
|---|----|--|-----|----|-----|----|-------|
| H | 1 | | | | | | |
| H | 1 | | B2 | 2 | A1 | | |
| O | 1 | | B3 | 2 | A2 | 3 | D1 0 |
| O | 1 | | B4 | 4 | A3 | 3 | D2 0 |
| H | 4 | | B5 | 1 | A4 | 5 | D3 0 |
| C | 4 | | B6 | 1 | A5 | 5 | D4 0 |
| H | 7 | | B7 | 4 | A6 | 1 | D5 0 |
| H | 7 | | B8 | 4 | A7 | 1 | D6 0 |
| O | 7 | | B9 | 4 | A8 | 1 | D7 0 |
| O | 7 | | B10 | 4 | A9 | 1 | D8 0 |
| O | 1 | | B11 | 5 | A10 | 4 | D9 0 |
| C | 12 | | B12 | 1 | A11 | 5 | D10 0 |
| H | 13 | | B13 | 12 | A12 | 1 | D11 0 |
| H | 13 | | B14 | 12 | A13 | 1 | D12 0 |
| O | 13 | | B15 | 12 | A14 | 1 | D13 0 |
| O | 16 | | B16 | 13 | A15 | 12 | D14 0 |
| H | 17 | | B17 | 16 | A16 | 13 | D15 0 |

Variables:

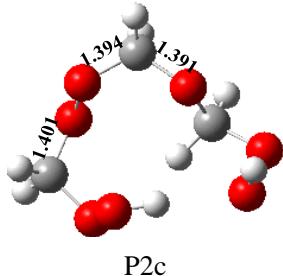
| | |
|----|------------|
| B1 | 1.08822105 |
| B2 | 1.09248724 |
| B3 | 2.29205468 |
| B4 | 1.40275015 |

| | |
|-----|---------------|
| B5 | 1.09651837 |
| B6 | 2.07146171 |
| B7 | 1.08539676 |
| B8 | 1.08431856 |
| B9 | 2.17197829 |
| B10 | 1.25381589 |
| B11 | 1.38807186 |
| B12 | 1.40660899 |
| B13 | 1.09237305 |
| B14 | 1.09030052 |
| B15 | 1.38788552 |
| B16 | 1.41449609 |
| B17 | 0.96710312 |
| A1 | 111.33825263 |
| A2 | 135.75219725 |
| A3 | 35.99138020 |
| A4 | 120.17714399 |
| A5 | 132.92302060 |
| A6 | 110.26438685 |
| A7 | 82.04308471 |
| A8 | 69.22682265 |
| A9 | 92.55809505 |
| A10 | 114.19942473 |
| A11 | 117.95478561 |
| A12 | 110.52380147 |
| A13 | 108.98011506 |
| A14 | 110.67815682 |
| A15 | 108.02146988 |
| A16 | 102.57729529 |
| D1 | -95.33460589 |
| D2 | 146.11137347 |
| D3 | -67.86854107 |
| D4 | 29.49492823 |
| D5 | 91.33413052 |
| D6 | -29.85607405 |
| D7 | -119.42611990 |
| D8 | -150.28906792 |
| D9 | -90.27296692 |
| D10 | 78.75076545 |
| D11 | 2.46988242 |
| D12 | 125.91857628 |
| D13 | -120.56991234 |
| D14 | 71.90661523 |
| D15 | -90.05706114 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 521.14 <i>i</i> | 60.42 | 73.14 | 96.87 | 121.27 | 154.30 | 180.40 | 205.45 | 337.52 | 362.68 | 383.27 |
| 388.08 | 441.97 | 468.13 | 559.95 | 597.94 | 628.83 | 846.51 | 908.05 | 942.68 | 965.92 | |
| 1002.96 | 1072.84 | 1118.98 | 1142.01 | 1153.50 | 1192.73 | 1217.33 | 1224.76 | 1251.51 | | |
| 1341.83 | 1350.29 | 1415.05 | 1431.90 | 1435.19 | 1450.90 | 1486.56 | 1512.98 | 1557.08 | | |
| 1640.72 | 1973.12 | 3080.76 | 3088.40 | 3146.38 | 3150.59 | 3160.74 | 3279.20 | 3799.25 | | |

Rotational constants (B/GHZ): 2.1368669 0.8386239 0.6464839



P2c

C

| | | | | | | |
|---|----|-----|----|-----|----|-----|
| H | 1 | B1 | | | | |
| H | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 |
| O | 1 | B4 | 4 | A3 | 3 | D2 |
| H | 5 | B5 | 1 | A4 | 4 | D3 |
| C | 4 | B6 | 1 | A5 | 5 | D4 |
| H | 7 | B7 | 4 | A6 | 1 | D5 |
| H | 7 | B8 | 4 | A7 | 1 | D6 |
| O | 7 | B9 | 4 | A8 | 1 | D7 |
| O | 7 | B10 | 4 | A9 | 1 | D8 |
| O | 1 | B11 | 5 | A10 | 4 | D9 |
| C | 12 | B12 | 1 | A11 | 5 | D10 |
| H | 13 | B13 | 12 | A12 | 1 | D11 |
| H | 13 | B14 | 12 | A13 | 1 | D12 |
| O | 13 | B15 | 12 | A14 | 1 | D13 |
| O | 16 | B16 | 13 | A15 | 12 | D14 |
| H | 17 | B17 | 16 | A16 | 13 | D15 |
| | | | | | | 0 |

Variables:

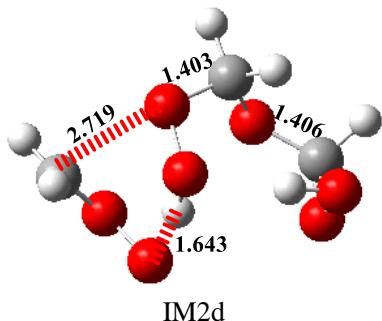
| | |
|-----|------------|
| B1 | 1.08804196 |
| B2 | 1.09491762 |
| B3 | 2.27492032 |
| B4 | 1.39372009 |
| B5 | 3.20695464 |
| B6 | 1.40061720 |
| B7 | 1.08973201 |
| B8 | 1.08965214 |
| B9 | 2.27878583 |
| B10 | 1.38871558 |
| B11 | 1.39135346 |

| | |
|-----|---------------|
| B12 | 1.40718095 |
| B13 | 1.09130927 |
| B14 | 1.09398138 |
| B15 | 1.38804938 |
| B16 | 1.41944571 |
| B17 | 0.96616097 |
| A1 | 111.00826776 |
| A2 | 138.51001701 |
| A3 | 36.87277193 |
| A4 | 89.16382476 |
| A5 | 132.45947809 |
| A6 | 104.70141827 |
| A7 | 109.70028309 |
| A8 | 106.31788028 |
| A9 | 114.41532465 |
| A10 | 114.13728410 |
| A11 | 116.16639715 |
| A12 | 111.27663138 |
| A13 | 111.15030493 |
| A14 | 107.75516983 |
| A15 | 107.11471579 |
| A16 | 101.55343398 |
| D1 | -102.06238759 |
| D2 | 138.34038038 |
| D3 | 76.73333567 |
| D4 | -56.63472133 |
| D5 | -173.80604446 |
| D6 | 65.36888885 |
| D7 | -21.90081340 |
| D8 | -59.73989428 |
| D9 | -80.86100177 |
| D10 | 86.34647865 |
| D11 | -63.10900622 |
| D12 | 61.11192440 |
| D13 | 175.41256076 |
| D14 | 68.09959073 |
| D15 | -97.62181004 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 56.64 | 99.70 | 115.04 | 128.67 | 157.70 | 175.85 | 189.49 | 292.64 | 353.62 | 360.84 | 396.61 |
| 446.88 | 461.30 | 497.57 | 556.01 | 631.36 | 686.12 | 887.38 | 962.60 | 968.62 | 1020.98 | |
| 1077.96 | 1130.34 | 1133.83 | 1141.82 | 1157.78 | 1174.32 | 1181.70 | 1223.52 | 1302.07 | | |
| 1342.74 | 1361.21 | 1413.93 | 1421.96 | 1429.11 | 1450.06 | 1457.67 | 1491.60 | 1507.42 | | |
| 1538.72 | 3063.26 | 3080.40 | 3102.23 | 3146.16 | 3161.26 | 3173.43 | 3742.99 | 3805.38 | | |

Rotational constants (B/GHZ): 1.7171591 1.0738626 0.7770133



IM2d

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| C | | | | | | |
| H | 1 | B1 | | | | |
| H | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| O | 1 | B4 | 4 | A3 | 2 | D2 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 0 |
| C | 5 | B6 | 1 | A5 | 4 | D4 0 |
| H | 7 | B7 | 5 | A6 | 1 | D5 0 |
| H | 7 | B8 | 5 | A7 | 1 | D6 0 |
| O | 7 | B9 | 5 | A8 | 1 | D7 0 |
| O | 7 | B10 | 5 | A9 | 1 | D8 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 0 |
| C | 12 | B12 | 1 | A11 | 5 | D10 0 |
| H | 13 | B13 | 12 | A12 | 1 | D11 0 |
| H | 13 | B14 | 12 | A13 | 1 | D12 0 |
| O | 13 | B15 | 12 | A14 | 1 | D13 0 |
| O | 16 | B16 | 13 | A15 | 12 | D14 0 |
| H | 17 | B17 | 16 | A16 | 13 | D15 0 |

Variables:

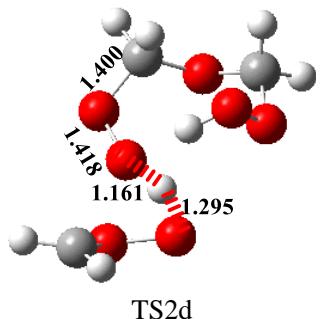
| | |
|-----|------------|
| B1 | 1.09230618 |
| B2 | 1.09152965 |
| B3 | 2.30712600 |
| B4 | 1.40339209 |
| B5 | 1.00358637 |
| B6 | 2.71928638 |
| B7 | 1.08298022 |
| B8 | 1.08478245 |
| B9 | 2.22786991 |
| B10 | 1.23283725 |
| B11 | 1.38988740 |
| B12 | 1.40618075 |
| B13 | 1.08735793 |
| B14 | 1.09272513 |
| B15 | 1.38978946 |
| B16 | 1.42037272 |
| B17 | 0.97170844 |

| | |
|-----|---------------|
| A1 | 111.15122046 |
| A2 | 138.03696929 |
| A3 | 35.45614286 |
| A4 | 98.02714931 |
| A5 | 121.92372641 |
| A6 | 112.60041067 |
| A7 | 66.63663805 |
| A8 | 77.10976933 |
| A9 | 91.91971324 |
| A10 | 111.17745592 |
| A11 | 118.06891513 |
| A12 | 105.26935443 |
| A13 | 110.48948435 |
| A14 | 115.10760989 |
| A15 | 108.93009905 |
| A16 | 100.92143105 |
| D1 | 113.57810685 |
| D2 | -129.02111946 |
| D3 | 99.26769621 |
| D4 | -102.83902346 |
| D5 | -74.47040132 |
| D6 | 166.14673737 |
| D7 | 73.76952847 |
| D8 | 44.28779259 |
| D9 | 68.38655223 |
| D10 | -114.07100982 |
| D11 | -172.75006226 |
| D12 | -52.05805084 |
| D13 | 71.97089060 |
| D14 | -86.61494647 |
| D15 | 98.61402746 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 51.63 | 67.67 | 84.47 | 130.39 | 147.39 | 173.10 | 189.60 | 212.21 | 243.54 | 283.78 | 351.96 |
| 431.17 | 457.85 | 550.78 | 605.23 | 609.59 | 650.22 | 711.33 | 876.70 | 903.01 | 943.94 | |
| 952.56 | 1006.74 | 1101.57 | 1105.39 | 1119.94 | 1139.49 | 1194.68 | 1220.63 | 1267.55 | | |
| 1329.67 | 1348.73 | 1423.54 | 1442.74 | 1454.52 | 1483.95 | 1489.03 | 1509.51 | 1638.73 | | |
| 1667.96 | 3011.00 | 3078.93 | 3085.14 | 3142.96 | 3145.11 | 3165.71 | 3289.07 | 3683.63 | | |

Rotational constants (B/GHZ): 1.9076250 0.9078872 0.8500031



TS2d

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| C | | | | | | |
| H | 1 | B1 | | | | |
| H | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| O | 1 | B4 | 4 | A3 | 2 | D2 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 0 |
| C | 4 | B6 | 1 | A5 | 5 | D4 0 |
| H | 7 | B7 | 4 | A6 | 1 | D5 0 |
| H | 7 | B8 | 4 | A7 | 1 | D6 0 |
| O | 7 | B9 | 4 | A8 | 1 | D7 0 |
| O | 7 | B10 | 4 | A9 | 1 | D8 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 0 |
| C | 12 | B12 | 1 | A11 | 5 | D10 0 |
| H | 13 | B13 | 12 | A12 | 1 | D11 0 |
| H | 13 | B14 | 12 | A13 | 1 | D12 0 |
| O | 13 | B15 | 12 | A14 | 1 | D13 0 |
| O | 16 | B16 | 13 | A15 | 12 | D14 0 |
| H | 17 | B17 | 16 | A16 | 13 | D15 0 |

Variables:

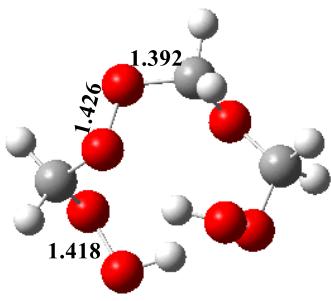
| | |
|-----|------------|
| B1 | 1.09367104 |
| B2 | 1.09074277 |
| B3 | 2.29192599 |
| B4 | 1.40042830 |
| B5 | 1.16093597 |
| B6 | 2.14527910 |
| B7 | 1.08508067 |
| B8 | 1.08212318 |
| B9 | 2.16523921 |
| B10 | 1.24990183 |
| B11 | 1.39167318 |
| B12 | 1.40093186 |
| B13 | 1.08757378 |
| B14 | 1.09277147 |
| B15 | 1.39383116 |
| B16 | 1.42031374 |
| B17 | 0.97225980 |

| | |
|-----|---------------|
| A1 | 111.15228335 |
| A2 | 138.52218970 |
| A3 | 35.85178712 |
| A4 | 97.59744781 |
| A5 | 132.88810683 |
| A6 | 111.47931341 |
| A7 | 80.02282469 |
| A8 | 67.24828457 |
| A9 | 90.61177313 |
| A10 | 111.56428225 |
| A11 | 118.11874004 |
| A12 | 105.58182353 |
| A13 | 110.98005521 |
| A14 | 114.59734224 |
| A15 | 108.91138900 |
| A16 | 101.19496613 |
| D1 | 116.61836747 |
| D2 | -126.35933158 |
| D3 | 102.13141964 |
| D4 | 31.03457895 |
| D5 | -68.81143216 |
| D6 | 169.93317752 |
| D7 | 80.23864756 |
| D8 | 49.30639345 |
| D9 | 64.69441313 |
| D10 | -115.06128116 |
| D11 | -168.87398847 |
| D12 | -47.77997472 |
| D13 | 76.06955785 |
| D14 | -86.88702127 |
| D15 | 94.21529419 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 842.60 <i>i</i> | 45.38 | 75.99 | 94.81 | 137.87 | 157.71 | 201.42 | 218.92 | 309.76 | 376.68 | 412.21 |
| 454.76 | 468.16 | 571.62 | 608.44 | 615.84 | 657.87 | 791.37 | 804.93 | 915.84 | 946.09 | |
| 971.18 | 1010.57 | 1107.48 | 1128.39 | 1138.23 | 1162.38 | 1195.79 | 1220.25 | 1250.91 | | |
| 1329.64 | 1344.08 | 1421.76 | 1437.82 | 1445.38 | 1485.06 | 1487.53 | 1516.13 | 1566.53 | | |
| 1634.61 | 1774.95 | 3076.33 | 3083.61 | 3151.78 | 3156.58 | 3168.93 | 3290.32 | 3656.04 | | |

Rotational constants (B/GHZ): 2.0039339 0.8782998 0.8104643



P2d

C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| H | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| O | 1 | B4 | 4 | A3 | 2 | D2 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 0 |
| C | 4 | B6 | 1 | A5 | 5 | D4 0 |
| H | 7 | B7 | 4 | A6 | 1 | D5 0 |
| H | 7 | B8 | 4 | A7 | 1 | D6 0 |
| O | 7 | B9 | 4 | A8 | 1 | D7 0 |
| O | 7 | B10 | 4 | A9 | 1 | D8 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 0 |
| C | 12 | B12 | 1 | A11 | 5 | D10 0 |
| H | 13 | B13 | 12 | A12 | 1 | D11 0 |
| H | 13 | B14 | 12 | A13 | 1 | D12 0 |
| O | 13 | B15 | 12 | A14 | 1 | D13 0 |
| O | 16 | B16 | 13 | A15 | 12 | D14 0 |
| H | 17 | B17 | 16 | A16 | 13 | D15 0 |

Variables:

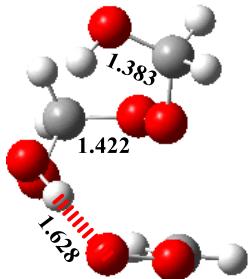
| | |
|-----|------------|
| B1 | 1.09309772 |
| B2 | 1.09100771 |
| B3 | 2.29414924 |
| B4 | 1.39192073 |
| B5 | 2.83987031 |
| B6 | 1.40870539 |
| B7 | 1.08905637 |
| B8 | 1.09062584 |
| B9 | 2.25155136 |
| B10 | 1.37965101 |
| B11 | 1.39878983 |
| B12 | 1.39203121 |
| B13 | 1.08803263 |
| B14 | 1.09196967 |
| B15 | 1.40090693 |
| B16 | 1.41817956 |

| | |
|-----|---------------|
| B17 | 0.97146288 |
| A1 | 111.11151288 |
| A2 | 137.48993681 |
| A3 | 35.98118791 |
| A4 | 88.65888437 |
| A5 | 128.38693063 |
| A6 | 109.70296427 |
| A7 | 104.03733893 |
| A8 | 98.58895242 |
| A9 | 113.42065813 |
| A10 | 111.69210369 |
| A11 | 118.28325766 |
| A12 | 106.85412716 |
| A13 | 111.87883549 |
| A14 | 113.12884958 |
| A15 | 108.55256572 |
| A16 | 102.48700391 |
| D1 | 108.77249315 |
| D2 | -133.69594214 |
| D3 | 123.79490551 |
| D4 | 61.26578478 |
| D5 | -72.84257660 |
| D6 | 166.41785372 |
| D7 | 80.90048485 |
| D8 | 45.49097179 |
| D9 | 73.82769244 |
| D10 | -126.40161905 |
| D11 | -157.64639852 |
| D12 | -35.23447306 |
| D13 | 87.88033664 |
| D14 | -81.82169669 |
| D15 | 91.20787985 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 67.95 | 70.34 | 92.00 | 145.56 | 185.43 | 210.22 | 242.88 | 275.79 | 377.58 | 400.76 | 462.28 |
| 504.46 | 516.17 | 588.53 | 619.04 | 650.40 | 679.53 | 893.44 | 947.19 | 969.44 | 1012.39 | |
| 1058.51 | 1101.68 | 1124.39 | 1139.97 | 1144.57 | 1173.58 | 1210.46 | 1231.14 | 1327.15 | | |
| 1346.08 | 1350.55 | 1409.66 | 1428.29 | 1451.21 | 1459.64 | 1466.44 | 1492.92 | 1495.42 | | |
| 1513.94 | 3076.60 | 3091.99 | 3102.62 | 3143.70 | 3172.18 | 3174.95 | 3698.15 | 3727.35 | | |

Rotational constants (B/GHZ): 1.6405933 1.2080624 0.9120953



IM2e

C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| H | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 0 |
| O | 1 | B4 | 4 | A3 | 2 | D2 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 0 |
| C | 5 | B6 | 1 | A5 | 4 | D4 0 |
| H | 7 | B7 | 5 | A6 | 1 | D5 0 |
| H | 7 | B8 | 5 | A7 | 1 | D6 0 |
| O | 7 | B9 | 5 | A8 | 1 | D7 0 |
| O | 7 | B10 | 5 | A9 | 1 | D8 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 0 |
| O | 12 | B12 | 1 | A11 | 5 | D10 0 |
| C | 13 | B13 | 12 | A12 | 1 | D11 0 |
| H | 14 | B14 | 13 | A13 | 12 | D12 0 |
| H | 14 | B15 | 13 | A14 | 12 | D13 0 |
| O | 14 | B16 | 13 | A15 | 12 | D14 0 |
| H | 17 | B17 | 14 | A16 | 13 | D15 0 |

Variables:

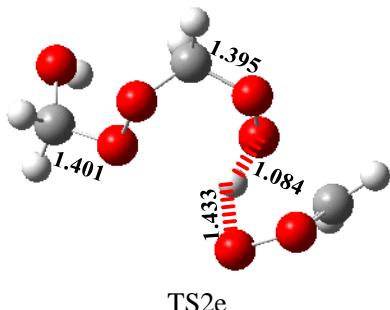
| | |
|-----|------------|
| B1 | 1.08612208 |
| B2 | 1.09029262 |
| B3 | 2.27923749 |
| B4 | 1.38262711 |
| B5 | 1.00102219 |
| B6 | 3.17989086 |
| B7 | 1.08308732 |
| B8 | 1.08639653 |
| B9 | 2.22949630 |
| B10 | 1.23244809 |
| B11 | 1.42234880 |
| B12 | 1.41793320 |
| B13 | 1.41067028 |
| B14 | 1.08917389 |
| B15 | 1.09452666 |
| B16 | 1.38261190 |

| | |
|-----|---------------|
| B17 | 0.96679914 |
| A1 | 112.18094293 |
| A2 | 79.08160700 |
| A3 | 36.37876894 |
| A4 | 117.41065646 |
| A5 | 101.43461274 |
| A6 | 137.57409026 |
| A7 | 26.55513924 |
| A8 | 70.76204339 |
| A9 | 101.84737662 |
| A10 | 113.35923781 |
| A11 | 109.99771538 |
| A12 | 111.11237852 |
| A13 | 110.02178604 |
| A14 | 102.06270164 |
| A15 | 113.07241891 |
| A16 | 108.62181219 |
| D1 | -138.30405178 |
| D2 | -149.10446672 |
| D3 | 69.50390516 |
| D4 | -92.93423693 |
| D5 | -28.78859466 |
| D6 | -101.16008569 |
| D7 | 134.04256453 |
| D8 | 122.82912041 |
| D9 | 92.65887420 |
| D10 | -53.96454365 |
| D11 | -89.53289303 |
| D12 | -49.16824222 |
| D13 | -167.23418630 |
| D14 | 71.18242593 |
| D15 | 46.07669395 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 18.74 | 62.73 | 93.56 | 112.18 | 134.59 | 152.20 | 200.02 | 225.26 | 248.99 | 267.68 | 350.47 |
| 384.50 | 482.22 | 509.90 | 544.98 | 633.06 | 668.30 | 726.94 | 873.25 | 889.63 | 910.48 | |
| 963.42 | 1022.69 | 1072.75 | 1115.25 | 1135.50 | 1151.35 | 1160.45 | 1183.86 | 1271.41 | | |
| 1293.62 | 1324.70 | 1378.24 | 1418.58 | 1448.98 | 1460.48 | 1495.79 | 1506.11 | 1619.70 | | |
| 1677.30 | 3066.91 | 3075.16 | 3110.59 | 3144.53 | 3145.62 | 3189.36 | 3288.77 | 3800.66 | | |

Rotational constants (B/GHZ): 1.5962138 0.9800565 0.8857907



TS2e

| C | | B1 | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | | | | | |
| H | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 0 |
| O | 1 | B4 | 4 | A3 | 2 | D2 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 0 |
| C | 4 | B6 | 1 | A5 | 5 | D4 0 |
| H | 7 | B7 | 4 | A6 | 1 | D5 0 |
| H | 7 | B8 | 4 | A7 | 1 | D6 0 |
| O | 7 | B9 | 4 | A8 | 1 | D7 0 |
| O | 7 | B10 | 4 | A9 | 1 | D8 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 0 |
| O | 12 | B12 | 1 | A11 | 5 | D10 0 |
| C | 13 | B13 | 12 | A12 | 1 | D11 0 |
| H | 14 | B14 | 13 | A13 | 12 | D12 0 |
| H | 14 | B15 | 13 | A14 | 12 | D13 0 |
| O | 14 | B16 | 13 | A15 | 12 | D14 0 |
| H | 17 | B17 | 14 | A16 | 13 | D15 0 |

Variables:

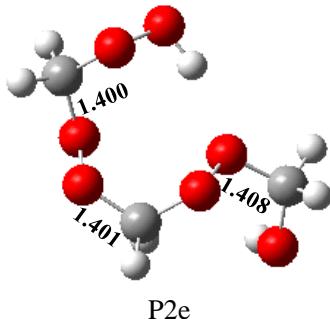
| | |
|-----|------------|
| B1 | 1.08923401 |
| B2 | 1.09009800 |
| B3 | 2.28173243 |
| B4 | 1.39493380 |
| B5 | 1.08394794 |
| B6 | 2.06772845 |
| B7 | 1.08527351 |
| B8 | 1.08303179 |
| B9 | 2.16473001 |
| B10 | 1.25271213 |
| B11 | 1.39370527 |
| B12 | 1.42174647 |
| B13 | 1.40069839 |
| B14 | 1.08821486 |
| B15 | 1.09222745 |
| B16 | 1.39235043 |
| B17 | 0.96045827 |

| | |
|-----|---------------|
| A1 | 112.44183552 |
| A2 | 83.04375779 |
| A3 | 36.13688195 |
| A4 | 98.38106256 |
| A5 | 135.75998694 |
| A6 | 108.70818668 |
| A7 | 82.38067310 |
| A8 | 69.97320235 |
| A9 | 93.28957040 |
| A10 | 113.71568944 |
| A11 | 108.95746625 |
| A12 | 107.17241240 |
| A13 | 109.72907776 |
| A14 | 103.35368248 |
| A15 | 113.17076732 |
| A16 | 109.03910104 |
| D1 | -140.71295350 |
| D2 | -139.43368109 |
| D3 | 102.47258006 |
| D4 | 26.25380766 |
| D5 | -66.01218646 |
| D6 | 172.56940833 |
| D7 | 83.91203637 |
| D8 | 52.86941997 |
| D9 | 81.49511747 |
| D10 | -80.05930208 |
| D11 | -112.03080042 |
| D12 | -45.86700062 |
| D13 | -164.49220104 |
| D14 | 73.41567897 |
| D15 | 69.34137392 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 479.67 <i>i</i> | 42.58 | 49.40 | 70.78 | 89.93 | 144.75 | 159.03 | 194.15 | 329.38 | 370.29 | 402.61 |
| 442.37 | 462.08 | 476.78 | 582.04 | 632.67 | 671.20 | 817.87 | 896.24 | 904.96 | 955.69 | |
| 1060.75 | 1069.80 | 1101.00 | 1122.26 | 1138.93 | 1156.21 | 1183.89 | 1232.02 | 1300.08 | | |
| 1301.41 | 1332.66 | 1384.12 | 1408.33 | 1437.32 | 1440.60 | 1457.24 | 1500.86 | 1584.36 | | |
| 1623.66 | 2047.92 | 3083.89 | 3105.96 | 3150.92 | 3165.02 | 3174.98 | 3281.72 | 3896.13 | | |

Rotational constants (B/GHZ): 2.5144665 0.6930923 0.6237335



P2e

| C | | B1 | | | | |
|---|----|-----|----|----|----|-------|
| H | 1 | | | | | |
| H | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 0 |
| O | 1 | B4 | 4 | A3 | 2 | D2 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 0 |
| C | 4 | B6 | 1 | A5 | 5 | D4 0 |
| H | 7 | B7 | 4 | A6 | 1 | D5 0 |
| H | 7 | B8 | 4 | A7 | 1 | D6 0 |
| O | 7 | B9 | 4 | A8 | 1 | D7 0 |
| O | 7 | B10 | 4 | A9 | 1 | D8 0 |
| O | 1 | B11 | 5 | 10 | 4 | D9 0 |
| O | 12 | B12 | 1 | 11 | 5 | D10 0 |
| C | 13 | B13 | 12 | 12 | 1 | D11 0 |
| H | 14 | B14 | 13 | 13 | 12 | D12 0 |
| H | 14 | B15 | 13 | 14 | 12 | D13 0 |
| O | 14 | B16 | 13 | 15 | 12 | D14 0 |
| H | 17 | B17 | 14 | 16 | 13 | D15 0 |

Variables:

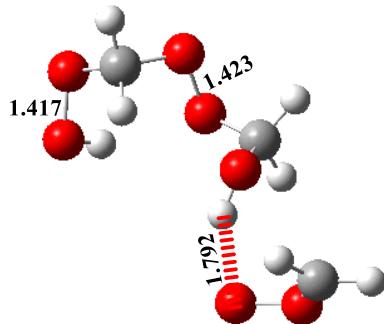
| | |
|-----|------------|
| B1 | 1.08891916 |
| B2 | 1.08968958 |
| B3 | 2.27065662 |
| B4 | 1.38754669 |
| B5 | 2.68713858 |
| B6 | 1.40044393 |
| B7 | 1.09038160 |
| B8 | 1.09068247 |
| B9 | 2.26491757 |
| B10 | 1.38426644 |
| B11 | 1.40114368 |
| B12 | 1.42057882 |
| B13 | 1.40828970 |
| B14 | 1.08765346 |
| B15 | 1.09240083 |
| B16 | 1.38617180 |
| B17 | 0.96060309 |

| | |
|-----|---------------|
| A1 | 112.12362214 |
| A2 | 84.39851150 |
| A3 | 36.81331179 |
| A4 | 84.78505923 |
| A5 | 129.06210279 |
| A6 | 110.43738593 |
| A7 | 103.88268553 |
| A8 | 98.04488206 |
| A9 | 113.56000497 |
| A10 | 113.96981209 |
| A11 | 109.54417534 |
| A12 | 107.31305993 |
| A13 | 109.40632468 |
| A14 | 103.37934023 |
| A15 | 112.66415694 |
| A16 | 109.45194888 |
| D1 | -142.25081628 |
| D2 | -137.16686151 |
| D3 | 121.12189566 |
| D4 | 60.31391196 |
| D5 | -77.88693348 |
| D6 | 161.13639535 |
| D7 | 74.62735218 |
| D8 | 40.09496279 |
| D9 | 78.28285708 |
| D10 | -90.68241610 |
| D11 | -112.85526833 |
| D12 | -46.22804825 |
| D13 | -164.83120013 |
| D14 | 72.94418472 |
| D15 | 70.84294455 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 41.45 | 56.84 | 89.21 | 107.18 | 148.65 | 190.21 | 238.15 | 273.49 | 340.14 | 414.07 | 428.68 |
| 471.14 | 502.64 | 527.73 | 626.92 | 658.35 | 686.63 | 882.30 | 918.49 | 965.75 | 1045.85 | |
| 1060.95 | 1079.08 | 1113.56 | 1134.80 | 1136.36 | 1141.42 | 1164.76 | 1213.13 | 1300.46 | | |
| 1324.56 | 1347.10 | 1392.02 | 1400.41 | 1422.61 | 1438.11 | 1457.42 | 1466.31 | 1501.72 | | |
| 1505.05 | 3091.26 | 3098.08 | 3108.12 | 3166.03 | 3167.91 | 3175.88 | 3737.06 | 3894.23 | | |

Rotational constants (B/GHZ): 2.1188528 0.8569316 0.6925481



IM2f

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | | | | | | | |
| O | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| C | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| O | 5 | B7 | 2 | A6 | 1 | D5 | 0 |
| O | 5 | B8 | 2 | A7 | 1 | D6 | 0 |
| H | 1 | B9 | 2 | A8 | 8 | D7 | 0 |
| H | 1 | B10 | 2 | A9 | 8 | D8 | 0 |
| O | 1 | B11 | 2 | A10 | 8 | D9 | 0 |
| C | 4 | B12 | 1 | A11 | 2 | D10 | 0 |
| H | 13 | B13 | 4 | A12 | 1 | D11 | 0 |
| H | 13 | B14 | 4 | A13 | 1 | D12 | 0 |
| O | 13 | B15 | 4 | A14 | 1 | D13 | 0 |
| O | 16 | B16 | 13 | A15 | 4 | D14 | 0 |
| H | 17 | B17 | 16 | A16 | 13 | D15 | 0 |

Variables:

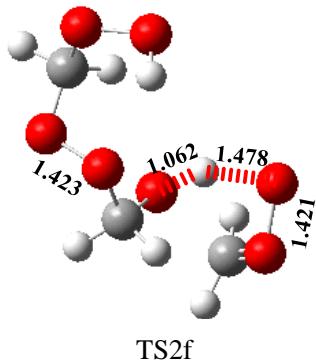
| | |
|-----|------------|
| B1 | 1.38541949 |
| B2 | 0.97881337 |
| B3 | 2.27986516 |
| B4 | 2.85195410 |
| B5 | 1.08281979 |
| B6 | 1.08406020 |
| B7 | 2.22515895 |
| B8 | 1.23488140 |
| B9 | 1.08920564 |
| B10 | 1.09371930 |
| B11 | 1.40676994 |
| B12 | 1.40377379 |
| B13 | 1.08892979 |
| B14 | 1.09022278 |
| B15 | 1.38916304 |

| | |
|-----|---------------|
| B16 | 1.41743589 |
| B17 | 0.96689024 |
| A1 | 107.88364174 |
| A2 | 98.97126201 |
| A3 | 118.60526939 |
| A4 | 128.04137336 |
| A5 | 62.88419809 |
| A6 | 62.39075969 |
| A7 | 81.48096122 |
| A8 | 108.19585792 |
| A9 | 112.10662447 |
| A10 | 113.11187194 |
| A11 | 116.58836494 |
| A12 | 110.74221169 |
| A13 | 103.60174462 |
| A14 | 113.06229427 |
| A15 | 109.01415233 |
| A16 | 102.44190489 |
| D1 | 114.44477801 |
| D2 | -175.34010402 |
| D3 | 58.01265176 |
| D4 | 172.45032314 |
| D5 | -86.01791353 |
| D6 | -57.85909124 |
| D7 | -139.81605346 |
| D8 | -16.56835866 |
| D9 | 99.65813261 |
| D10 | -31.88923729 |
| D11 | 15.33568935 |
| D12 | 136.60401672 |
| D13 | -109.06072058 |
| D14 | 88.48242965 |
| D15 | -77.33818027 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 32.45 | 38.20 | 60.54 | 83.33 | 94.99 | 133.96 | 165.32 | 190.61 | 197.23 | 251.06 | 363.22 |
| 396.34 | 401.69 | 494.97 | 542.92 | 630.74 | 664.85 | 705.89 | 794.45 | 894.60 | 912.69 | |
| 966.80 | 1050.80 | 1082.92 | 1110.22 | 1113.80 | 1134.71 | 1142.36 | 1188.63 | 1268.30 | | |
| 1326.70 | 1335.88 | 1407.30 | 1434.12 | 1450.33 | 1463.64 | 1467.83 | 1480.08 | 1498.30 | | |
| 1658.51 | 3082.16 | 3112.34 | 3152.53 | 3154.83 | 3183.50 | 3301.60 | 3487.41 | 3822.53 | | |

Rotational constants (B/GHZ): 2.4734210 0.5244542 0.4772716



| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | | | | | | | |
| O | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| C | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| O | 5 | B7 | 2 | A6 | 1 | D5 | 0 |
| O | 5 | B8 | 2 | A7 | 1 | D6 | 0 |
| H | 1 | B9 | 2 | A8 | 5 | D7 | 0 |
| H | 1 | B10 | 2 | A9 | 5 | D8 | 0 |
| O | 1 | B11 | 2 | A10 | 5 | D9 | 0 |
| C | 4 | B12 | 1 | A11 | 12 | D10 | 0 |
| H | 13 | B13 | 4 | A12 | 1 | D11 | 0 |
| H | 13 | B14 | 4 | A13 | 1 | D12 | 0 |
| O | 13 | B15 | 4 | A14 | 1 | D13 | 0 |
| O | 16 | B16 | 13 | A15 | 4 | D14 | 0 |
| H | 17 | B17 | 16 | A16 | 13 | D15 | 0 |

Variables:

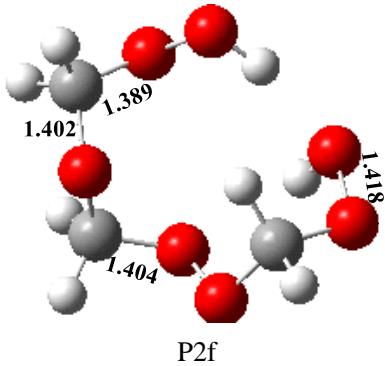
| | |
|-----|------------|
| B1 | 1.39961428 |
| B2 | 1.06230827 |
| B3 | 2.27469756 |
| B4 | 2.02225615 |
| B5 | 1.08600759 |
| B6 | 1.08273072 |
| B7 | 2.16672676 |
| B8 | 1.25760257 |
| B9 | 1.08954590 |
| B10 | 1.09438224 |
| B11 | 1.39494950 |
| B12 | 1.40641657 |
| B13 | 1.08920709 |
| B14 | 1.09012719 |
| B15 | 1.38691368 |
| B16 | 1.41721953 |

| | |
|-----|---------------|
| B17 | 0.96665240 |
| A1 | 106.91873974 |
| A2 | 98.51220404 |
| A3 | 112.18553269 |
| A4 | 108.73508948 |
| A5 | 83.74583601 |
| A6 | 71.26994541 |
| A7 | 94.45826679 |
| A8 | 108.35761304 |
| A9 | 111.22899059 |
| A10 | 111.73604657 |
| A11 | 116.89660233 |
| A12 | 110.84006237 |
| A13 | 103.28386193 |
| A14 | 113.12151268 |
| A15 | 109.00330423 |
| A16 | 102.55150867 |
| D1 | 102.71963239 |
| D2 | -176.82991113 |
| D3 | 54.15560690 |
| D4 | 175.35081731 |
| D5 | -96.47401378 |
| D6 | -65.12487889 |
| D7 | -91.09240334 |
| D8 | 32.22709201 |
| D9 | 147.70420891 |
| D10 | 84.27230204 |
| D11 | 17.90426513 |
| D12 | 138.88468532 |
| D13 | -106.44822035 |
| D14 | 90.22906792 |
| D15 | -81.53657170 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 420.24 <i>i</i> | 24.74 | 53.34 | 92.84 | 109.60 | 150.44 | 169.51 | 196.96 | 328.73 | 363.63 | 395.24 |
| 402.67 | 468.24 | 500.11 | 569.79 | 640.57 | 667.15 | 850.24 | 898.34 | 910.17 | 967.97 | |
| 1059.22 | 1069.61 | 1125.31 | 1128.51 | 1143.47 | 1191.06 | 1201.95 | 1227.86 | 1287.64 | | |
| 1332.36 | 1356.94 | 1412.18 | 1420.50 | 1448.55 | 1457.98 | 1476.54 | 1499.78 | 1547.63 | | |
| 1610.13 | 2187.80 | 3076.48 | 3116.86 | 3146.00 | 3148.12 | 3188.00 | 3276.65 | 3824.95 | | |

Rotational constants (B/GHZ): 2.3942415 0.6652077 0.5803588



C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| O | 1 | B1 | | | | |
| H | 2 | B2 | 1 | A1 | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 0 |
| C | 2 | B4 | 1 | A3 | 4 | D2 0 |
| H | 5 | B5 | 2 | A4 | 1 | D3 0 |
| H | 5 | B6 | 2 | A5 | 1 | D4 0 |
| O | 5 | B7 | 2 | A6 | 1 | D5 0 |
| O | 5 | B8 | 2 | A7 | 1 | D6 0 |
| H | 1 | B9 | 2 | A8 | 5 | D7 0 |
| H | 1 | B10 | 2 | A9 | 5 | D8 0 |
| O | 1 | B11 | 2 | A10 | 5 | D9 0 |
| C | 4 | B12 | 1 | A11 | 2 | D10 0 |
| H | 13 | B13 | 4 | A12 | 1 | D11 0 |
| H | 13 | B14 | 4 | A13 | 1 | D12 0 |
| O | 13 | B15 | 4 | A14 | 1 | D13 0 |
| O | 16 | B16 | 13 | A15 | 4 | D14 0 |
| H | 17 | B17 | 16 | A16 | 13 | D15 0 |

Variables:

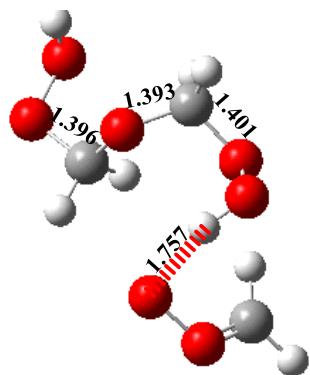
| | |
|-----|------------|
| B1 | 1.39016151 |
| B2 | 3.17128950 |
| B3 | 2.28378685 |
| B4 | 1.40213902 |
| B5 | 1.09381529 |
| B6 | 1.08795931 |
| B7 | 2.26618927 |
| B8 | 1.38905157 |
| B9 | 1.08838158 |
| B10 | 1.09364724 |
| B11 | 1.40427350 |
| B12 | 1.40134802 |
| B13 | 1.08979752 |
| B14 | 1.08978026 |
| B15 | 1.39478933 |
| B16 | 1.41782831 |

| | |
|-----|---------------|
| B17 | 0.96837901 |
| A1 | 99.81199139 |
| A2 | 100.36555267 |
| A3 | 115.28611557 |
| A4 | 110.45574588 |
| A5 | 106.18580949 |
| A6 | 101.73168033 |
| A7 | 114.36884630 |
| A8 | 107.66155829 |
| A9 | 111.69357720 |
| A10 | 113.26034996 |
| A11 | 114.69693545 |
| A12 | 110.72534321 |
| A13 | 104.18113993 |
| A14 | 112.90563740 |
| A15 | 109.43100524 |
| A16 | 103.06092293 |
| D1 | 59.59624301 |
| D2 | 125.58457954 |
| D3 | 51.64532794 |
| D4 | 172.78300804 |
| D5 | -101.57273673 |
| D6 | -65.09533819 |
| D7 | -149.81749699 |
| D8 | -26.93769359 |
| D9 | 89.86669200 |
| D10 | -28.03390935 |
| D11 | 15.68529921 |
| D12 | 136.88246327 |
| D13 | -109.46425857 |
| D14 | 83.52303734 |
| D15 | -75.21026115 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 52.91 | 95.56 | 111.93 | 132.16 | 178.78 | 197.26 | 236.35 | 319.29 | 371.98 | 402.47 | 446.61 |
| 486.16 | 519.34 | 582.49 | 613.86 | 667.11 | 685.08 | 895.34 | 956.86 | 957.99 | 994.35 | |
| 1055.88 | 1106.03 | 1111.17 | 1126.66 | 1136.57 | 1182.62 | 1199.50 | 1224.93 | 1329.27 | | |
| 1338.13 | 1362.85 | 1413.36 | 1427.77 | 1444.14 | 1449.49 | 1470.95 | 1484.88 | 1505.65 | | |
| 1518.67 | 3082.24 | 3088.08 | 3108.05 | 3161.03 | 3166.16 | 3178.87 | 3667.48 | 3767.38 | | |

Rotational constants (B/GHZ): 1.7576020 1.1421941 0.8117293



IM2g

| C | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 1 | B1 | | | | | |
| H | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 | 0 |
| O | 1 | B4 | 4 | A3 | 3 | D2 | 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 | 0 |
| C | 4 | B6 | 1 | A5 | 5 | D4 | 0 |
| H | 7 | B7 | 4 | A6 | 1 | D5 | 0 |
| H | 7 | B8 | 4 | A7 | 1 | D6 | 0 |
| O | 7 | B9 | 4 | A8 | 1 | D7 | 0 |
| O | 7 | B10 | 4 | A9 | 1 | D8 | 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 | 0 |
| C | 12 | B12 | 1 | A11 | 5 | D10 | 0 |
| H | 13 | B13 | 12 | A12 | 1 | D11 | 0 |
| H | 13 | B14 | 12 | A13 | 1 | D12 | 0 |
| O | 13 | B15 | 12 | A14 | 1 | D13 | 0 |
| O | 16 | B16 | 13 | A15 | 12 | D14 | 0 |
| H | 17 | B17 | 16 | A16 | 13 | D15 | 0 |

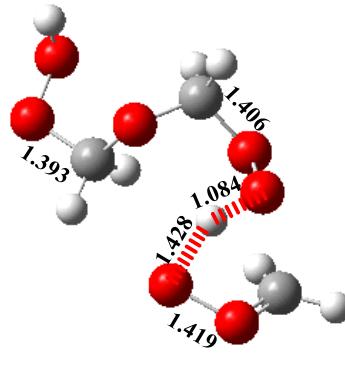
Variables:

| | |
|-----|------------|
| B1 | 1.09251099 |
| B2 | 1.08857672 |
| B3 | 2.28184846 |
| B4 | 1.40104938 |
| B5 | 0.98793151 |
| B6 | 2.91142732 |
| B7 | 1.08333958 |
| B8 | 1.08666208 |
| B9 | 2.22617563 |
| B10 | 1.23529145 |
| B11 | 1.39336495 |
| B12 | 1.39873873 |
| B13 | 1.09338349 |
| B14 | 1.08793991 |

| | |
|-----|---------------|
| B15 | 1.39594118 |
| B16 | 1.41932363 |
| B17 | 0.96444280 |
| A1 | 112.29161584 |
| A2 | 86.49480522 |
| A3 | 36.19947374 |
| A4 | 93.62676194 |
| A5 | 109.19439623 |
| A6 | 133.30938701 |
| A7 | 56.12162122 |
| A8 | 61.14500383 |
| A9 | 83.55764158 |
| A10 | 112.33947202 |
| A11 | 115.72248522 |
| A12 | 110.53858517 |
| A13 | 109.19011473 |
| A14 | 111.43558064 |
| A15 | 107.29833333 |
| A16 | 101.47327251 |
| D1 | 143.24263789 |
| D2 | 131.30999379 |
| D3 | -104.43033882 |
| D4 | -41.64727776 |
| D5 | 136.41637140 |
| D6 | 27.59241056 |
| D7 | -79.45326753 |
| D8 | -104.94110326 |
| D9 | -65.49269616 |
| D10 | -71.37026394 |
| D11 | 14.73887242 |
| D12 | 136.78862317 |
| D13 | -108.24045279 |
| D14 | 67.69223761 |
| D15 | -103.34990991 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-------------------------------|---------|---------|-----------|---------|-----------|---------|-----------|---------|--------|--------|
| 46.21 | 66.36 | 76.76 | 99.71 | 117.70 | 127.51 | 164.59 | 192.81 | 207.05 | 265.81 | 296.07 |
| 349.87 | 398.31 | 491.96 | 546.01 | 598.84 | 691.64 | 702.03 | 843.86 | 908.97 | 956.44 | |
| 959.98 | 1013.02 | 1098.00 | 1102.94 | 1114.39 | 1126.36 | 1196.16 | 1221.22 | 1281.06 | | |
| 1322.84 | 1349.48 | 1412.90 | 1415.48 | 1443.48 | 1459.35 | 1491.24 | 1516.57 | 1537.98 | | |
| 1659.80 | 3072.75 | 3094.81 | 3134.12 | 3165.17 | 3182.78 | 3282.19 | 3355.77 | 3832.79 | | |
| Rotational constants (B/GHZ): | | | 2.0751858 | | 0.6898281 | | 0.5863434 | | | |



TS2g

C

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 1 | B1 | | | | | |
| H | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 | 0 |
| O | 1 | B4 | 4 | A3 | 3 | D2 | 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 | 0 |
| C | 4 | B6 | 1 | A5 | 5 | D4 | 0 |
| H | 7 | B7 | 4 | A6 | 1 | D5 | 0 |
| H | 7 | B8 | 4 | A7 | 1 | D6 | 0 |
| O | 7 | B9 | 4 | A8 | 1 | D7 | 0 |
| O | 7 | B10 | 4 | A9 | 1 | D8 | 0 |
| O | 1 | B11 | 5 | A10 | 4 | D9 | 0 |
| C | 12 | B12 | 1 | A11 | 5 | D10 | 0 |
| H | 13 | B13 | 12 | A12 | 1 | D11 | 0 |
| H | 13 | B14 | 12 | A13 | 1 | D12 | 0 |
| O | 13 | B15 | 12 | A14 | 1 | D13 | 0 |
| O | 16 | B16 | 13 | A15 | 12 | D14 | 0 |
| H | 17 | B17 | 16 | A16 | 13 | D15 | 0 |

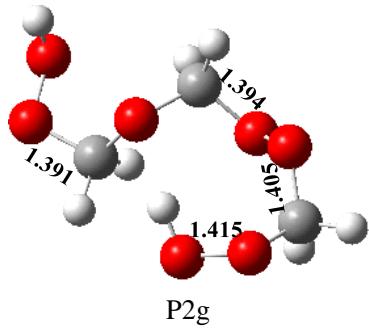
Variables:

| | |
|-----|------------|
| B1 | 1.09255349 |
| B2 | 1.08880208 |
| B3 | 2.27735311 |
| B4 | 1.40560362 |
| B5 | 1.08429991 |
| B6 | 2.05063373 |
| B7 | 1.08531656 |
| B8 | 1.08428220 |
| B9 | 2.16784408 |
| B10 | 1.25646182 |
| B11 | 1.38989073 |
| B12 | 1.40270194 |
| B13 | 1.09298237 |
| B14 | 1.08874137 |
| B15 | 1.39321724 |

| | |
|-----|---------------|
| B16 | 1.41990570 |
| B17 | 0.96444818 |
| A1 | 112.21428794 |
| A2 | 88.41870957 |
| A3 | 36.37581507 |
| A4 | 89.14953315 |
| A5 | 130.25346852 |
| A6 | 109.45917960 |
| A7 | 82.71542406 |
| A8 | 70.10523631 |
| A9 | 93.41373454 |
| A10 | 111.99920686 |
| A11 | 115.90753998 |
| A12 | 110.53177004 |
| A13 | 108.89039209 |
| A14 | 111.26312212 |
| A15 | 107.10448192 |
| A16 | 101.37931161 |
| D1 | 144.48717432 |
| D2 | 128.17118389 |
| D3 | -112.24729833 |
| D4 | -43.28307859 |
| D5 | 134.06370574 |
| D6 | 12.64959652 |
| D7 | -76.21104489 |
| D8 | -107.37611105 |
| D9 | -61.53055399 |
| D10 | -69.57946020 |
| D11 | 13.25499114 |
| D12 | 135.36579299 |
| D13 | -109.67520965 |
| D14 | 68.56946770 |
| D15 | -106.64554466 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-------------------------------|---------|-----------|---------|-----------|---------|-----------|---------|---------|--------|--------|
| 480.25 <i>i</i> | 48.26 | 64.12 | 72.78 | 115.01 | 156.90 | 178.67 | 219.92 | 297.00 | 334.03 | 382.58 |
| 399.30 | 444.36 | 474.42 | 558.72 | 597.44 | 702.54 | 851.96 | 910.73 | 956.36 | 967.34 | |
| 1004.76 | 1081.33 | 1109.81 | 1129.81 | 1168.14 | 1194.16 | 1218.94 | 1228.05 | 1263.09 | | |
| 1319.98 | 1344.81 | 1413.67 | 1420.53 | 1430.76 | 1445.13 | 1494.17 | 1515.07 | 1579.79 | | |
| 1669.50 | 2011.72 | 3080.15 | 3091.69 | 3144.56 | 3158.77 | 3162.57 | 3275.66 | 3850.65 | | |
| Rotational constants (B/GHZ): | | 2.5857978 | | 0.6776697 | | 0.5836400 | | | | |



P2g

| C | | B1 | | | | |
|---|----|-----|----|-----|----|-----|
| H | 1 | | | | | |
| H | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 |
| O | 1 | B4 | 4 | A3 | 3 | D2 |
| H | 4 | B5 | 1 | A4 | 5 | D3 |
| C | 4 | B6 | 1 | A5 | 5 | D4 |
| H | 7 | B7 | 4 | A6 | 1 | D5 |
| H | 7 | B8 | 4 | A7 | 1 | D6 |
| O | 7 | B9 | 4 | A8 | 1 | D7 |
| O | 7 | B10 | 4 | A9 | 1 | D8 |
| O | 1 | B11 | 5 | A10 | 4 | D9 |
| C | 12 | B12 | 1 | A11 | 5 | D10 |
| H | 13 | B13 | 12 | A12 | 1 | D11 |
| H | 13 | B14 | 12 | A13 | 1 | D12 |
| O | 13 | B15 | 12 | A14 | 1 | D13 |
| O | 16 | B16 | 13 | A15 | 12 | D14 |
| H | 17 | B17 | 16 | A16 | 13 | D15 |
| | | | | | | 0 |

Variables:

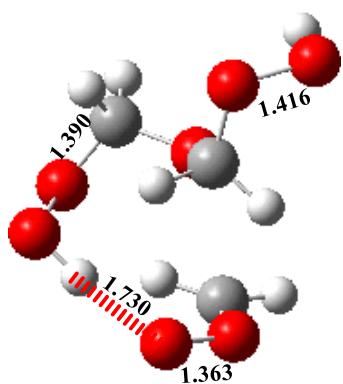
| | |
|-----|------------|
| B1 | 1.09103800 |
| B2 | 1.08796265 |
| B3 | 2.27623751 |
| B4 | 1.39395661 |
| B5 | 2.62642987 |
| B6 | 1.40546038 |
| B7 | 1.08987311 |
| B8 | 1.08960326 |
| B9 | 2.27070349 |
| B10 | 1.38779544 |
| B11 | 1.40283305 |
| B12 | 1.40603069 |
| B13 | 1.09270609 |
| B14 | 1.08985450 |
| B15 | 1.39054820 |
| B16 | 1.41922653 |
| B17 | 0.96456561 |

| | |
|-----|---------------|
| A1 | 111.79194762 |
| A2 | 80.67936969 |
| A3 | 36.74951676 |
| A4 | 69.59693642 |
| A5 | 130.07016792 |
| A6 | 106.32062282 |
| A7 | 109.22904256 |
| A8 | 99.01915591 |
| A9 | 112.71971506 |
| A10 | 112.98726579 |
| A11 | 115.04877759 |
| A12 | 110.35423705 |
| A13 | 109.40362864 |
| A14 | 111.30136070 |
| A15 | 107.01317549 |
| A16 | 101.50851226 |
| D1 | 137.94182976 |
| D2 | 143.37539711 |
| D3 | -105.16687005 |
| D4 | -64.81225627 |
| D5 | 176.29465784 |
| D6 | 54.66300917 |
| D7 | -34.81203912 |
| D8 | -69.92150218 |
| D9 | -80.59422487 |
| D10 | -77.50311667 |
| D11 | 13.94032389 |
| D12 | 135.98580146 |
| D13 | -109.32325411 |
| D14 | 68.70910568 |
| D15 | -108.04090264 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 55.26 | 67.33 | 95.53 | 115.19 | 145.26 | 172.37 | 197.67 | 265.66 | 319.69 | 391.55 | 393.86 |
| 445.40 | 473.18 | 516.78 | 578.66 | 627.55 | 682.22 | 897.91 | 957.76 | 971.25 | 996.07 | |
| 1064.82 | 1098.79 | 1127.59 | 1132.20 | 1139.79 | 1170.32 | 1185.30 | 1228.99 | 1321.87 | | |
| 1336.31 | 1362.46 | 1403.43 | 1422.23 | 1423.36 | 1449.01 | 1464.02 | 1490.39 | 1508.87 | | |
| 1523.76 | 3082.99 | 3101.23 | 3105.61 | 3154.56 | 3170.14 | 3170.53 | 3740.03 | 3846.15 | | |

Rotational constants (B/GHZ): 2.6948311 0.7063897 0.5917402



IM2h

C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 0 |
| C | 4 | B5 | 1 | A4 | 3 | D3 0 |
| O | 6 | B6 | 4 | A5 | 1 | D4 0 |
| O | 6 | B7 | 4 | A6 | 1 | D5 0 |
| H | 6 | B8 | 4 | A7 | 1 | D6 0 |
| O | 1 | B9 | 4 | A8 | 3 | D7 0 |
| C | 10 | B10 | 1 | A9 | 4 | D8 0 |
| H | 11 | B11 | 10 | A10 | 1 | D9 0 |
| O | 11 | B12 | 10 | A11 | 1 | D10 0 |
| O | 13 | B13 | 11 | A12 | 10 | D11 0 |
| H | 14 | B14 | 13 | A13 | 11 | D12 0 |
| H | 6 | B15 | 4 | A14 | 1 | D13 0 |
| H | 1 | B16 | 4 | A15 | 3 | D14 0 |
| H | 11 | B17 | 10 | A16 | 1 | D15 0 |

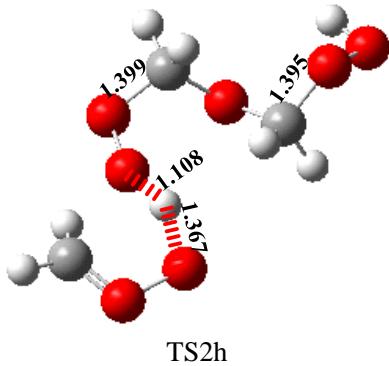
Variables:

| | |
|-----|------------|
| B1 | 1.08971566 |
| B2 | 2.27253275 |
| B3 | 1.39010865 |
| B4 | 0.98769047 |
| B5 | 3.15440970 |
| B6 | 2.22974974 |
| B7 | 1.23417325 |
| B8 | 1.08321969 |
| B9 | 1.40755424 |
| B10 | 1.40860821 |
| B11 | 1.09000645 |
| B12 | 1.39385093 |
| B13 | 1.41648418 |
| B14 | 0.96491137 |

| | |
|-----|---------------|
| B15 | 1.08567381 |
| B16 | 1.09194504 |
| B17 | 1.08792016 |
| A1 | 139.89223970 |
| A2 | 36.43624281 |
| A3 | 99.55580024 |
| A4 | 89.68900009 |
| A5 | 73.26297427 |
| A6 | 103.02761207 |
| A7 | 134.13522847 |
| A8 | 111.47502245 |
| A9 | 115.76480717 |
| A10 | 111.52522327 |
| A11 | 111.23720722 |
| A12 | 107.81788764 |
| A13 | 102.44573130 |
| A14 | 29.50851920 |
| A15 | 110.39820795 |
| A16 | 106.82828904 |
| D1 | -19.06547212 |
| D2 | 97.63418694 |
| D3 | -93.77028877 |
| D4 | 100.08621750 |
| D5 | 86.63980538 |
| D6 | -59.75685416 |
| D7 | 75.91639981 |
| D8 | -103.62298906 |
| D9 | 38.28301404 |
| D10 | -78.72373717 |
| D11 | -70.86071400 |
| D12 | 86.63424103 |
| D13 | -144.25822477 |
| D14 | -47.41013193 |
| D15 | 160.41736294 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-------------------------------|---------|---------|-----------|---------|-----------|---------|-----------|---------|--------|--------|
| 63.01 | 96.56 | 101.18 | 112.73 | 135.00 | 150.20 | 172.78 | 189.46 | 238.90 | 249.70 | 259.90 |
| 342.47 | 419.74 | 517.21 | 559.22 | 591.11 | 689.18 | 703.57 | 759.75 | 917.57 | 956.05 | |
| 964.42 | 985.14 | 1086.25 | 1095.61 | 1118.11 | 1140.32 | 1178.22 | 1222.63 | 1276.04 | | |
| 1324.77 | 1351.96 | 1418.18 | 1429.22 | 1443.23 | 1462.70 | 1482.44 | 1507.39 | 1606.93 | | |
| 1669.06 | 3089.67 | 3114.87 | 3141.22 | 3156.10 | 3184.69 | 3288.70 | 3334.45 | 3825.83 | | |
| Rotational constants (B/GHZ): | | | 1.5653054 | | 0.8960914 | | 0.7090610 | | | |



TS2h

C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 0 |
| C | 3 | B5 | 1 | A4 | 4 | D3 0 |
| O | 6 | B6 | 3 | A5 | 1 | D4 0 |
| O | 6 | B7 | 3 | A6 | 1 | D5 0 |
| H | 6 | B8 | 3 | A7 | 1 | D6 0 |
| O | 1 | B9 | 4 | A8 | 3 | D7 0 |
| C | 10 | B10 | 1 | A9 | 4 | D8 0 |
| H | 11 | B11 | 10 | A10 | 1 | D9 0 |
| O | 11 | B12 | 10 | A11 | 1 | D10 0 |
| O | 13 | B13 | 11 | A12 | 10 | D11 0 |
| H | 14 | B14 | 13 | A13 | 11 | D12 0 |
| H | 6 | B15 | 3 | A14 | 1 | D13 0 |
| H | 1 | B16 | 10 | A15 | 11 | D14 0 |
| H | 11 | B17 | 10 | A16 | 1 | D15 0 |

Variables:

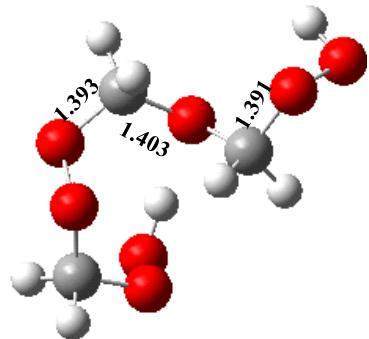
| | |
|-----|------------|
| B1 | 1.08918921 |
| B2 | 2.26991947 |
| B3 | 1.39919125 |
| B4 | 1.10798769 |
| B5 | 2.08121138 |
| B6 | 2.16695998 |
| B7 | 1.25553177 |
| B8 | 1.08509206 |
| B9 | 1.39446402 |
| B10 | 1.40449342 |
| B11 | 1.09180998 |
| B12 | 1.39458612 |
| B13 | 1.41596698 |
| B14 | 0.96581822 |
| B15 | 1.08455134 |
| B16 | 1.09333226 |

| | |
|-----|---------------|
| B17 | 1.08792582 |
| A1 | 139.97834002 |
| A2 | 36.53355088 |
| A3 | 92.52524319 |
| A4 | 131.57776929 |
| A5 | 68.93566771 |
| A6 | 92.09186719 |
| A7 | 110.47761309 |
| A8 | 111.40216306 |
| A9 | 116.18639986 |
| A10 | 111.90979077 |
| A11 | 111.29608539 |
| A12 | 107.67231763 |
| A13 | 102.55390087 |
| A14 | 81.75860943 |
| A15 | 111.00467033 |
| A16 | 106.57033144 |
| D1 | -9.45173549 |
| D2 | 110.86891332 |
| D3 | 43.13314291 |
| D4 | 81.24394911 |
| D5 | 112.60440441 |
| D6 | -129.13157205 |
| D7 | 68.99287148 |
| D8 | -104.42811431 |
| D9 | 35.45960935 |
| D10 | -80.98099262 |
| D11 | -70.40695770 |
| D12 | 78.26282618 |
| D13 | -7.74798712 |
| D14 | 18.60760720 |
| D15 | 158.05968250 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 549.49 <i>i</i> | 33.55 | 67.89 | 76.07 | 94.02 | 136.29 | 160.73 | 195.71 | 270.92 | 351.39 | 370.04 |
| 408.02 | 449.10 | 510.08 | 551.76 | 598.56 | 688.47 | 842.37 | 912.08 | 960.19 | 964.27 | |
| 1000.43 | 1073.52 | 1110.24 | 1120.12 | 1154.09 | 1189.09 | 1219.79 | 1233.45 | 1299.58 | | |
| 1326.35 | 1354.13 | 1414.09 | 1428.17 | 1444.30 | 1456.05 | 1488.19 | 1506.86 | 1514.47 | | |
| 1636.06 | 1931.93 | 3075.48 | 3101.07 | 3149.11 | 3150.66 | 3175.01 | 3282.00 | 3801.91 | | |

Rotational constants (B/GHZ): 2.6170536 0.6374371 0.5516667



P2h

C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| H | 4 | B4 | 1 | A3 | 3 | D2 0 |
| C | 3 | B5 | 1 | A4 | 4 | D3 0 |
| O | 6 | B6 | 3 | A5 | 1 | D4 0 |
| O | 6 | B7 | 3 | A6 | 1 | D5 0 |
| H | 6 | B8 | 3 | A7 | 1 | D6 0 |
| O | 1 | B9 | 4 | A8 | 3 | D7 0 |
| C | 10 | B10 | 1 | A9 | 4 | D8 0 |
| H | 11 | B11 | 10 | A10 | 1 | D9 0 |
| O | 11 | B12 | 10 | A11 | 1 | D10 0 |
| O | 13 | B13 | 11 | A12 | 10 | D11 0 |
| H | 14 | B14 | 13 | A13 | 11 | D12 0 |
| H | 6 | B15 | 3 | A14 | 1 | D13 0 |
| H | 1 | B16 | 4 | A15 | 3 | D14 0 |
| H | 11 | B17 | 10 | A16 | 1 | D15 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.08877532 |
| B2 | 2.26930949 |
| B3 | 1.39311289 |
| B4 | 2.60325504 |
| B5 | 1.40328883 |
| B6 | 2.29327111 |
| B7 | 1.39002715 |
| B8 | 1.09013041 |
| B9 | 1.40308882 |
| B10 | 1.41270503 |
| B11 | 1.08960069 |
| B12 | 1.39064916 |
| B13 | 1.41592648 |
| B14 | 0.96542230 |
| B15 | 1.08910671 |

| | |
|-----|---------------|
| B16 | 1.09235409 |
| B17 | 1.08800381 |
| A1 | 139.83750564 |
| A2 | 36.90786676 |
| A3 | 79.00641048 |
| A4 | 122.95847928 |
| A5 | 110.44440725 |
| A6 | 113.70385650 |
| A7 | 103.51745521 |
| A8 | 111.84987135 |
| A9 | 115.80114981 |
| A10 | 111.29150182 |
| A11 | 111.00868536 |
| A12 | 107.75688776 |
| A13 | 102.58653419 |
| A14 | 110.46809897 |
| A15 | 110.60726161 |
| A16 | 106.54763988 |
| D1 | -16.83301383 |
| D2 | -86.30584833 |
| D3 | 75.00811407 |
| D4 | 3.82125513 |
| D5 | 42.23051816 |
| D6 | 156.99521408 |
| D7 | 74.16713403 |
| D8 | -102.87408219 |
| D9 | 35.50686411 |
| D10 | -81.40705961 |
| D11 | -71.64962251 |
| D12 | 84.40368265 |
| D13 | -82.27628607 |
| D14 | -49.42964535 |
| D15 | 157.60846268 |

Harmonic Vibrational Frequencies (cm⁻¹):

62.61 95.37 96.61 137.04 165.34 183.54 223.39 271.71 321.30 344.66 438.00

485.19 515.12 548.16 601.37 641.25 691.64 891.03 963.61 965.40 981.57

1063.41 1092.97 1125.06 1130.25 1136.19 1168.25 1198.38 1224.40 1320.88

1342.85 1355.74 1408.88 1422.13 1434.65 1445.05 1470.08 1484.39 1494.07

1511.90 3087.34 3114.50 3118.45 3158.17 3184.10 3186.59 3701.23 3814.21

Rotational constants (B/GHZ): 2.2190058 0.8036039 0.7076173

Figure S6. Optimized geometries, z-matrices and vibrational frequencies of all stationary points in the reaction of 2*anti*-CH₃CHO with HO-CH(CH₃)OO-H(Pa₂ and Pb₂) at the M06-2X/6-311+G(2df,2p) level of theory



C

| | | | | | | | |
|---|---|----|---|----|---|----|---|
| C | 1 | B1 | | | | | |
| O | 2 | B2 | 1 | A1 | | | |
| O | 3 | B3 | 2 | A2 | 1 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| H | 1 | B5 | 2 | A4 | 3 | D3 | 0 |
| H | 1 | B6 | 2 | A5 | 3 | D4 | 0 |
| H | 1 | B7 | 2 | A6 | 3 | D5 | 0 |

Variables:

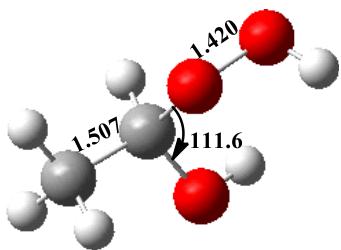
| | |
|----|---------------|
| B1 | 1.47773142 |
| B2 | 1.23946346 |
| B3 | 1.35750070 |
| B4 | 1.08771168 |
| B5 | 1.08635238 |
| B6 | 1.09128861 |
| B7 | 1.09128861 |
| A1 | 119.45495955 |
| A2 | 118.49336247 |
| A3 | 124.16595089 |
| A4 | 110.51284798 |
| A5 | 109.76373093 |
| A6 | 109.76373093 |
| D1 | 180.00000000 |
| D2 | 180.00000000 |
| D3 | 0.00000000 |
| D4 | 121.23944242 |
| D5 | -121.23944242 |

Harmonic Vibrational Frequencies (cm⁻¹):

123.60 267.33 326.90 569.53 885.58 907.63 994.50 1094.19 1168.65 1361.95

1421.37 1464.01 1466.30 1669.61 3041.35 3100.89 3154.85 3185.97

Rotational constants (B/GHZ): 50.3397406 4.4856969 4.2257340



Pa2(*anti*-HO-C(CH₃)HOO-H)

| C | | B1 | | A1 | | D1 | 0 |
|---|---|-----|---|----|---|----|---|
| O | 1 | | | | | | |
| O | 2 | B2 | 1 | A1 | | | |
| H | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| O | 1 | B4 | 2 | A3 | 3 | D2 | 0 |
| H | 3 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 5 | B6 | 1 | A5 | 2 | D4 | 0 |
| C | 1 | B7 | 5 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 1 | A7 | 5 | D6 | 0 |
| H | 8 | B9 | 1 | A8 | 5 | D7 | 0 |
| H | 8 | B10 | 1 | A9 | 5 | D8 | 0 |

Variables:

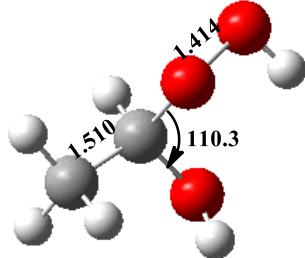
| | |
|-----|---------------|
| B1 | 1.41569532 |
| B2 | 1.42017416 |
| B3 | 1.09482603 |
| B4 | 1.39030971 |
| B5 | 0.96410626 |
| B6 | 0.96025509 |
| B7 | 1.50671757 |
| B8 | 1.08714989 |
| B9 | 1.08735218 |
| B10 | 1.08861151 |
| A1 | 106.67614608 |
| A2 | 107.36440783 |
| A3 | 111.57568824 |
| A4 | 101.25233335 |
| A5 | 108.50688635 |
| A6 | 109.19015556 |
| A7 | 110.32004034 |
| A8 | 109.28533909 |
| A9 | 109.19173123 |
| D1 | -56.73123655 |
| D2 | 64.50648454 |
| D3 | -115.03145039 |
| D4 | -73.83304950 |
| D5 | -116.37221789 |

D6 176.51039554
D7 -63.03391591
D8 56.09516575

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 168.88 | 206.99 | 270.98 | 301.52 | 386.96 | 487.11 | 542.40 | 621.29 | 881.39 | 944.49 |
| 1050.37 | 1085.29 | 1149.31 | 1197.29 | 1287.22 | 1382.43 | 1405.19 | 1423.97 | 1474.84 | |
| 1490.31 | 1497.81 | 3062.41 | 3076.94 | 3159.39 | 3166.55 | 3841.24 | 3901.81 | | |

Rotational constants (B/GHZ): 8.9648260 4.0384667 3.0258813



Pb2(*anti*-HO-C(CH₃)HOO-H)

| C | | B1 | | | | |
|---|---|-----|---|----|---|----|
| O | 1 | | | | | |
| O | 2 | B2 | 1 | A1 | | |
| H | 1 | B3 | 2 | A2 | 3 | D1 |
| O | 1 | B4 | 2 | A3 | 3 | D2 |
| H | 3 | B5 | 2 | A4 | 1 | D3 |
| H | 5 | B6 | 1 | A5 | 2 | D4 |
| C | 1 | B7 | 5 | A6 | 2 | D5 |
| H | 8 | B8 | 1 | A7 | 5 | D6 |
| H | 8 | B9 | 1 | A8 | 5 | D7 |
| H | 8 | B10 | 1 | A9 | 5 | D8 |
| | | | | | | 0 |

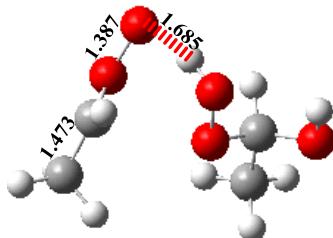
Variables:

| | |
|-----|--------------|
| B1 | 1.40563851 |
| B2 | 1.41436283 |
| B3 | 1.09042144 |
| B4 | 1.40172694 |
| B5 | 0.96713594 |
| B6 | 0.96232772 |
| B7 | 1.51031333 |
| B8 | 1.08742974 |
| B9 | 1.08760410 |
| B10 | 1.09109605 |
| A1 | 107.90919012 |
| A2 | 108.92681699 |
| A3 | 110.31500838 |
| A4 | 102.43358095 |
| A5 | 108.67336606 |
| A6 | 113.23886840 |

| | |
|----|---------------|
| A7 | 110.39831349 |
| A8 | 109.43760934 |
| A9 | 109.91873676 |
| D1 | -49.35090905 |
| D2 | 66.01742464 |
| D3 | -69.81772721 |
| D4 | 73.46672198 |
| D5 | -118.58772121 |
| D6 | -178.27029831 |
| D7 | -57.81897386 |
| D8 | 62.08270738 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|-------------------------------|---------|---------|---------|---------|-----------|-----------|-----------|---------|--------|
| 168.12 | 232.23 | 288.62 | 363.46 | 403.13 | 437.44 | 552.43 | 615.43 | 884.89 | 938.21 |
| 1058.32 | 1081.91 | 1145.96 | 1190.98 | 1305.12 | 1375.74 | 1414.66 | 1446.95 | 1450.02 | |
| 1492.38 | 1500.00 | 3064.20 | 3122.16 | 3147.46 | 3168.68 | 3791.89 | 3868.85 | | |
| Rotational constants (B/GHZ): | | | | | 8.7844581 | 4.0553836 | 3.0361122 | | |



IM3a

| C | | B1 | | | | | |
|---|----|-----|---|-----|---|-----|---|
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| C | 7 | B7 | 5 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 7 | A7 | 5 | D6 | 0 |
| H | 8 | B9 | 7 | A8 | 5 | D7 | 0 |
| H | 8 | B10 | 7 | A9 | 5 | D8 | 0 |
| O | 7 | B11 | 5 | A10 | 2 | D9 | 0 |
| O | 7 | B12 | 5 | A11 | 2 | D10 | 0 |
| H | 7 | B13 | 5 | A12 | 2 | D11 | 0 |
| H | 1 | B14 | 2 | A13 | 5 | D12 | 0 |
| H | 1 | B15 | 2 | A14 | 5 | D13 | 0 |
| H | 1 | B16 | 2 | A15 | 5 | D14 | 0 |
| O | 2 | B17 | 1 | A16 | 5 | D15 | 0 |
| H | 18 | B18 | 2 | A17 | 1 | D16 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.50667016 |
|----|------------|

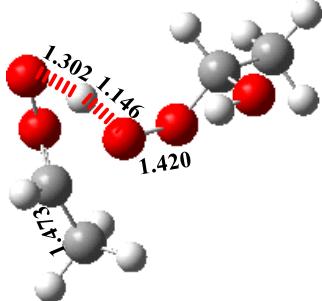
| | |
|-----|---------------|
| B2 | 1.09588134 |
| B3 | 2.28606161 |
| B4 | 1.41705760 |
| B5 | 0.99701842 |
| B6 | 2.59897264 |
| B7 | 1.47301445 |
| B8 | 1.08601017 |
| B9 | 1.09244501 |
| B10 | 1.09033213 |
| B11 | 2.23959042 |
| B12 | 1.23746317 |
| B13 | 1.08743103 |
| B14 | 1.08744946 |
| B15 | 1.08897381 |
| B16 | 1.08887468 |
| B17 | 1.38882283 |
| B18 | 0.96279214 |
| A1 | 112.13754806 |
| A2 | 142.64497767 |
| A3 | 106.41150456 |
| A4 | 95.72684391 |
| A5 | 125.61685596 |
| A6 | 108.65017375 |
| A7 | 111.10967367 |
| A8 | 107.60088200 |
| A9 | 109.81576832 |
| A10 | 75.56088665 |
| A11 | 88.94494959 |
| A12 | 71.51387444 |
| A13 | 109.20222614 |
| A14 | 109.39308447 |
| A15 | 110.34489610 |
| A16 | 109.16737299 |
| A17 | 107.36515794 |
| D1 | 111.71784539 |
| D2 | 5.16348217 |
| D3 | -91.08735906 |
| D4 | -70.09383366 |
| D5 | 88.74610847 |
| D6 | -102.78034882 |
| D7 | 17.89552690 |
| D8 | 134.57356470 |
| D9 | -63.12231281 |
| D10 | -32.08261190 |

D11 -151.68081177
 D12 -178.87559666
 D13 -59.80323837
 D14 61.32949895
 D15 119.67301473
 D16 -174.10957451

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 47.71 | 59.00 | 76.97 | 107.97 | 188.52 | 192.14 | 220.40 | 246.89 | 252.67 | 298.71 | 308.41 |
| 360.37 | 383.00 | 440.77 | 550.52 | 568.35 | 626.28 | 874.46 | 886.13 | 896.09 | 933.03 | |
| 946.12 | 997.64 | 1045.06 | 1083.50 | 1122.51 | 1158.81 | 1184.54 | 1203.62 | 1292.90 | | |
| 1382.97 | 1395.65 | 1408.10 | 1431.47 | 1468.30 | 1475.05 | 1477.58 | 1493.81 | 1496.03 | | |
| 1593.99 | 1694.84 | 3061.88 | 3066.98 | 3067.59 | 3134.37 | 3147.02 | 3158.88 | 3167.83 | | |
| 3174.55 | 3199.28 | 3864.38 | | | | | | | | |

Rotational constants (B/GHZ): 2.2080409 1.0023933 0.8428133



TS3a

| C | | B1 | | | | |
|---|----|-----|---|-----|---|-------|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 0 |
| C | 7 | B7 | 4 | A6 | 2 | D5 0 |
| H | 8 | B8 | 7 | A7 | 4 | D6 0 |
| H | 8 | B9 | 7 | A8 | 4 | D7 0 |
| H | 8 | B10 | 7 | A9 | 4 | D8 0 |
| O | 7 | B11 | 4 | A10 | 2 | D9 0 |
| O | 7 | B12 | 4 | A11 | 2 | D10 0 |
| H | 7 | B13 | 4 | A12 | 2 | D11 0 |
| H | 1 | B14 | 2 | A13 | 5 | D12 0 |
| H | 1 | B15 | 2 | A14 | 5 | D13 0 |
| H | 1 | B16 | 2 | A15 | 5 | D14 0 |
| O | 2 | B17 | 1 | A16 | 5 | D15 0 |
| H | 18 | B18 | 2 | A17 | 1 | D16 0 |

Variables:

B1 1.50591939

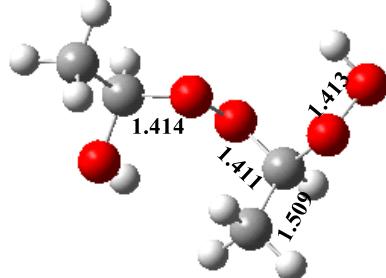
| | |
|-----|--------------|
| B2 | 1.09680033 |
| B3 | 2.27537540 |
| B4 | 1.41267018 |
| B5 | 1.14629694 |
| B6 | 2.09266996 |
| B7 | 1.47314801 |
| B8 | 1.08562748 |
| B9 | 1.09139659 |
| B10 | 1.08954279 |
| B11 | 2.17830566 |
| B12 | 1.26509406 |
| B13 | 1.08442645 |
| B14 | 1.08740960 |
| B15 | 1.08872873 |
| B16 | 1.08728928 |
| B17 | 1.39196119 |
| B18 | 0.96206416 |
| A1 | 112.12615210 |
| A2 | 142.99993630 |
| A3 | 106.45456874 |
| A4 | 98.52823318 |
| A5 | 132.39413035 |
| A6 | 109.42652762 |
| A7 | 110.69685909 |
| A8 | 106.94235463 |
| A9 | 110.14408341 |
| A10 | 67.73088327 |
| A11 | 91.56398322 |
| A12 | 81.72079728 |
| A13 | 109.16316794 |
| A14 | 109.19415616 |
| A15 | 110.32371413 |
| A16 | 109.05867000 |
| A17 | 107.56277655 |
| D1 | 113.41450101 |
| D2 | 3.72670173 |
| D3 | -95.07909793 |
| D4 | -21.63742703 |
| D5 | 68.83295965 |
| D6 | -98.50512974 |
| D7 | 20.53512345 |
| D8 | 138.04082086 |
| D9 | -82.48237143 |
| D10 | -52.02823463 |

| | |
|-----|---------------|
| D11 | -169.94234885 |
| D12 | -179.76790553 |
| D13 | -60.81273213 |
| D14 | 59.88635127 |
| D15 | 120.02083831 |
| D16 | -175.20892712 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 760.59 <i>i</i> | 31.44 | 71.46 | 83.50 | 133.16 | 182.72 | 211.84 | 228.31 | 312.04 | 328.67 | 370.32 |
| 395.31 | 450.26 | 515.55 | 551.06 | 574.16 | 630.10 | 848.54 | 890.14 | 892.66 | 945.48 | |
| 978.12 | 1004.62 | 1068.06 | 1093.53 | 1143.18 | 1167.27 | 1181.59 | 1204.03 | 1289.46 | | |
| 1362.14 | 1394.15 | 1399.75 | 1420.52 | 1455.39 | 1470.77 | 1471.41 | 1490.72 | 1496.52 | | |
| 1577.39 | 1620.43 | 1793.12 | 3050.67 | 3069.61 | 3072.46 | 3143.83 | 3152.24 | 3159.82 | | |
| 3180.57 | 3213.23 | 3879.88 | | | | | | | | |

Rotational constants (B/GHZ): 2.6545881 0.8829012 0.8283969



P3a

| C | | B1 | | | | |
|---|----|-----|---|-----|---|-----|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 |
| O | 2 | B4 | 1 | A3 | 4 | D2 |
| H | 4 | B5 | 2 | A4 | 1 | D3 |
| C | 4 | B6 | 2 | A5 | 1 | D4 |
| C | 7 | B7 | 4 | A6 | 2 | D5 |
| H | 8 | B8 | 7 | A7 | 4 | D6 |
| H | 8 | B9 | 7 | A8 | 4 | D7 |
| H | 8 | B10 | 7 | A9 | 4 | D8 |
| O | 7 | B11 | 4 | A10 | 2 | D9 |
| O | 7 | B12 | 4 | A11 | 2 | D10 |
| H | 7 | B13 | 4 | A12 | 2 | D11 |
| H | 1 | B14 | 2 | A13 | 5 | D12 |
| H | 1 | B15 | 2 | A14 | 5 | D13 |
| H | 1 | B16 | 2 | A15 | 5 | D14 |
| O | 2 | B17 | 1 | A16 | 5 | D15 |
| H | 18 | B18 | 2 | A17 | 1 | D16 |

Variables:

| | |
|----|------------|
| B1 | 1.50666212 |
|----|------------|

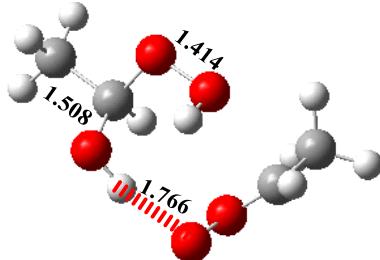
| | |
|-----|---------------|
| B2 | 1.09491115 |
| B3 | 2.26630708 |
| B4 | 1.41372421 |
| B5 | 2.49099596 |
| B6 | 1.41142786 |
| B7 | 1.50946176 |
| B8 | 1.08627522 |
| B9 | 1.08763812 |
| B10 | 1.08753086 |
| B11 | 2.27669741 |
| B12 | 1.39592198 |
| B13 | 1.09294165 |
| B14 | 1.08715034 |
| B15 | 1.08859529 |
| B16 | 1.08717461 |
| B17 | 1.39223791 |
| B18 | 0.96066653 |
| A1 | 112.35980412 |
| A2 | 142.83491688 |
| A3 | 105.73052198 |
| A4 | 122.40293209 |
| A5 | 132.66947382 |
| A6 | 114.52002117 |
| A7 | 110.28259467 |
| A8 | 109.60337723 |
| A9 | 109.20949822 |
| A10 | 92.04386608 |
| A11 | 110.87381857 |
| A12 | 101.75024035 |
| A13 | 109.08803930 |
| A14 | 109.25921967 |
| A15 | 110.45558069 |
| A16 | 109.00843256 |
| A17 | 108.35450949 |
| D1 | 112.61435024 |
| D2 | 4.50037556 |
| D3 | -35.39188089 |
| D4 | 66.19824516 |
| D5 | 22.75594823 |
| D6 | -66.60412420 |
| D7 | 53.23355628 |
| D8 | 173.03325184 |
| D9 | -129.53463826 |
| D10 | -97.90640667 |

D11 145.30971230
 D12 178.82165302
 D13 -62.11988246
 D14 58.37736945
 D15 120.19231452
 D16 171.69769825

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 49.07 | 72.08 | 109.32 | 159.58 | 199.78 | 211.56 | 247.01 | 273.05 | 321.64 | 363.27 | 376.25 |
| 390.49 | 430.45 | 520.05 | 586.09 | 615.27 | 698.51 | 879.77 | 897.41 | 933.68 | 949.05 | |
| 1013.58 | 1062.37 | 1086.76 | 1137.70 | 1150.45 | 1157.58 | 1188.85 | 1220.13 | 1291.81 | | |
| 1365.80 | 1391.02 | 1400.64 | 1408.40 | 1429.49 | 1441.78 | 1476.11 | 1488.89 | 1492.48 | | |
| 1495.08 | 1498.79 | 3066.69 | 3073.40 | 3085.37 | 3111.40 | 3153.93 | 3168.12 | 3168.81 | | |
| 3174.59 | 3822.63 | 3892.80 | | | | | | | | |

Rotational constants (B/GHZ): 2.9762768 0.9426122 0.8230956



IM3b

| C | | B1 | | | | |
|---|----|-----|---|-----|---|-------|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 0 |
| O | 1 | B5 | 2 | A4 | 3 | D3 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 0 |
| C | 8 | B8 | 1 | A7 | 6 | D6 0 |
| C | 9 | B9 | 8 | A8 | 1 | D7 0 |
| H | 10 | B10 | 9 | A9 | 8 | D8 0 |
| H | 10 | B11 | 9 | A10 | 8 | D9 0 |
| H | 10 | B12 | 9 | A11 | 8 | D10 0 |
| O | 9 | B13 | 8 | A12 | 1 | D11 0 |
| O | 9 | B14 | 8 | A13 | 1 | D12 0 |
| H | 9 | B15 | 8 | A14 | 1 | D13 0 |
| H | 1 | B16 | 6 | A15 | 2 | D14 0 |
| O | 8 | B17 | 1 | A16 | 6 | D15 0 |
| H | 8 | B18 | 1 | A17 | 6 | D16 0 |

Variables:

| | |
|----|------------|
| B1 | 1.50825435 |
| B2 | 1.08742419 |

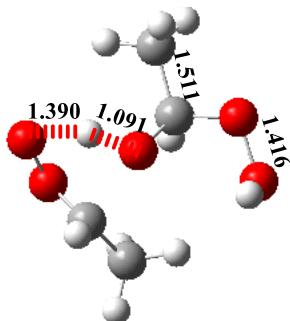
| | |
|-----|---------------|
| B3 | 1.08849329 |
| B4 | 1.08801695 |
| B5 | 1.37963044 |
| B6 | 0.98140154 |
| B7 | 2.29812352 |
| B8 | 2.61762296 |
| B9 | 1.47212864 |
| B10 | 1.09291525 |
| B11 | 1.09006863 |
| B12 | 1.08583169 |
| B13 | 2.22848650 |
| B14 | 1.23644418 |
| B15 | 1.08641135 |
| B16 | 1.09605670 |
| B17 | 1.41388068 |
| B18 | 0.96988235 |
| A1 | 109.04063971 |
| A2 | 109.00976048 |
| A3 | 110.83837920 |
| A4 | 110.69646544 |
| A5 | 109.56835659 |
| A6 | 90.06949017 |
| A7 | 98.04100798 |
| A8 | 105.48106580 |
| A9 | 107.23490174 |
| A10 | 110.05995475 |
| A11 | 111.12688858 |
| A12 | 78.37575326 |
| A13 | 92.09357087 |
| A14 | 71.68440492 |
| A15 | 110.77549308 |
| A16 | 36.32329653 |
| A17 | 87.12518764 |
| D1 | 118.80009668 |
| D2 | -120.64392270 |
| D3 | -64.02594521 |
| D4 | 152.51063018 |
| D5 | 145.58714926 |
| D6 | 86.49384873 |
| D7 | 93.51104707 |
| D8 | 14.97659590 |
| D9 | 131.71522148 |
| D10 | -105.36166400 |
| D11 | -59.57857943 |

D12 -28.25144516
 D13 -146.03504076
 D14 -125.02492738
 D15 -127.16654047
 D16 -12.27407397

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 48.80 | 58.14 | 107.77 | 120.57 | 132.66 | 187.07 | 190.50 | 232.68 | 247.56 | 298.83 | 328.29 |
| 339.80 | 395.23 | 468.03 | 548.30 | 568.34 | 625.06 | 835.37 | 875.57 | 877.41 | 905.48 | |
| 946.51 | 992.40 | 1058.26 | 1117.03 | 1122.63 | 1146.30 | 1179.94 | 1203.32 | 1366.89 | | |
| 1373.09 | 1393.82 | 1410.21 | 1420.47 | 1442.30 | 1462.87 | 1473.30 | 1489.60 | 1499.05 | | |
| 1527.16 | 1703.80 | 3052.21 | 3055.92 | 3075.25 | 3122.17 | 3157.34 | 3163.19 | 3172.25 | | |
| 3207.48 | 3417.56 | 3748.50 | | | | | | | | |

Rotational constants (B/GHZ): 2.2886834 0.9674864 0.8347377



TS3b

| C | | B1 | | | | |
|---|----|-----|---|-----|---|-------|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 0 |
| O | 1 | B5 | 2 | A4 | 5 | D3 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 0 |
| C | 6 | B8 | 1 | A7 | 2 | D6 0 |
| C | 9 | B9 | 6 | A8 | 1 | D7 0 |
| H | 10 | B10 | 9 | A9 | 6 | D8 0 |
| H | 10 | B11 | 9 | A10 | 6 | D9 0 |
| H | 10 | B12 | 9 | A11 | 6 | D10 0 |
| O | 9 | B13 | 6 | A12 | 1 | D11 0 |
| O | 9 | B14 | 6 | A13 | 1 | D12 0 |
| H | 9 | B15 | 6 | A14 | 1 | D13 0 |
| H | 1 | B16 | 6 | A15 | 9 | D14 0 |
| O | 1 | B17 | 6 | A16 | 9 | D15 0 |
| H | 8 | B18 | 1 | A17 | 6 | D16 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51062631 |
| B2 | 1.08894606 |

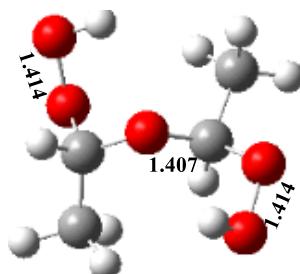
| | |
|-----|---------------|
| B3 | 1.08900550 |
| B4 | 1.08757170 |
| B5 | 1.39929354 |
| B6 | 1.09113654 |
| B7 | 2.28023194 |
| B8 | 2.03408399 |
| B9 | 1.47661477 |
| B10 | 1.09235790 |
| B11 | 1.08957650 |
| B12 | 1.08662645 |
| B13 | 2.18171319 |
| B14 | 1.26979616 |
| B15 | 1.08415993 |
| B16 | 1.09872965 |
| B17 | 1.40485157 |
| B18 | 0.96555941 |
| A1 | 109.01941750 |
| A2 | 109.38592021 |
| A3 | 110.27797062 |
| A4 | 112.40756686 |
| A5 | 110.46802222 |
| A6 | 89.71843740 |
| A7 | 113.07122217 |
| A8 | 110.52064325 |
| A9 | 108.01940160 |
| A10 | 109.72632567 |
| A11 | 110.76039368 |
| A12 | 69.24310544 |
| A13 | 93.06772810 |
| A14 | 82.65874760 |
| A15 | 109.66074057 |
| A16 | 108.73198273 |
| A17 | 99.79921535 |
| D1 | 119.39230675 |
| D2 | -120.28745656 |
| D3 | 178.77025123 |
| D4 | 36.93816828 |
| D5 | 148.69453395 |
| D6 | 118.44094878 |
| D7 | 50.01032463 |
| D8 | 19.26879146 |
| D9 | 137.11342074 |
| D10 | -100.69445777 |
| D11 | -102.08684848 |

| | |
|-----|---------------|
| D12 | -71.55593788 |
| D13 | 171.06876081 |
| D14 | -6.04388695 |
| D15 | -124.25596382 |
| D16 | -27.43712274 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 474.45 <i>i</i> | 62.09 | 97.56 | 123.53 | 165.09 | 185.11 | 208.12 | 248.10 | 295.94 | 314.49 | 362.82 |
| 393.60 | 431.70 | 507.10 | 542.37 | 560.69 | 632.44 | 865.08 | 894.08 | 942.11 | 986.23 | |
| 996.69 | 1050.51 | 1094.51 | 1138.22 | 1177.78 | 1182.24 | 1194.41 | 1249.18 | 1348.53 | | |
| 1358.39 | 1403.00 | 1415.93 | 1423.96 | 1433.14 | 1464.67 | 1476.49 | 1481.10 | 1493.14 | | |
| 1513.21 | 1609.62 | 1970.27 | 3037.07 | 3059.73 | 3063.19 | 3131.25 | 3145.94 | 3155.89 | | |
| 3167.76 | 3204.51 | 3816.84 | | | | | | | | |

Rotational constants (B/GHZ): 2.1197962 1.2237817 0.8718358



P3b

| C | | B1 | | | | |
|---|----|-----|---|-----|----|-----|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 |
| H | 2 | B4 | 1 | A3 | 3 | D2 |
| O | 1 | B5 | 2 | A4 | 5 | D3 |
| H | 6 | B6 | 1 | A5 | 2 | D4 |
| O | 1 | B7 | 6 | A6 | 2 | D5 |
| C | 6 | B8 | 1 | A7 | 2 | D6 |
| C | 9 | B9 | 6 | A8 | 1 | D7 |
| H | 10 | B10 | 9 | A9 | 6 | D8 |
| H | 10 | B11 | 9 | A10 | 6 | D9 |
| H | 10 | B12 | 9 | A11 | 6 | D10 |
| O | 9 | B13 | 6 | A12 | 1 | D11 |
| O | 9 | B14 | 6 | A13 | 1 | D12 |
| H | 9 | B15 | 6 | A14 | 1 | D13 |
| H | 1 | B16 | 6 | A15 | 9 | D14 |
| O | 1 | B17 | 6 | A16 | 9 | D15 |
| H | 8 | B18 | 1 | A17 | 18 | D16 |
| | | | | | | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51068400 |
| B2 | 1.08948177 |
| B3 | 1.08964319 |

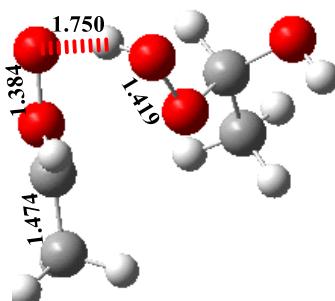
| | |
|-----|---------------|
| B4 | 1.08797851 |
| B5 | 1.41354738 |
| B6 | 2.37964189 |
| B7 | 2.27279279 |
| B8 | 1.40730535 |
| B9 | 1.51599776 |
| B10 | 1.08810642 |
| B11 | 1.08719265 |
| B12 | 1.08776051 |
| B13 | 2.28350987 |
| B14 | 1.40455768 |
| B15 | 1.09017820 |
| B16 | 1.09117736 |
| B17 | 1.39742619 |
| B18 | 0.96582125 |
| A1 | 109.25678648 |
| A2 | 109.40120634 |
| A3 | 110.35780723 |
| A4 | 111.50523270 |
| A5 | 102.66767236 |
| A6 | 90.90151083 |
| A7 | 117.72303081 |
| A8 | 115.65532016 |
| A9 | 109.64118902 |
| A10 | 108.94687840 |
| A11 | 111.64286441 |
| A12 | 93.46293253 |
| A13 | 110.14539866 |
| A14 | 104.02643067 |
| A15 | 110.19153149 |
| A16 | 107.38733033 |
| A17 | 96.83812200 |
| D1 | 120.45693880 |
| D2 | -119.55490049 |
| D3 | 174.17223229 |
| D4 | 20.89587741 |
| D5 | 148.84115021 |
| D6 | 101.40900703 |
| D7 | 53.91118029 |
| D8 | 41.20979940 |
| D9 | 161.02335061 |
| D10 | -79.76057145 |
| D11 | -99.20642815 |
| D12 | -66.41172449 |

D13 176.82418888
 D14 -23.86872240
 D15 -142.63706892
 D16 100.55168646

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 41.22 | 77.44 | 148.20 | 170.40 | 195.42 | 221.03 | 259.35 | 281.52 | 297.98 | 339.47 | 352.64 |
| 375.25 | 438.01 | 517.45 | 554.97 | 586.72 | 695.19 | 855.83 | 896.05 | 925.73 | 970.53 | |
| 1055.61 | 1058.87 | 1107.49 | 1133.25 | 1149.10 | 1186.69 | 1194.34 | 1226.73 | 1357.54 | | |
| 1368.53 | 1406.03 | 1413.35 | 1429.66 | 1437.03 | 1440.74 | 1455.38 | 1487.56 | 1500.81 | | |
| 1501.82 | 1512.39 | 3065.42 | 3070.69 | 3119.97 | 3130.97 | 3146.88 | 3154.98 | 3158.09 | | |
| 3165.83 | 3777.32 | 3812.77 | | | | | | | | |

Rotational constants (B/GHZ): 2.4247505 1.1625174 0.8900905



IM3c

| | | | | | | | |
|---|----|-----|---|-----|---|-----|---|
| C | | | | | | | |
| C | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| C | 7 | B7 | 5 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 7 | A7 | 5 | D6 | 0 |
| H | 8 | B9 | 7 | A8 | 5 | D7 | 0 |
| H | 8 | B10 | 7 | A9 | 5 | D8 | 0 |
| O | 7 | B11 | 5 | A10 | 2 | D9 | 0 |
| O | 7 | B12 | 5 | A11 | 2 | D10 | 0 |
| H | 7 | B13 | 5 | A12 | 2 | D11 | 0 |
| H | 1 | B14 | 2 | A13 | 5 | D12 | 0 |
| H | 1 | B15 | 2 | A14 | 5 | D13 | 0 |
| H | 1 | B16 | 2 | A15 | 5 | D14 | 0 |
| O | 2 | B17 | 1 | A16 | 5 | D15 | 0 |
| H | 18 | B18 | 2 | A17 | 1 | D16 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51557311 |
| B2 | 1.09090764 |
| B3 | 2.31387011 |

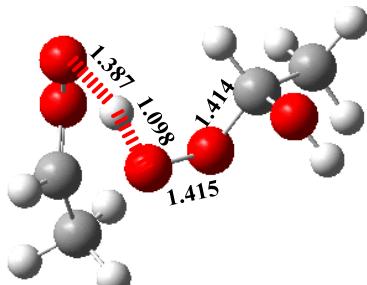
| | |
|-----|---------------|
| B4 | 1.41340867 |
| B5 | 0.98968588 |
| B6 | 2.60636525 |
| B7 | 1.47374587 |
| B8 | 1.08615479 |
| B9 | 1.09252696 |
| B10 | 1.09015192 |
| B11 | 2.23980231 |
| B12 | 1.23764064 |
| B13 | 1.08733254 |
| B14 | 1.08731829 |
| B15 | 1.09160500 |
| B16 | 1.08941931 |
| B17 | 1.38994353 |
| B18 | 0.96183438 |
| A1 | 111.96190063 |
| A2 | 138.90040289 |
| A3 | 104.91744742 |
| A4 | 92.69338531 |
| A5 | 121.93956092 |
| A6 | 109.44285781 |
| A7 | 111.06296548 |
| A8 | 107.65100903 |
| A9 | 109.98393190 |
| A10 | 74.67227951 |
| A11 | 88.29793044 |
| A12 | 71.25950956 |
| A13 | 109.22096192 |
| A14 | 110.01436840 |
| A15 | 110.62038368 |
| A16 | 113.16459695 |
| A17 | 108.59782348 |
| D1 | 106.22672556 |
| D2 | 11.69280182 |
| D3 | -83.81560938 |
| D4 | -61.93995909 |
| D5 | 90.52522798 |
| D6 | -103.62338377 |
| D7 | 16.90104495 |
| D8 | 133.70127963 |
| D9 | -60.86894526 |
| D10 | -30.02052062 |
| D11 | -149.99250764 |
| D12 | -176.52125053 |

D13 -57.18926337
 D14 63.51990960
 D15 122.03227877
 D16 -63.69917379

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 46.89 | 58.09 | 63.24 | 106.00 | 166.90 | 189.04 | 222.61 | 227.77 | 236.13 | 287.39 | 299.82 |
| 324.06 | 361.28 | 393.61 | 550.62 | 568.92 | 594.12 | 842.02 | 875.55 | 887.66 | 912.13 | |
| 941.21 | 997.12 | 1057.44 | 1083.89 | 1115.13 | 1130.17 | 1182.18 | 1193.48 | 1316.56 | | |
| 1375.59 | 1385.72 | 1408.93 | 1434.10 | 1435.32 | 1466.98 | 1472.85 | 1487.90 | 1498.18 | | |
| 1573.86 | 1692.68 | 3046.56 | 3060.89 | 3118.41 | 3128.51 | 3136.50 | 3149.22 | 3171.22 | | |
| 3204.53 | 3310.30 | 3872.96 | | | | | | | | |

Rotational constants (B/GHZ): 2.1902236 1.0176992 0.8757031



TS3c

| C | | B1 | | | | |
|---|----|-----|---|-----|---|-------|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 0 |
| C | 7 | B7 | 4 | A6 | 2 | D5 0 |
| H | 8 | B8 | 7 | A7 | 4 | D6 0 |
| H | 8 | B9 | 7 | A8 | 4 | D7 0 |
| H | 8 | B10 | 7 | A9 | 4 | D8 0 |
| O | 7 | B11 | 4 | A10 | 2 | D9 0 |
| O | 7 | B12 | 4 | A11 | 2 | D10 0 |
| H | 7 | B13 | 4 | A12 | 2 | D11 0 |
| H | 1 | B14 | 2 | A13 | 5 | D12 0 |
| H | 1 | B15 | 2 | A14 | 5 | D13 0 |
| H | 1 | B16 | 2 | A15 | 5 | D14 0 |
| O | 2 | B17 | 1 | A16 | 5 | D15 0 |
| H | 18 | B18 | 2 | A17 | 1 | D16 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51347450 |
| B2 | 1.09200831 |
| B3 | 2.30796299 |

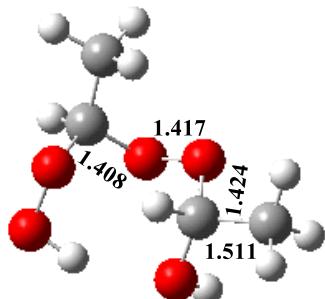
| | |
|-----|---------------|
| B4 | 1.41401246 |
| B5 | 1.09820114 |
| B6 | 2.06523848 |
| B7 | 1.47530888 |
| B8 | 1.08551818 |
| B9 | 1.08953515 |
| B10 | 1.09072505 |
| B11 | 2.17903111 |
| B12 | 1.26492397 |
| B13 | 1.08522293 |
| B14 | 1.08734268 |
| B15 | 1.09118181 |
| B16 | 1.08761227 |
| B17 | 1.39016122 |
| B18 | 0.96193845 |
| A1 | 111.85102583 |
| A2 | 139.56881374 |
| A3 | 104.89303342 |
| A4 | 85.19227706 |
| A5 | 124.01680680 |
| A6 | 108.94402735 |
| A7 | 110.66712727 |
| A8 | 107.80724483 |
| A9 | 109.55842511 |
| A10 | 69.09863294 |
| A11 | 92.40710665 |
| A12 | 82.87124982 |
| A13 | 108.99644049 |
| A14 | 109.88902269 |
| A15 | 110.65551456 |
| A16 | 113.35950288 |
| A17 | 108.71714304 |
| D1 | 109.52610156 |
| D2 | 8.45140619 |
| D3 | -106.39983305 |
| D4 | -40.49880834 |
| D5 | 84.82122756 |
| D6 | -88.75849014 |
| D7 | 31.51701080 |
| D8 | 148.95966522 |
| D9 | -67.22279330 |
| D10 | -36.38631620 |
| D11 | -154.04165291 |
| D12 | -178.59743440 |

D13 -59.28127759
D14 60.97819578
D15 122.33459091
D16 -57.91138606

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|--------|---------|---------|---------|---------|---------|---------|--------|
| 478.26 <i>i</i> | 35.65 | 73.12 | 80.16 | 123.78 | 176.55 | 219.32 | 246.76 | 309.23 | 321.92 | 343.85 |
| 378.31 | 437.87 | 520.74 | 563.75 | 578.05 | 603.56 | 885.27 | 893.39 | 941.11 | 974.45 | |
| 999.95 | 1040.67 | 1089.99 | | 1114.60 | 1131.25 | 1182.55 | 1194.46 | 1277.56 | 1318.88 | |
| 1365.43 | 1389.78 | 1415.91 | | 1421.19 | 1447.23 | 1453.36 | 1474.75 | 1489.68 | 1502.94 | |
| 1611.34 | 1628.35 | 1887.50 | | 3065.65 | 3067.16 | 3122.48 | 3141.54 | 3148.00 | 3163.51 | |
| 3183.30 | 3207.58 | 3875.75 | | | | | | | | |

Rotational constants (B/GHZ): 2.6131001 0.9239361 0.8711024



P3c

| C | | B1 | | | | |
|---|----|-----|---|-----|---|-------|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 0 |
| O | 4 | B4 | 2 | A3 | 1 | D2 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 0 |
| C | 7 | B7 | 4 | A6 | 2 | D5 0 |
| H | 8 | B8 | 7 | A7 | 4 | D6 0 |
| H | 8 | B9 | 7 | A8 | 4 | D7 0 |
| H | 8 | B10 | 7 | A9 | 4 | D8 0 |
| O | 7 | B11 | 4 | A10 | 2 | D9 0 |
| O | 7 | B12 | 4 | A11 | 2 | D10 0 |
| H | 7 | B13 | 4 | A12 | 2 | D11 0 |
| H | 1 | B14 | 2 | A13 | 5 | D12 0 |
| H | 1 | B15 | 2 | A14 | 5 | D13 0 |
| H | 1 | B16 | 2 | A15 | 5 | D14 0 |
| O | 2 | B17 | 1 | A16 | 5 | D15 0 |
| H | 18 | B18 | 2 | A17 | 1 | D16 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51072575 |
| B2 | 1.08912457 |
| B3 | 2.34851031 |

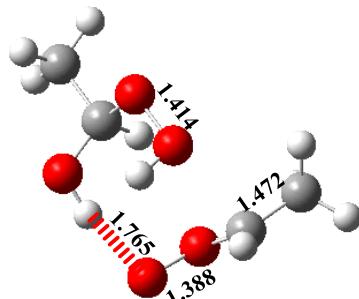
| | |
|-----|---------------|
| B4 | 1.41662705 |
| B5 | 2.47427596 |
| B6 | 1.40844697 |
| B7 | 1.50877995 |
| B8 | 1.08741022 |
| B9 | 1.08743051 |
| B10 | 1.08713084 |
| B11 | 2.28344763 |
| B12 | 1.40021873 |
| B13 | 1.09293893 |
| B14 | 1.08761040 |
| B15 | 1.09021355 |
| B16 | 1.08828438 |
| B17 | 1.39633155 |
| B18 | 0.96351575 |
| A1 | 112.06604004 |
| A2 | 136.97320321 |
| A3 | 34.35559065 |
| A4 | 67.54573384 |
| A5 | 104.34354920 |
| A6 | 114.34998474 |
| A7 | 110.40288894 |
| A8 | 109.28093071 |
| A9 | 109.43187243 |
| A10 | 91.77378084 |
| A11 | 111.29316642 |
| A12 | 101.58133542 |
| A13 | 109.18061569 |
| A14 | 109.87176982 |
| A15 | 110.44422465 |
| A16 | 113.51786416 |
| A17 | 109.01895802 |
| D1 | 131.45671080 |
| D2 | -21.11341616 |
| D3 | 162.04968288 |
| D4 | -129.31785414 |
| D5 | 81.85744072 |
| D6 | -69.76624023 |
| D7 | 50.06738650 |
| D8 | 170.16532842 |
| D9 | -70.31944503 |
| D10 | -39.24070240 |
| D11 | -155.76145142 |
| D12 | 178.47100275 |

D13 -61.52582127
 D14 58.33366633
 D15 121.66821320
 D16 -62.48549906

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 59.06 | 100.54 | 144.23 | 172.05 | 219.95 | 239.94 | 261.82 | 280.99 | 318.08 | 338.27 |
| 408.94 | 425.65 | 520.26 | 538.81 | 578.60 | 621.30 | 724.66 | 853.62 | 885.79 | 920.87 |
| 935.39 | 1016.58 | 1060.61 | 1085.22 | 1126.05 | 1138.01 | 1150.73 | 1193.99 | 1210.27 | |
| 1305.75 | 1358.68 | 1375.10 | 1396.83 | 1420.48 | 1424.34 | 1461.46 | 1483.00 | 1489.09 | |
| 1495.83 | 1501.89 | 1517.25 | 3067.49 | 3069.59 | 3104.35 | 3130.63 | 3152.01 | 3153.17 | |
| 3158.98 | 3168.66 | 3704.64 | 3852.07 | | | | | | |

Rotational constants (B/GHZ): 2.3376001 1.2905174 1.0017937



IM3d

| | | | | | | |
|---|----|-----|---|-----|---|-------|
| C | | | | | | |
| C | 1 | B1 | | | | |
| H | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 0 |
| O | 1 | B5 | 2 | A4 | 5 | D3 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 0 |
| C | 8 | B8 | 1 | A7 | 6 | D6 0 |
| C | 9 | B9 | 8 | A8 | 1 | D7 0 |
| H | 10 | B10 | 9 | A9 | 8 | D8 0 |
| H | 10 | B11 | 9 | A10 | 8 | D9 0 |
| H | 10 | B12 | 9 | A11 | 8 | D10 0 |
| O | 9 | B13 | 8 | A12 | 1 | D11 0 |
| O | 9 | B14 | 8 | A13 | 1 | D12 0 |
| H | 9 | B15 | 8 | A14 | 1 | D13 0 |
| H | 1 | B16 | 6 | A15 | 2 | D14 0 |
| O | 8 | B17 | 1 | A16 | 6 | D15 0 |
| H | 8 | B18 | 1 | A17 | 6 | D16 0 |

Variables:

| | |
|----|------------|
| B1 | 1.50826493 |
| B2 | 1.08849529 |
| B3 | 1.08801670 |

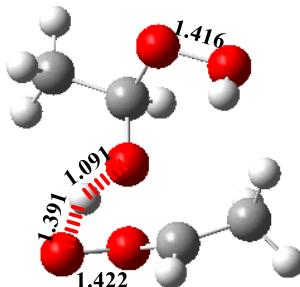
| | |
|-----|---------------|
| B4 | 1.08742205 |
| B5 | 1.37962600 |
| B6 | 0.98142278 |
| B7 | 2.29806678 |
| B8 | 2.61776907 |
| B9 | 1.47212942 |
| B10 | 1.09290962 |
| B11 | 1.09006994 |
| B12 | 1.08583184 |
| B13 | 2.22846638 |
| B14 | 1.23643882 |
| B15 | 1.08641314 |
| B16 | 1.09605777 |
| B17 | 1.41388495 |
| B18 | 0.96988115 |
| A1 | 109.01036072 |
| A2 | 110.84148501 |
| A3 | 109.03763998 |
| A4 | 110.69434922 |
| A5 | 109.57607280 |
| A6 | 90.05983673 |
| A7 | 98.01723396 |
| A8 | 105.47799746 |
| A9 | 107.23694494 |
| A10 | 110.05720912 |
| A11 | 111.12794525 |
| A12 | 78.37768584 |
| A13 | 92.09396020 |
| A14 | 71.68952638 |
| A15 | 110.77581185 |
| A16 | 36.32281308 |
| A17 | 87.13287244 |
| D1 | 120.55712250 |
| D2 | -118.79854602 |
| D3 | -64.00008235 |
| D4 | 152.51486167 |
| D5 | 145.58311616 |
| D6 | 86.50072674 |
| D7 | 93.48177167 |
| D8 | 14.99025232 |
| D9 | 131.72828005 |
| D10 | -105.35056108 |
| D11 | -59.60987445 |
| D12 | -28.28139720 |

D13 -146.06327171
 D14 -125.01900609
 D15 -127.18120992
 D16 -12.30393477

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 48.70 | 58.15 | 107.79 | 120.47 | 132.63 | 187.12 | 190.52 | 232.69 | 247.40 | 298.78 | 328.26 |
| 339.79 | 395.24 | 467.75 | 548.30 | 568.33 | 625.09 | 835.47 | 875.63 | 877.40 | 905.42 | |
| 946.53 | 992.40 | 1058.25 | 1116.94 | 1122.66 | 1146.33 | 1179.94 | 1203.35 | 1366.90 | | |
| 1373.10 | 1393.85 | 1410.20 | 1420.48 | 1442.26 | 1462.87 | 1473.29 | 1489.60 | 1499.05 | | |
| 1527.18 | 1703.83 | 3052.27 | 3055.85 | 3075.24 | 3122.20 | 3157.33 | 3163.17 | 3172.24 | | |
| 3207.37 | 3417.10 | 3748.46 | | | | | | | | |

Rotational constants (B/GHZ): 2.2882567 0.9676758 0.8349229



TS3d

| C | | B1 | | | | | |
|---|----|-----|---|-----|---|-----|---|
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| O | 1 | B5 | 2 | A4 | 4 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 | 0 |
| C | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| C | 9 | B9 | 6 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 9 | A9 | 6 | D8 | 0 |
| H | 10 | B11 | 9 | A10 | 6 | D9 | 0 |
| H | 10 | B12 | 9 | A11 | 6 | D10 | 0 |
| O | 9 | B13 | 6 | A12 | 1 | D11 | 0 |
| O | 9 | B14 | 6 | A13 | 1 | D12 | 0 |
| H | 9 | B15 | 6 | A14 | 1 | D13 | 0 |
| H | 1 | B16 | 6 | A15 | 9 | D14 | 0 |
| O | 1 | B17 | 6 | A16 | 9 | D15 | 0 |
| H | 8 | B18 | 1 | A17 | 6 | D16 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51062721 |
| B2 | 1.08899963 |
| B3 | 1.08754863 |

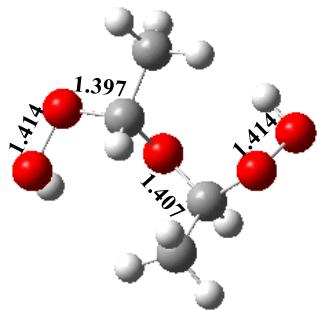
| | |
|-----|---------------|
| B4 | 1.08890640 |
| B5 | 1.39944841 |
| B6 | 1.09076945 |
| B7 | 2.28016169 |
| B8 | 2.03285956 |
| B9 | 1.47667443 |
| B10 | 1.09231438 |
| B11 | 1.08958067 |
| B12 | 1.08662402 |
| B13 | 2.18183027 |
| B14 | 1.26986233 |
| B15 | 1.08417695 |
| B16 | 1.09869541 |
| B17 | 1.40479016 |
| B18 | 0.96552862 |
| A1 | 109.39921212 |
| A2 | 110.26379595 |
| A3 | 109.01878635 |
| A4 | 112.46332959 |
| A5 | 110.52821037 |
| A6 | 89.74982896 |
| A7 | 113.12856475 |
| A8 | 110.51338887 |
| A9 | 108.02666454 |
| A10 | 109.72007093 |
| A11 | 110.75824359 |
| A12 | 69.27338968 |
| A13 | 93.10712764 |
| A14 | 82.67386623 |
| A15 | 109.64796687 |
| A16 | 108.70777143 |
| A17 | 99.96845148 |
| D1 | 120.32575407 |
| D2 | -119.39763046 |
| D3 | 179.37812485 |
| D4 | 36.79687479 |
| D5 | 148.73522994 |
| D6 | 118.34880438 |
| D7 | 50.11453130 |
| D8 | 19.40476679 |
| D9 | 137.27097159 |
| D10 | -100.55672073 |
| D11 | -101.98145046 |
| D12 | -71.46640659 |

D13 171.15901035
 D14 -6.15783029
 D15 -124.34519710
 D16 -27.57342043

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 473.45 <i>i</i> | 62.49 | 98.03 | 123.37 | 165.61 | 185.49 | 208.87 | 248.37 | 296.01 | 314.43 | 362.94 |
| 394.65 | 431.58 | 507.10 | 542.48 | 560.59 | 632.45 | 865.10 | 894.24 | 941.62 | 986.56 | |
| 996.59 | 1050.51 | 1094.91 | 1137.71 | 1177.82 | 1182.67 | 1194.81 | 1248.99 | 1348.35 | | |
| 1358.43 | 1403.00 | 1415.77 | 1424.17 | 1433.04 | 1464.64 | 1476.06 | 1481.07 | 1493.79 | | |
| 1513.03 | 1609.43 | 1973.17 | 3037.43 | 3059.86 | 3062.85 | 3131.43 | 3146.14 | 3154.55 | | |
| 3167.57 | 3204.15 | 3816.88 | | | | | | | | |

Rotational constants (B/GHZ): 2.1199984 1.2235984 0.8716425



P3d

| | | | | | | |
|---|----|-----|---|-----|----|----------|
| C | | | | | | |
| C | 1 | B1 | | | | |
| H | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 0 |
| O | 1 | B5 | 2 | A4 | 4 | D3 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 0 |
| C | 6 | B8 | 1 | A7 | 2 | D6 0 |
| C | 9 | B9 | 6 | A8 | 1 | D7 0 |
| H | 10 | B10 | 9 | A9 | 6 | D8 0 |
| H | 10 | B11 | 9 | A10 | 6 | D9 0 |
| H | 10 | B12 | 9 | A11 | 6 | D10 0 |
| O | 9 | B13 | 6 | A12 | 1 | D11 0 |
| O | 9 | B14 | 6 | A13 | 1 | D12 0 |
| H | 9 | B15 | 6 | A14 | 1 | D13 0 |
| H | 1 | B16 | 6 | A15 | 9 | D14 0 |
| O | 1 | B17 | 6 | A16 | 9 | D15 0 |
| H | 8 | B18 | 1 | A17 | 18 | D16 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51068459 |
| B2 | 1.08964289 |
| B3 | 1.08797811 |

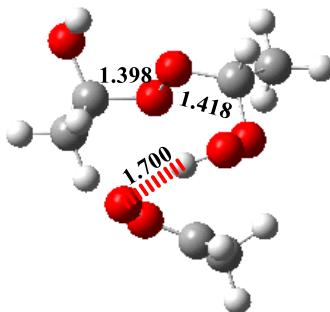
| | |
|-----|---------------|
| B4 | 1.08948149 |
| B5 | 1.41354785 |
| B6 | 2.37962991 |
| B7 | 2.27279198 |
| B8 | 1.40730527 |
| B9 | 1.51599687 |
| B10 | 1.08810672 |
| B11 | 1.08719344 |
| B12 | 1.08776085 |
| B13 | 2.28351177 |
| B14 | 1.40455757 |
| B15 | 1.09017848 |
| B16 | 1.09117794 |
| B17 | 1.39742566 |
| B18 | 0.96582080 |
| A1 | 109.40116474 |
| A2 | 110.35773269 |
| A3 | 109.25677114 |
| A4 | 111.50530483 |
| A5 | 102.66783615 |
| A6 | 90.90180133 |
| A7 | 117.72290565 |
| A8 | 115.65533261 |
| A9 | 109.64116860 |
| A10 | 108.94691120 |
| A11 | 111.64286050 |
| A12 | 93.46277603 |
| A13 | 110.14548391 |
| A14 | 104.02638792 |
| A15 | 110.19142788 |
| A16 | 107.38727151 |
| A17 | 96.83861467 |
| D1 | 119.98813338 |
| D2 | -120.45693187 |
| D3 | 174.17320839 |
| D4 | 20.89402614 |
| D5 | 148.84146645 |
| D6 | 101.40736069 |
| D7 | 53.91099463 |
| D8 | 41.20929583 |
| D9 | 161.02283642 |
| D10 | -79.76114649 |
| D11 | -99.20655459 |
| D12 | -66.41199542 |

D13 176.82391288
 D14 -23.87044330
 D15 -142.63861301
 D16 100.55099936

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 41.22 | 77.45 | 148.20 | 170.39 | 195.42 | 221.03 | 259.36 | 281.53 | 297.99 | 339.48 | 352.64 |
| 375.25 | 438.01 | 517.45 | 554.97 | 586.72 | 695.19 | 855.83 | 896.05 | 925.73 | 970.53 | |
| 1055.61 | 1058.87 | 1107.49 | 1133.25 | 1149.10 | 1186.69 | 1194.34 | 1226.73 | 1357.55 | | |
| 1368.53 | 1406.03 | 1413.35 | 1429.66 | 1437.03 | 1440.74 | 1455.39 | 1487.56 | 1500.81 | | |
| 1501.82 | 1512.39 | 3065.42 | 3070.69 | 3119.97 | 3130.97 | 3146.88 | 3154.98 | 3158.09 | | |
| 3165.84 | 3777.32 | 3812.77 | | | | | | | | |

Rotational constants (B/GHZ): 2.4247574 1.1625116 0.8900912



IM4a

| C | | | | | | |
|---|----|-----|----|-----|----|----------|
| H | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 0 |
| C | 4 | B5 | 1 | A4 | 3 | D3 0 |
| O | 6 | B6 | 4 | A5 | 1 | D4 0 |
| O | 6 | B7 | 4 | A6 | 1 | D5 0 |
| C | 1 | B8 | 4 | A7 | 3 | D6 0 |
| H | 9 | B9 | 1 | A8 | 4 | D7 0 |
| H | 9 | B10 | 1 | A9 | 4 | D8 0 |
| H | 9 | B11 | 1 | A10 | 4 | D9 0 |
| O | 1 | B12 | 4 | A11 | 3 | D10 0 |
| C | 6 | B13 | 4 | A12 | 1 | D11 0 |
| H | 14 | B14 | 6 | A13 | 4 | D12 0 |
| H | 14 | B15 | 6 | A14 | 4 | D13 0 |
| H | 14 | B16 | 6 | A15 | 4 | D14 0 |
| H | 6 | B17 | 4 | A16 | 1 | D15 0 |
| O | 13 | B18 | 1 | A17 | 4 | D16 0 |
| C | 19 | B19 | 13 | A18 | 1 | D17 0 |
| H | 20 | B20 | 19 | A19 | 13 | D18 0 |
| C | 20 | B21 | 19 | A20 | 13 | D19 0 |
| H | 22 | B22 | 20 | A21 | 19 | D20 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 22 | B23 | 20 | A22 | 19 | D21 | 0 |
| H | 22 | B24 | 20 | A23 | 19 | D22 | 0 |
| O | 20 | B25 | 19 | A24 | 13 | D23 | 0 |
| H | 26 | B26 | 20 | A25 | 19 | D24 | 0 |

Variables:

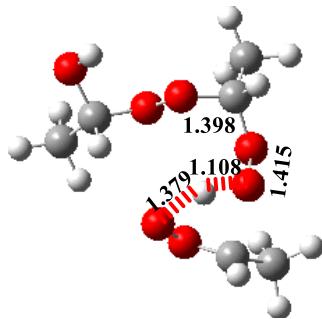
| | |
|-----|--------------|
| B1 | 1.09166775 |
| B2 | 2.29317669 |
| B3 | 1.40104503 |
| B4 | 0.99490733 |
| B5 | 2.62278378 |
| B6 | 2.24168914 |
| B7 | 1.23673777 |
| B8 | 1.51213066 |
| B9 | 1.08729069 |
| B10 | 1.08727747 |
| B11 | 1.08744854 |
| B12 | 1.39845904 |
| B13 | 1.47288773 |
| B14 | 1.09064633 |
| B15 | 1.08602217 |
| B16 | 1.09175634 |
| B17 | 1.08748199 |
| B18 | 1.43068689 |
| B19 | 1.41845233 |
| B20 | 1.09273645 |
| B21 | 1.50712955 |
| B22 | 1.08695033 |
| B23 | 1.08729256 |
| B24 | 1.08909615 |
| B25 | 1.39355163 |
| B26 | 0.96076856 |
| A1 | 81.90897612 |
| A2 | 35.88077040 |
| A3 | 101.31834786 |
| A4 | 131.44360136 |
| A5 | 79.66216246 |
| A6 | 93.39425061 |
| A7 | 106.82501598 |
| A8 | 109.55879262 |
| A9 | 110.36091113 |
| A10 | 109.23362074 |
| A11 | 111.93621621 |
| A12 | 105.60526548 |
| A13 | 109.88073810 |

| | |
|-----|---------------|
| A14 | 111.04562011 |
| A15 | 107.55418559 |
| A16 | 70.00450110 |
| A17 | 108.10333547 |
| A18 | 104.58906658 |
| A19 | 107.25223492 |
| A20 | 105.85349491 |
| A21 | 110.49336836 |
| A22 | 108.80333331 |
| A23 | 109.44885763 |
| A24 | 110.94573523 |
| A25 | 108.25525287 |
| D1 | 138.88980310 |
| D2 | -94.84525347 |
| D3 | 107.30526467 |
| D4 | -73.69143791 |
| D5 | -43.11851795 |
| D6 | 165.71105953 |
| D7 | -66.18987301 |
| D8 | 54.46006409 |
| D9 | 173.65981488 |
| D10 | -69.07274747 |
| D11 | 78.53534425 |
| D12 | 133.82235279 |
| D13 | -103.42640012 |
| D14 | 17.06617301 |
| D15 | -161.12785937 |
| D16 | -71.30904863 |
| D17 | 164.53806241 |
| D18 | -56.00117457 |
| D19 | -176.63502519 |
| D20 | 61.63454919 |
| D21 | -178.60745167 |
| D22 | -59.73308936 |
| D23 | 65.92930384 |
| D24 | -67.46179980 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 40.01 | 53.06 | 73.16 | 81.06 | 97.16 | 111.48 | 120.06 | 141.56 | 158.72 | 206.97 | 219.15 |
| 229.12 | 233.63 | 254.40 | 287.07 | 304.46 | 327.77 | 353.49 | 386.89 | 411.05 | 424.79 | |
| 520.43 | 567.14 | 579.64 | 601.10 | 699.97 | 823.22 | 878.22 | 886.27 | 901.62 | 905.09 | |
| 937.09 | 954.15 | 994.24 | 1006.60 | 1060.33 | 1088.76 | 1111.31 | 1143.82 | 1150.60 | | |
| 1161.98 | 1182.34 | 1185.69 | 1213.59 | 1297.07 | 1346.72 | 1373.68 | 1393.34 | 1398.23 | | |
| 1422.26 | 1423.32 | 1423.89 | 1463.61 | 1468.81 | 1483.71 | 1485.21 | 1496.59 | 1497.81 | | |
| 1500.44 | 1617.78 | 1695.77 | 3055.82 | 3077.49 | 3081.33 | 3114.26 | 3117.08 | 3127.61 | | |

3159.62 3161.57 3168.56 3170.70 3176.89 3185.26 3201.17 3896.98
 Rotational constants (B/GHZ): 0.8404079 0.6655326 0.5199558



TS4a

C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 0 |
| C | 3 | B5 | 1 | A4 | 4 | D3 0 |
| O | 6 | B6 | 3 | A5 | 1 | D4 0 |
| O | 6 | B7 | 3 | A6 | 1 | D5 0 |
| C | 1 | B8 | 4 | A7 | 3 | D6 0 |
| H | 9 | B9 | 1 | A8 | 4 | D7 0 |
| H | 9 | B10 | 1 | A9 | 4 | D8 0 |
| H | 9 | B11 | 1 | A10 | 4 | D9 0 |
| O | 1 | B12 | 4 | A11 | 3 | D10 0 |
| C | 6 | B13 | 3 | A12 | 1 | D11 0 |
| H | 14 | B14 | 6 | A13 | 3 | D12 0 |
| H | 14 | B15 | 6 | A14 | 3 | D13 0 |
| H | 14 | B16 | 6 | A15 | 3 | D14 0 |
| H | 6 | B17 | 3 | A16 | 1 | D15 0 |
| O | 13 | B18 | 1 | A17 | 4 | D16 0 |
| C | 19 | B19 | 13 | A18 | 1 | D17 0 |
| H | 20 | B20 | 19 | A19 | 13 | D18 0 |
| C | 20 | B21 | 19 | A20 | 13 | D19 0 |
| H | 22 | B22 | 20 | A21 | 19 | D20 0 |
| H | 22 | B23 | 20 | A22 | 19 | D21 0 |
| H | 22 | B24 | 20 | A23 | 19 | D22 0 |
| O | 20 | B25 | 19 | A24 | 13 | D23 0 |
| H | 26 | B26 | 20 | A25 | 19 | D24 0 |

Variables:

| | |
|----|------------|
| B1 | 1.09305760 |
| B2 | 2.28920986 |
| B3 | 1.40251695 |
| B4 | 1.10803985 |
| B5 | 2.04784044 |

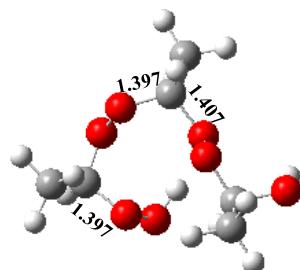
| | |
|-----|--------------|
| B6 | 2.17345685 |
| B7 | 1.26616672 |
| B8 | 1.51146059 |
| B9 | 1.08750242 |
| B10 | 1.08663416 |
| B11 | 1.08755991 |
| B12 | 1.39787808 |
| B13 | 1.47523420 |
| B14 | 1.09110229 |
| B15 | 1.08542504 |
| B16 | 1.08914207 |
| B17 | 1.08509114 |
| B18 | 1.43087617 |
| B19 | 1.41171451 |
| B20 | 1.09090000 |
| B21 | 1.50573353 |
| B22 | 1.08727855 |
| B23 | 1.08732745 |
| B24 | 1.08906741 |
| B25 | 1.39718939 |
| B26 | 0.96040756 |
| A1 | 85.63299725 |
| A2 | 35.82719462 |
| A3 | 93.38569115 |
| A4 | 129.97126223 |
| A5 | 69.35897017 |
| A6 | 92.91593901 |
| A7 | 106.11341755 |
| A8 | 109.66420352 |
| A9 | 110.07153147 |
| A10 | 109.04012241 |
| A11 | 111.66210862 |
| A12 | 108.87267572 |
| A13 | 109.18338956 |
| A14 | 110.66379939 |
| A15 | 108.07029571 |
| A16 | 83.20141216 |
| A17 | 107.48035991 |
| A18 | 105.16912477 |
| A19 | 107.44743296 |
| A20 | 105.67402457 |
| A21 | 109.47506435 |
| A22 | 109.04108824 |
| A23 | 109.72218512 |

| | |
|-----|---------------|
| A24 | 111.13681846 |
| A25 | 108.29576429 |
| D1 | 132.93866792 |
| D2 | -110.93651103 |
| D3 | -38.54409198 |
| D4 | -79.73361701 |
| D5 | -48.76383637 |
| D6 | 173.15024269 |
| D7 | -66.20545521 |
| D8 | 54.35860537 |
| D9 | 173.88149122 |
| D10 | -61.89888204 |
| D11 | 72.67064407 |
| D12 | 151.80761150 |
| D13 | -86.20023555 |
| D14 | 34.36895698 |
| D15 | -166.17766104 |
| D16 | -65.53116459 |
| D17 | 169.22210117 |
| D18 | -48.74501194 |
| D19 | -168.27994875 |
| D20 | 62.00204995 |
| D21 | -178.13719277 |
| D22 | -58.92423512 |
| D23 | 73.30128810 |
| D24 | -67.80762676 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 559.33 <i>i</i> | 36.51 | 52.98 | 64.01 | 73.78 | 92.29 | 112.52 | 137.55 | 160.33 | 204.54 | 212.44 |
| 219.36 | 250.06 | 290.36 | 324.25 | 337.91 | 377.15 | 392.71 | 400.32 | 435.35 | 522.50 | |
| 539.32 | 565.46 | 585.81 | 599.34 | 707.39 | 886.97 | 894.52 | 908.08 | 939.39 | 954.90 | |
| 967.96 | 995.19 | 1009.06 | 1013.52 | 1088.15 | 1109.31 | 1140.55 | 1146.56 | 1162.71 | | |
| 1178.68 | 1184.37 | 1209.50 | 1229.67 | 1290.54 | 1351.60 | 1355.86 | 1393.97 | 1396.09 | | |
| 1400.33 | 1418.32 | 1426.94 | 1450.86 | 1471.47 | 1474.60 | 1489.64 | 1490.28 | 1496.68 | | |
| 1503.36 | 1582.72 | 1623.30 | 1854.33 | 3063.79 | 3071.18 | 3085.54 | 3104.27 | 3124.55 | | |
| 3143.57 | 3155.06 | 3163.03 | 3166.72 | 3175.52 | 3180.90 | 3211.16 | 3900.90 | | | |

Rotational constants (B/GHZ): 1.0502275 0.5675060 0.4326991



P4a

| C | | B1 | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 0 |
| C | 3 | B5 | 1 | A4 | 4 | D3 0 |
| O | 6 | B6 | 3 | A5 | 1 | D4 0 |
| O | 6 | B7 | 3 | A6 | 1 | D5 0 |
| C | 1 | B8 | 4 | A7 | 3 | D6 0 |
| H | 9 | B9 | 1 | A8 | 4 | D7 0 |
| H | 9 | B10 | 1 | A9 | 4 | D8 0 |
| H | 9 | B11 | 1 | A10 | 4 | D9 0 |
| O | 1 | B12 | 4 | A11 | 3 | D10 0 |
| C | 6 | B13 | 3 | A12 | 1 | D11 0 |
| H | 14 | B14 | 6 | A13 | 3 | D12 0 |
| H | 14 | B15 | 6 | A14 | 3 | D13 0 |
| H | 14 | B16 | 6 | A15 | 3 | D14 0 |
| H | 6 | B17 | 3 | A16 | 1 | D15 0 |
| O | 13 | B18 | 1 | A17 | 4 | D16 0 |
| C | 19 | B19 | 13 | A18 | 1 | D17 0 |
| H | 20 | B20 | 19 | A19 | 13 | D18 0 |
| C | 20 | B21 | 19 | A20 | 13 | D19 0 |
| H | 22 | B22 | 20 | A21 | 19 | D20 0 |
| H | 22 | B23 | 20 | A22 | 19 | D21 0 |
| H | 22 | B24 | 20 | A23 | 19 | D22 0 |
| O | 20 | B25 | 19 | A24 | 13 | D23 0 |
| H | 26 | B26 | 20 | A25 | 19 | D24 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.09236410 |
| B2 | 2.27624819 |
| B3 | 1.39659979 |
| B4 | 2.53268836 |
| B5 | 1.40991757 |
| B6 | 2.27741737 |
| B7 | 1.39746599 |
| B8 | 1.51130089 |
| B9 | 1.08708862 |
| B10 | 1.08635936 |
| B11 | 1.08748501 |
| B12 | 1.40742215 |
| B13 | 1.50939067 |
| B14 | 1.08730608 |
| B15 | 1.08713452 |
| B16 | 1.08753335 |

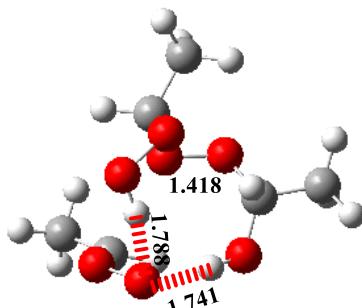
| | |
|-----|---------------|
| B17 | 1.09267857 |
| B18 | 1.43043745 |
| B19 | 1.41230303 |
| B20 | 1.09291560 |
| B21 | 1.50683556 |
| B22 | 1.08719759 |
| B23 | 1.08714733 |
| B24 | 1.08876305 |
| B25 | 1.39432692 |
| B26 | 0.96039074 |
| A1 | 81.97205284 |
| A2 | 36.53396844 |
| A3 | 73.83803625 |
| A4 | 124.25240040 |
| A5 | 92.91926410 |
| A6 | 112.00617768 |
| A7 | 106.50856878 |
| A8 | 109.32301756 |
| A9 | 110.29129115 |
| A10 | 109.15510741 |
| A11 | 112.03526591 |
| A12 | 114.00690044 |
| A13 | 109.42351105 |
| A14 | 109.88740119 |
| A15 | 109.38988789 |
| A16 | 101.40730278 |
| A17 | 107.01788247 |
| A18 | 106.01005338 |
| A19 | 107.85648477 |
| A20 | 105.39320408 |
| A21 | 110.06078305 |
| A22 | 108.96569767 |
| A23 | 109.40964461 |
| A24 | 111.41360556 |
| A25 | 108.94946055 |
| D1 | 139.64237489 |
| D2 | -133.95408747 |
| D3 | -75.35413053 |
| D4 | -67.27321830 |
| D5 | -35.62985652 |
| D6 | 165.17342551 |
| D7 | -68.52740365 |
| D8 | 51.76353862 |
| D9 | 171.50680838 |

| | |
|-----|---------------|
| D10 | -70.06800310 |
| D11 | 85.39489019 |
| D12 | 169.35294427 |
| D13 | -70.52489663 |
| D14 | 49.38585820 |
| D15 | -152.40756194 |
| D16 | -67.71068351 |
| D17 | 174.96989933 |
| D18 | -51.93411078 |
| D19 | -171.76797334 |
| D20 | 60.37926654 |
| D21 | -179.45991700 |
| D22 | -60.41974203 |
| D23 | 70.29652453 |
| D24 | -68.56422670 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 34.03 | 41.01 | 73.16 | 99.64 | 128.17 | 138.78 | 157.80 | 173.79 | 186.74 | 214.15 | 219.67 |
| 266.07 | 287.73 | 307.95 | 314.55 | 353.82 | 383.09 | 413.96 | 431.68 | 503.31 | 519.55 | |
| 569.26 | 587.19 | 594.39 | 697.53 | 699.28 | 875.92 | 891.23 | 908.87 | 929.83 | 939.46 | |
| 953.30 | 1006.23 | 1020.91 | 1059.14 | 1083.26 | 134.11 | 1141.67 | 1147.59 | 1150.92 | | |
| 1156.53 | 1179.82 | 1201.96 | 1230.09 | 1285.22 | 1357.07 | 1364.07 | 1393.53 | 1396.18 | | |
| 1401.87 | 1410.27 | 1420.22 | 1425.92 | 1460.73 | 1469.39 | 1483.24 | 1484.42 | 1490.30 | | |
| 1495.12 | 1497.34 | 1498.17 | 3073.94 | 3077.01 | 3077.77 | 3108.15 | 3110.02 | 3112.27 | | |
| 3158.13 | 3159.82 | 3159.91 | 3163.38 | 3167.54 | 3168.97 | 3765.41 | 3901.87 | | | |

Rotational constants (B/GHZ): 0.9989220 0.6205029 0.4912401



IM4b

| C | | B1 | | | | |
|---|---|----|---|----|---|------|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 0 |
| O | 1 | B5 | 2 | A4 | 3 | D3 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 0 |
| C | 6 | B7 | 1 | A6 | 2 | D5 0 |
| C | 8 | B8 | 6 | A7 | 1 | D6 0 |
| H | 9 | B9 | 8 | A8 | 6 | D7 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 9 | B10 | 8 | A9 | 6 | D8 | 0 |
| H | 9 | B11 | 8 | A10 | 6 | D9 | 0 |
| O | 8 | B12 | 6 | A11 | 1 | D10 | 0 |
| O | 8 | B13 | 6 | A12 | 1 | D11 | 0 |
| H | 8 | B14 | 6 | A13 | 1 | D12 | 0 |
| H | 1 | B15 | 6 | A14 | 2 | D13 | 0 |
| O | 1 | B16 | 6 | A15 | 2 | D14 | 0 |
| O | 17 | B17 | 1 | A16 | 6 | D15 | 0 |
| C | 18 | B18 | 17 | A17 | 1 | D16 | 0 |
| H | 19 | B19 | 18 | A18 | 17 | D17 | 0 |
| C | 19 | B20 | 18 | A19 | 17 | D18 | 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 | 0 |
| H | 21 | B22 | 19 | A21 | 18 | D20 | 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 | 0 |
| O | 19 | B24 | 18 | A23 | 17 | D22 | 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 | 0 |

Variables:

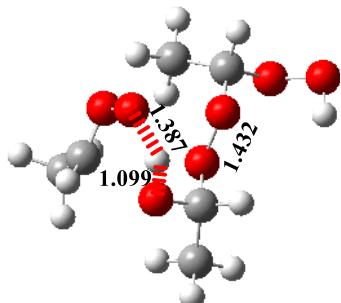
| | |
|-----|------------|
| B1 | 1.50971389 |
| B2 | 1.08731480 |
| B3 | 1.08893475 |
| B4 | 1.08783924 |
| B5 | 1.38126481 |
| B6 | 0.97997535 |
| B7 | 3.09683344 |
| B8 | 1.47208233 |
| B9 | 1.09199636 |
| B10 | 1.09067128 |
| B11 | 1.08573996 |
| B12 | 2.24965673 |
| B13 | 1.23877899 |
| B14 | 1.08821958 |
| B15 | 1.09209117 |
| B16 | 1.43363029 |
| B17 | 1.41761745 |
| B18 | 1.42376575 |
| B19 | 1.09248423 |
| B20 | 1.50972754 |
| B21 | 1.08705435 |
| B22 | 1.08725755 |
| B23 | 1.08726875 |
| B24 | 1.39136939 |
| B25 | 1.41639088 |
| B26 | 0.98337025 |

| | |
|-----|---------------|
| A1 | 108.87248638 |
| A2 | 109.22580512 |
| A3 | 110.92826347 |
| A4 | 109.98380516 |
| A5 | 109.27330830 |
| A6 | 106.93379592 |
| A7 | 147.20662058 |
| A8 | 107.31325578 |
| A9 | 109.51363687 |
| A10 | 111.32287060 |
| A11 | 58.22785283 |
| A12 | 90.90545366 |
| A13 | 30.82054598 |
| A14 | 110.98798739 |
| A15 | 111.64623190 |
| A16 | 110.19204826 |
| A17 | 111.15543258 |
| A18 | 102.30121766 |
| A19 | 113.42440636 |
| A20 | 108.83008232 |
| A21 | 110.27952279 |
| A22 | 109.93569481 |
| A23 | 111.80295282 |
| A24 | 108.74772470 |
| A25 | 104.21966745 |
| D1 | 118.73839395 |
| D2 | -120.52078093 |
| D3 | -61.95233780 |
| D4 | 157.13852095 |
| D5 | -146.89835259 |
| D6 | 64.65969904 |
| D7 | -31.85145049 |
| D8 | 84.36506363 |
| D9 | -152.84950939 |
| D10 | -98.63323274 |
| D11 | -91.23153019 |
| D12 | 114.31367953 |
| D13 | -125.10161198 |
| D14 | 114.78552957 |
| D15 | 66.55979873 |
| D16 | 94.70615654 |
| D17 | 159.76604016 |
| D18 | 37.74099439 |
| D19 | 166.25762108 |

| | |
|-----|--------------|
| D20 | -74.17596929 |
| D21 | 45.81783677 |
| D22 | -83.84925776 |
| D23 | -75.23575748 |
| D24 | 87.03251440 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-------------------------------|---------|---------|---------|-----------|-----------|-----------|---------|---------|--------|--------|
| 34.30 | 63.36 | 78.34 | 99.69 | 118.45 | 121.17 | 129.17 | 149.64 | 179.36 | 211.79 | 219.88 |
| 235.22 | 240.87 | 273.44 | 303.47 | 317.64 | 333.39 | 362.58 | 397.46 | 426.64 | 530.64 | |
| 566.74 | 578.08 | 621.37 | 707.45 | 780.95 | 852.16 | 875.47 | 887.20 | 899.36 | 915.60 | |
| 925.75 | 955.09 | 1009.29 | 1014.82 | 1062.08 | 1108.48 | 1119.68 | 1128.41 | 1140.11 | | |
| 1160.06 | 1187.17 | 1197.20 | 1206.04 | 1356.42 | 1361.35 | 1388.17 | 1393.31 | 1402.31 | | |
| 1410.99 | 1425.34 | 1444.34 | 1465.44 | 1467.50 | 1485.38 | 1490.86 | 1493.45 | 1496.01 | | |
| 1508.31 | 1530.24 | 1697.23 | 3057.56 | 3071.21 | 3078.63 | 3099.53 | 3101.43 | 3122.74 | | |
| 3151.85 | 3162.00 | 3165.71 | 3166.38 | 3173.89 | 3197.03 | 3404.80 | 3455.08 | | | |
| Rotational constants (B/GHZ): | | | | 0.8262655 | 0.6476380 | 0.5240421 | | | | |



TS4b

| C | | B1 | | | | |
|---|----|-----|----|-----|----|-------|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 0 |
| O | 1 | B5 | 2 | A4 | 3 | D3 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 0 |
| C | 6 | B7 | 1 | A6 | 2 | D5 0 |
| C | 8 | B8 | 6 | A7 | 1 | D6 0 |
| H | 9 | B9 | 8 | A8 | 6 | D7 0 |
| H | 9 | B10 | 8 | A9 | 6 | D8 0 |
| H | 9 | B11 | 8 | A10 | 6 | D9 0 |
| O | 8 | B12 | 6 | A11 | 1 | D10 0 |
| O | 8 | B13 | 6 | A12 | 1 | D11 0 |
| H | 8 | B14 | 6 | A13 | 1 | D12 0 |
| H | 1 | B15 | 6 | A14 | 8 | D13 0 |
| O | 1 | B16 | 6 | A15 | 8 | D14 0 |
| O | 17 | B17 | 1 | A16 | 6 | D15 0 |
| C | 18 | B18 | 17 | A17 | 1 | D16 0 |
| H | 19 | B19 | 18 | A18 | 17 | D17 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 19 | B20 | 18 | A19 | 17 | D18 | 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 | 0 |
| H | 21 | B22 | 19 | A21 | 18 | D20 | 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 | 0 |
| O | 19 | B24 | 18 | A23 | 17 | D22 | 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 | 0 |

Variables:

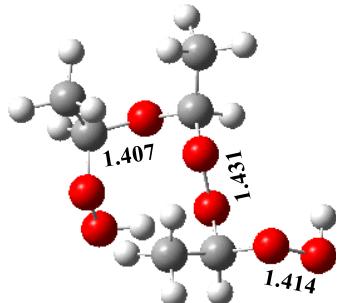
| | |
|-----|--------------|
| B1 | 1.51135490 |
| B2 | 1.08719356 |
| B3 | 1.08941491 |
| B4 | 1.08750585 |
| B5 | 1.39206112 |
| B6 | 1.09904681 |
| B7 | 2.01655519 |
| B8 | 1.47946920 |
| B9 | 1.08702995 |
| B10 | 1.09250770 |
| B11 | 1.08583226 |
| B12 | 2.17914880 |
| B13 | 1.26731438 |
| B14 | 1.08439845 |
| B15 | 1.09504521 |
| B16 | 1.40976923 |
| B17 | 1.43191750 |
| B18 | 1.40352881 |
| B19 | 1.09209770 |
| B20 | 1.51001292 |
| B21 | 1.08726424 |
| B22 | 1.08781966 |
| B23 | 1.08715779 |
| B24 | 1.39950397 |
| B25 | 1.41330314 |
| B26 | 0.96577011 |
| A1 | 109.06279137 |
| A2 | 109.86680895 |
| A3 | 110.57334854 |
| A4 | 110.01984734 |
| A5 | 115.37864391 |
| A6 | 123.21133579 |
| A7 | 111.90883330 |
| A8 | 109.36933558 |
| A9 | 108.16701845 |
| A10 | 110.73345272 |

| | |
|-----|---------------|
| A11 | 69.54778778 |
| A12 | 94.42132904 |
| A13 | 81.54202377 |
| A14 | 108.78237289 |
| A15 | 112.68614711 |
| A16 | 105.44692004 |
| A17 | 108.37616026 |
| A18 | 101.67839617 |
| A19 | 114.54676231 |
| A20 | 109.25889162 |
| A21 | 110.12328795 |
| A22 | 108.85927813 |
| A23 | 111.34170866 |
| A24 | 108.27062600 |
| A25 | 102.35174224 |
| D1 | 119.22524315 |
| D2 | -120.60214204 |
| D3 | -54.97744044 |
| D4 | 177.55608707 |
| D5 | -93.27045911 |
| D6 | 41.40139413 |
| D7 | 50.14021398 |
| D8 | 167.55375535 |
| D9 | -71.98651333 |
| D10 | -111.41375750 |
| D11 | -81.54589758 |
| D12 | 161.58855492 |
| D13 | 143.79777570 |
| D14 | 24.40159460 |
| D15 | 75.36780610 |
| D16 | 178.03295493 |
| D17 | 173.54672870 |
| D18 | 51.44608850 |
| D19 | 170.35419264 |
| D20 | -70.06144343 |
| D21 | 50.64003125 |
| D22 | -69.44014438 |
| D23 | -65.30630775 |
| D24 | 79.74807401 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 531.58 <i>i</i> | 51.24 | 56.67 | 67.11 | 88.35 | 112.60 | 140.82 | 162.11 | 175.28 | 206.43 | 221.54 |
| 236.26 | 254.77 | 258.60 | 285.35 | 316.24 | 342.31 | 354.95 | 399.28 | 421.86 | 480.86 | |
| 527.55 | 571.75 | 582.94 | 617.52 | 703.88 | 869.05 | 890.60 | 899.37 | 927.82 | 943.78 | |
| 951.15 | 1012.66 | 1017.87 | 1061.73 | 1091.11 | 1124.84 | 1144.44 | 1152.31 | 1158.94 | | |

| | | | | | | | | |
|-------------------------------|---------|---------|---------|-----------|-----------|-----------|---------|---------|
| 1181.89 | 1199.36 | 1215.53 | 1238.95 | 1346.42 | 1360.55 | 1362.52 | 1390.77 | 1393.74 |
| 1405.03 | 1414.98 | 1419.91 | 1430.18 | 1446.40 | 1454.86 | 1481.16 | 1490.46 | 1494.72 |
| 1499.94 | 1506.18 | 1615.35 | 1968.74 | 3057.14 | 3072.40 | 3072.74 | 3075.86 | 3115.20 |
| 3138.04 | 3152.74 | 3154.41 | 3168.04 | 3169.91 | 3180.36 | 3209.75 | 3826.63 | |
| Rotational constants (B/GHZ): | | | | 1.0669644 | 0.5352829 | 0.4656729 | | |



P4b

C

| | | | | | | | | |
|---|----|-----|----|-----|----|-----|---|--|
| C | 1 | B1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 | |
| H | 2 | B4 | 1 | A3 | 3 | D2 | 0 | |
| O | 1 | B5 | 2 | A4 | 4 | D3 | 0 | |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 | |
| C | 6 | B7 | 1 | A6 | 2 | D5 | 0 | |
| C | 8 | B8 | 6 | A7 | 1 | D6 | 0 | |
| H | 9 | B9 | 8 | A8 | 6 | D7 | 0 | |
| H | 9 | B10 | 8 | A9 | 6 | D8 | 0 | |
| H | 9 | B11 | 8 | A10 | 6 | D9 | 0 | |
| O | 8 | B12 | 6 | A11 | 1 | D10 | 0 | |
| O | 8 | B13 | 6 | A12 | 1 | D11 | 0 | |
| H | 8 | B14 | 6 | A13 | 1 | D12 | 0 | |
| H | 1 | B15 | 6 | A14 | 8 | D13 | 0 | |
| O | 1 | B16 | 6 | A15 | 8 | D14 | 0 | |
| O | 17 | B17 | 1 | A16 | 6 | D15 | 0 | |
| C | 18 | B18 | 17 | A17 | 1 | D16 | 0 | |
| H | 19 | B19 | 18 | A18 | 17 | D17 | 0 | |
| C | 19 | B20 | 18 | A19 | 17 | D18 | 0 | |
| H | 21 | B21 | 19 | A20 | 18 | D19 | 0 | |
| H | 21 | B22 | 19 | A21 | 18 | D20 | 0 | |
| H | 21 | B23 | 19 | A22 | 18 | D21 | 0 | |
| O | 19 | B24 | 18 | A23 | 17 | D22 | 0 | |
| O | 25 | B25 | 19 | A24 | 18 | D23 | 0 | |
| H | 26 | B26 | 25 | A25 | 19 | D24 | 0 | |

Variables:

| | |
|----|------------|
| B1 | 1.51778472 |
| B2 | 1.08781576 |

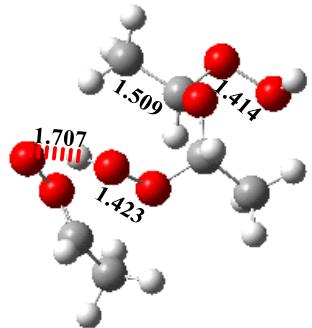
| | |
|-----|--------------|
| B3 | 1.08592820 |
| B4 | 1.08802912 |
| B5 | 1.40471297 |
| B6 | 2.47347935 |
| B7 | 1.40670352 |
| B8 | 1.51408940 |
| B9 | 1.08763919 |
| B10 | 1.08776992 |
| B11 | 1.08836529 |
| B12 | 2.28963871 |
| B13 | 1.40472425 |
| B14 | 1.09097849 |
| B15 | 1.09229739 |
| B16 | 1.40049727 |
| B17 | 1.43068758 |
| B18 | 1.41373867 |
| B19 | 1.09252189 |
| B20 | 1.50862462 |
| B21 | 1.08718239 |
| B22 | 1.08710720 |
| B23 | 1.08681197 |
| B24 | 1.39576218 |
| B25 | 1.41387598 |
| B26 | 0.96519263 |
| A1 | 108.81488813 |
| A2 | 112.01611333 |
| A3 | 109.19802834 |
| A4 | 115.23172648 |
| A5 | 101.13924911 |
| A6 | 122.78553737 |
| A7 | 116.97727072 |
| A8 | 110.17478636 |
| A9 | 108.64193458 |
| A10 | 110.59049177 |
| A11 | 91.47342435 |
| A12 | 111.66080708 |
| A13 | 102.98865479 |
| A14 | 103.23348437 |
| A15 | 113.45198599 |
| A16 | 106.23972759 |
| A17 | 107.87736588 |
| A18 | 101.67656647 |
| A19 | 114.43187866 |
| A20 | 108.91260130 |

| | |
|-----|---------------|
| A21 | 110.16493996 |
| A22 | 109.14585399 |
| A23 | 110.84622903 |
| A24 | 108.32342169 |
| A25 | 102.30925376 |
| D1 | 120.92997456 |
| D2 | -118.96586348 |
| D3 | 77.28792069 |
| D4 | -160.22610906 |
| D5 | -79.18683181 |
| D6 | 47.19177581 |
| D7 | 51.20582404 |
| D8 | 170.51649771 |
| D9 | -70.50979939 |
| D10 | -103.72892230 |
| D11 | -73.45359851 |
| D12 | 170.07108324 |
| D13 | 160.71757623 |
| D14 | 43.05162316 |
| D15 | 66.40232755 |
| D16 | 179.21301691 |
| D17 | 172.45939587 |
| D18 | 50.22675868 |
| D19 | 169.50672787 |
| D20 | -70.77569657 |
| D21 | 49.15602421 |
| D22 | -70.92089317 |
| D23 | -65.79342151 |
| D24 | 85.65306895 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 41.73 | 49.93 | 79.89 | 107.21 | 124.79 | 159.28 | 182.13 | 191.62 | 209.26 | 250.57 | 252.74 |
| 266.69 | 292.32 | 309.35 | 321.44 | 335.89 | 352.23 | 413.86 | 432.13 | 487.40 | 515.13 | |
| 523.31 | 585.20 | 590.34 | 681.39 | 756.21 | 805.24 | 886.68 | 898.22 | 920.09 | 940.51 | |
| 952.40 | 1014.97 | 1060.08 | 1063.71 | 1114.74 | 1133.20 | 1136.44 | 1152.50 | 1157.41 | | |
| 1170.07 | 1200.42 | 1208.75 | 1232.12 | 1361.67 | 1363.69 | 1377.88 | 1406.84 | 1411.92 | | |
| 1415.29 | 1426.82 | 1430.16 | 1434.41 | 1449.82 | 1474.24 | 1485.54 | 1487.06 | 1488.74 | | |
| 1499.51 | 1505.25 | 1516.41 | 3069.67 | 3075.98 | 3077.17 | 3098.27 | 3111.47 | 3118.27 | | |
| 3149.41 | 3150.71 | 3156.93 | 3159.87 | 3176.11 | 3177.27 | 3761.21 | 3818.68 | | | |

Rotational constants (B/GHZ): 1.1588304 0.5531838 0.4628137



IM4c

| C | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 1 | B1 | | | | | |
| O | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 | 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 | 0 |
| C | 4 | B5 | 1 | A4 | 3 | D3 | 0 |
| O | 6 | B6 | 4 | A5 | 1 | D4 | 0 |
| O | 6 | B7 | 4 | A6 | 1 | D5 | 0 |
| C | 1 | B8 | 4 | A7 | 3 | D6 | 0 |
| H | 9 | B9 | 1 | A8 | 4 | D7 | 0 |
| H | 9 | B10 | 1 | A9 | 4 | D8 | 0 |
| H | 9 | B11 | 1 | A10 | 4 | D9 | 0 |
| O | 1 | B12 | 4 | A11 | 3 | D10 | 0 |
| C | 13 | B13 | 1 | A12 | 4 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 1 | D12 | 0 |
| C | 14 | B15 | 13 | A14 | 1 | D13 | 0 |
| H | 16 | B16 | 14 | A15 | 13 | D14 | 0 |
| H | 16 | B17 | 14 | A16 | 13 | D15 | 0 |
| H | 16 | B18 | 14 | A17 | 13 | D16 | 0 |
| O | 14 | B19 | 13 | A18 | 1 | D17 | 0 |
| O | 20 | B20 | 14 | A19 | 13 | D18 | 0 |
| H | 21 | B21 | 20 | A20 | 14 | D19 | 0 |
| C | 6 | B22 | 4 | A21 | 1 | D20 | 0 |
| H | 23 | B23 | 6 | A22 | 4 | D21 | 0 |
| H | 23 | B24 | 6 | A23 | 4 | D22 | 0 |
| H | 23 | B25 | 6 | A24 | 4 | D23 | 0 |
| H | 6 | B26 | 4 | A25 | 1 | D24 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.08988603 |
| B2 | 2.29960509 |
| B3 | 1.40574902 |
| B4 | 0.99271921 |
| B5 | 2.59745988 |
| B6 | 2.23565349 |

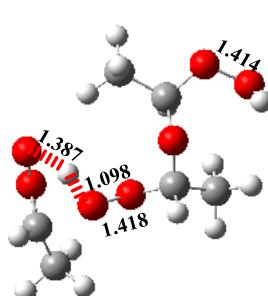
| | |
|-----|--------------|
| B7 | 1.23696252 |
| B8 | 1.51678566 |
| B9 | 1.08834973 |
| B10 | 1.08832284 |
| B11 | 1.08735019 |
| B12 | 1.40183326 |
| B13 | 1.40807472 |
| B14 | 1.09402576 |
| B15 | 1.50852929 |
| B16 | 1.08871594 |
| B17 | 1.08832217 |
| B18 | 1.08764312 |
| B19 | 1.40484278 |
| B20 | 1.41402464 |
| B21 | 0.96517079 |
| B22 | 1.47267808 |
| B23 | 1.08607725 |
| B24 | 1.09183282 |
| B25 | 1.09094578 |
| B26 | 1.08799804 |
| A1 | 80.59763462 |
| A2 | 35.88210385 |
| A3 | 118.61058201 |
| A4 | 151.09511942 |
| A5 | 79.63349535 |
| A6 | 90.51805067 |
| A7 | 105.48599470 |
| A8 | 109.24674426 |
| A9 | 111.69896699 |
| A10 | 109.40370252 |
| A11 | 112.48522537 |
| A12 | 118.04993538 |
| A13 | 110.06607374 |
| A14 | 110.46620569 |
| A15 | 108.83260544 |
| A16 | 110.21101903 |
| A17 | 109.74733276 |
| A18 | 109.34439981 |
| A19 | 108.71266761 |
| A20 | 101.55195751 |
| A21 | 103.98011563 |
| A22 | 111.09364650 |
| A23 | 107.78421319 |
| A24 | 109.69459378 |

| | |
|-----|---------------|
| A25 | 74.35202657 |
| D1 | 140.51155807 |
| D2 | -67.96473918 |
| D3 | 139.14702820 |
| D4 | -103.97079536 |
| D5 | -71.85864678 |
| D6 | 160.65084845 |
| D7 | -59.91206576 |
| D8 | 61.38837581 |
| D9 | -179.04126659 |
| D10 | -73.60180211 |
| D11 | -53.53927270 |
| D12 | -4.80830856 |
| D13 | 119.89401887 |
| D14 | 55.01528347 |
| D15 | 175.00004187 |
| D16 | -64.83461936 |
| D17 | -124.70145506 |
| D18 | 65.71984230 |
| D19 | -90.93592897 |
| D20 | 48.78474884 |
| D21 | -98.51260590 |
| D22 | 22.51852363 |
| D23 | 139.20594197 |
| D24 | 170.04876827 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 26.86 | 47.88 | 69.44 | 80.97 | 110.38 | 120.64 | 147.77 | 166.59 | 181.43 | 206.90 | 225.63 |
| 227.88 | 253.31 | 266.99 | 269.80 | 308.24 | 318.19 | 338.47 | 349.96 | 362.62 | 434.08 | |
| 514.98 | 555.47 | 566.95 | 578.60 | 679.20 | 771.20 | 856.49 | 886.99 | 895.78 | 900.65 | |
| 929.94 | 966.81 | 991.27 | 1056.17 | 1062.39 | 1102.75 | 1118.04 | 1137.80 | 1141.70 | | |
| 1181.28 | 1187.39 | 1198.96 | 1219.44 | 1354.24 | 1369.97 | 1374.98 | 1408.27 | 1419.08 | | |
| 1420.92 | 1425.49 | 1427.21 | 1436.44 | 1467.34 | 1471.01 | 1487.44 | 1497.06 | 1501.07 | | |
| 1502.48 | 1614.43 | 1700.01 | 3064.53 | 3069.58 | 3074.40 | 3081.75 | 3123.61 | 3131.67 | | |
| 3151.31 | 3157.44 | 3158.21 | 3169.27 | 3171.31 | 3191.81 | 3220.42 | 3822.76 | | | |

Rotational constants (B/GHZ): 0.9835528 0.5122121 0.4796666



TS4c

| C | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 0 |
| C | 3 | B5 | 1 | A4 | 4 | D3 0 |
| O | 6 | B6 | 3 | A5 | 1 | D4 0 |
| O | 6 | B7 | 3 | A6 | 1 | D5 0 |
| C | 1 | B8 | 4 | A7 | 3 | D6 0 |
| H | 9 | B9 | 1 | A8 | 4 | D7 0 |
| H | 9 | B10 | 1 | A9 | 4 | D8 0 |
| H | 9 | B11 | 1 | A10 | 4 | D9 0 |
| O | 1 | B12 | 4 | A11 | 3 | D10 0 |
| C | 13 | B13 | 1 | A12 | 4 | D11 0 |
| H | 14 | B14 | 13 | A13 | 1 | D12 0 |
| C | 14 | B15 | 13 | A14 | 1 | D13 0 |
| H | 16 | B16 | 14 | A15 | 13 | D14 0 |
| H | 16 | B17 | 14 | A16 | 13 | D15 0 |
| H | 16 | B18 | 14 | A17 | 13 | D16 0 |
| O | 14 | B19 | 13 | A18 | 1 | D17 0 |
| O | 20 | B20 | 14 | A19 | 13 | D18 0 |
| H | 21 | B21 | 20 | A20 | 14 | D19 0 |
| C | 6 | B22 | 3 | A21 | 1 | D20 0 |
| H | 23 | B23 | 6 | A22 | 3 | D21 0 |
| H | 23 | B24 | 6 | A23 | 3 | D22 0 |
| H | 23 | B25 | 6 | A24 | 3 | D23 0 |
| H | 6 | B26 | 3 | A25 | 1 | D24 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.09027824 |
| B2 | 2.28871652 |
| B3 | 1.41025512 |
| B4 | 1.09822617 |
| B5 | 2.04638788 |
| B6 | 2.17627638 |
| B7 | 1.26598624 |
| B8 | 1.51632880 |
| B9 | 1.08807711 |
| B10 | 1.08711601 |
| B11 | 1.08719138 |
| B12 | 1.39874708 |
| B13 | 1.41172244 |
| B14 | 1.09174360 |
| B15 | 1.50841540 |
| B16 | 1.08857215 |

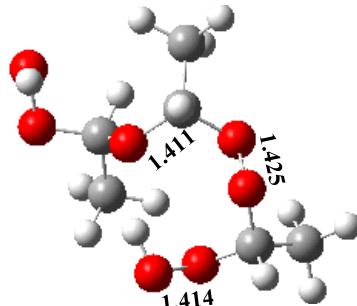
| | |
|-----|---------------|
| B17 | 1.08811697 |
| B18 | 1.08821200 |
| B19 | 1.40358429 |
| B20 | 1.41430354 |
| B21 | 0.96495567 |
| B22 | 1.47520706 |
| B23 | 1.08550621 |
| B24 | 1.08948570 |
| B25 | 1.09071355 |
| B26 | 1.08516488 |
| A1 | 80.90599422 |
| A2 | 36.09220734 |
| A3 | 114.02711144 |
| A4 | 136.71198258 |
| A5 | 69.20430217 |
| A6 | 92.89436318 |
| A7 | 105.52604985 |
| A8 | 109.04547160 |
| A9 | 111.99899896 |
| A10 | 109.37121565 |
| A11 | 111.87758695 |
| A12 | 118.22057919 |
| A13 | 110.18705608 |
| A14 | 110.66988430 |
| A15 | 109.24252325 |
| A16 | 109.98568527 |
| A17 | 109.61231449 |
| A18 | 108.91441600 |
| A19 | 108.48915612 |
| A20 | 101.53388125 |
| A21 | 108.92357287 |
| A22 | 110.71040380 |
| A23 | 107.83469815 |
| A24 | 109.41746432 |
| A25 | 83.06401722 |
| D1 | 139.70022270 |
| D2 | -81.14862053 |
| D3 | 11.86121007 |
| D4 | -106.76811185 |
| D5 | -75.98559807 |
| D6 | 161.44254417 |
| D7 | -59.62631169 |
| D8 | 61.12157823 |
| D9 | -178.76397902 |

| | |
|-----|---------------|
| D10 | -72.23568393 |
| D11 | -59.19140006 |
| D12 | -5.50395753 |
| D13 | 118.97155337 |
| D14 | 52.11950511 |
| D15 | 172.18648570 |
| D16 | -68.13675924 |
| D17 | -125.50807962 |
| D18 | 66.58663246 |
| D19 | -93.21220483 |
| D20 | 45.46956963 |
| D21 | -89.07354800 |
| D22 | 31.27686293 |
| D23 | 148.63928212 |
| D24 | 166.57886308 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 505.89 <i>i</i> | 23.71 | 45.59 | 70.52 | 95.30 | 104.94 | 119.21 | 126.71 | 154.50 | 180.78 | 225.58 |
| 232.48 | 258.36 | 278.48 | 309.61 | 323.48 | 347.98 | 362.94 | 409.65 | 429.91 | 507.99 | |
| 531.23 | 545.34 | 578.05 | 597.41 | 684.76 | 857.11 | 889.45 | 896.51 | 928.00 | 965.62 | |
| 975.57 | 999.14 | 1012.81 | 1059.93 | 1097.71 | 1125.38 | 1137.93 | 1141.08 | 1182.45 | | |
| 1185.69 | 1197.12 | 1219.32 | 1240.41 | 1357.38 | 1363.36 | 1371.92 | 1412.11 | 1414.88 | | |
| 1421.35 | 1424.08 | 1434.14 | 1440.68 | 1452.31 | 1474.94 | 1484.18 | 1492.48 | 1493.27 | | |
| 1503.53 | 1577.25 | 1619.99 | 1921.59 | 3067.11 | 3068.84 | 3079.96 | 3118.32 | 3128.47 | | |
| 3135.79 | 3153.78 | 3158.32 | 3160.93 | 3171.61 | 3185.57 | 3200.64 | 3829.34 | | | |

Rotational constants (B/GHZ): 1.3716013 0.4360083 0.3611265



P4c

| C | | | | | | |
|---|---|----|---|----|---|------|
| H | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 0 |
| C | 3 | B5 | 1 | A4 | 4 | D3 0 |
| O | 6 | B6 | 3 | A5 | 1 | D4 0 |
| O | 6 | B7 | 3 | A6 | 1 | D5 0 |
| C | 1 | B8 | 4 | A7 | 3 | D6 0 |
| H | 9 | B9 | 1 | A8 | 4 | D7 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 9 | B10 | 1 | A9 | 4 | D8 | 0 |
| H | 9 | B11 | 1 | A10 | 4 | D9 | 0 |
| O | 1 | B12 | 4 | A11 | 3 | D10 | 0 |
| C | 13 | B13 | 1 | A12 | 4 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 1 | D12 | 0 |
| C | 14 | B15 | 13 | A14 | 1 | D13 | 0 |
| H | 16 | B16 | 14 | A15 | 13 | D14 | 0 |
| H | 16 | B17 | 14 | A16 | 13 | D15 | 0 |
| H | 16 | B18 | 14 | A17 | 13 | D16 | 0 |
| O | 14 | B19 | 13 | A18 | 1 | D17 | 0 |
| O | 20 | B20 | 14 | A19 | 13 | D18 | 0 |
| H | 21 | B21 | 20 | A20 | 14 | D19 | 0 |
| C | 6 | B22 | 3 | A21 | 1 | D20 | 0 |
| H | 23 | B23 | 6 | A22 | 3 | D21 | 0 |
| H | 23 | B24 | 6 | A23 | 3 | D22 | 0 |
| H | 23 | B25 | 6 | A24 | 3 | D23 | 0 |
| H | 6 | B26 | 3 | A25 | 1 | D24 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.08984330 |
| B2 | 2.26901889 |
| B3 | 1.40466683 |
| B4 | 2.57786830 |
| B5 | 1.40785886 |
| B6 | 2.28159555 |
| B7 | 1.39393412 |
| B8 | 1.51624121 |
| B9 | 1.08702961 |
| B10 | 1.08847577 |
| B11 | 1.08782404 |
| B12 | 1.41111931 |
| B13 | 1.41769577 |
| B14 | 1.08915038 |
| B15 | 1.50762473 |
| B16 | 1.08887701 |
| B17 | 1.08789489 |
| B18 | 1.08668875 |
| B19 | 1.40002383 |
| B20 | 1.41462377 |
| B21 | 0.96537340 |
| B22 | 1.51030104 |
| B23 | 1.08739578 |
| B24 | 1.08748156 |
| B25 | 1.08722841 |
| B26 | 1.09316273 |

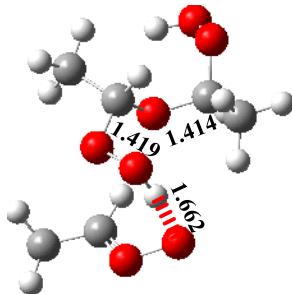
| | |
|-----|---------------|
| A1 | 77.72733929 |
| A2 | 37.01732810 |
| A3 | 70.91714484 |
| A4 | 127.63523441 |
| A5 | 92.45262552 |
| A6 | 112.04838758 |
| A7 | 105.80271809 |
| A8 | 108.13683857 |
| A9 | 111.52423977 |
| A10 | 110.26737557 |
| A11 | 111.49360852 |
| A12 | 120.41187612 |
| A13 | 109.77976998 |
| A14 | 112.21195588 |
| A15 | 110.19990321 |
| A16 | 109.49192381 |
| A17 | 109.28809164 |
| A18 | 107.49928572 |
| A19 | 108.11938108 |
| A20 | 101.75734298 |
| A21 | 113.77402109 |
| A22 | 110.03810860 |
| A23 | 109.26792542 |
| A24 | 109.61596832 |
| A25 | 101.33262410 |
| D1 | 144.23648516 |
| D2 | -123.54921823 |
| D3 | -71.07298332 |
| D4 | -61.21761047 |
| D5 | -30.20297612 |
| D6 | 155.78733177 |
| D7 | -72.98047146 |
| D8 | 45.53923364 |
| D9 | 167.18252740 |
| D10 | -76.89803133 |
| D11 | -87.46669639 |
| D12 | -12.45243848 |
| D13 | 112.91008497 |
| D14 | 55.11212562 |
| D15 | 175.66756697 |
| D16 | -63.70804031 |
| D17 | -130.74372586 |
| D18 | 66.54326520 |
| D19 | -91.22770080 |

D20 90.69001424
 D21 -67.45750011
 D22 52.32064257
 D23 172.35577850
 D24 -147.60391668

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 38.99 | 49.34 | 97.71 | 114.58 | 126.67 | 168.63 | 198.49 | 206.95 | 227.98 | 237.59 | 239.92 |
| 258.94 | 293.61 | 307.79 | 320.41 | 359.23 | 365.41 | 415.98 | 437.88 | 501.76 | 544.14 | |
| 576.62 | 583.29 | 597.64 | 673.63 | 703.75 | 843.37 | 880.01 | 903.02 | 920.52 | 939.41 | |
| 968.90 | 1011.41 | 1057.48 | 1063.11 | 107.65 | 1137.69 | 1138.75 | 1148.55 | 1153.81 | | |
| 1176.98 | 1185.72 | 1216.69 | 1225.97 | 1347.07 | 1360.65 | 1377.84 | 1399.31 | 1411.42 | | |
| 1420.10 | 1424.16 | 1426.11 | 1431.22 | 1439.13 | 1477.80 | 1484.31 | 1488.18 | 1493.21 | | |
| 1495.22 | 1502.37 | 1513.19 | 3067.59 | 3070.54 | 3078.39 | 3101.13 | 3121.07 | 3132.38 | | |
| 3150.12 | 3155.15 | 3157.69 | 3162.04 | 3169.34 | 3170.97 | 3697.55 | 3817.60 | | | |

Rotational constants (B/GHZ): 1.2463340 0.5375475 0.4463976



IM4d

| C | | B1 | | | | |
|---|----|-----|----|-----|----|-------|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 0 |
| C | 5 | B6 | 2 | A5 | 1 | D4 0 |
| O | 7 | B7 | 5 | A6 | 2 | D5 0 |
| O | 7 | B8 | 5 | A7 | 2 | D6 0 |
| H | 1 | B9 | 2 | A8 | 5 | D7 0 |
| H | 1 | B10 | 2 | A9 | 5 | D8 0 |
| H | 1 | B11 | 2 | A10 | 5 | D9 0 |
| O | 2 | B12 | 1 | A11 | 5 | D10 0 |
| C | 13 | B13 | 2 | A12 | 1 | D11 0 |
| H | 14 | B14 | 13 | A13 | 2 | D12 0 |
| C | 14 | B15 | 13 | A14 | 2 | D13 0 |
| H | 16 | B16 | 14 | A15 | 13 | D14 0 |
| H | 16 | B17 | 14 | A16 | 13 | D15 0 |
| H | 16 | B18 | 14 | A17 | 13 | D16 0 |
| O | 14 | B19 | 13 | A18 | 2 | D17 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 20 | B20 | 14 | A19 | 13 | D18 | 0 |
| H | 21 | B21 | 20 | A20 | 14 | D19 | 0 |
| C | 7 | B22 | 5 | A21 | 2 | D20 | 0 |
| H | 23 | B23 | 7 | A22 | 5 | D21 | 0 |
| H | 23 | B24 | 7 | A23 | 5 | D22 | 0 |
| H | 23 | B25 | 7 | A24 | 5 | D23 | 0 |
| H | 7 | B26 | 5 | A25 | 2 | D24 | 0 |

Variables:

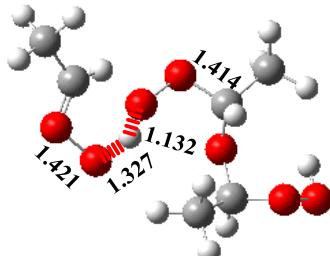
| | |
|-----|--------------|
| B1 | 1.51253247 |
| B2 | 1.09002450 |
| B3 | 2.29688285 |
| B4 | 1.39852099 |
| B5 | 0.99644826 |
| B6 | 2.74829119 |
| B7 | 2.22986604 |
| B8 | 1.23683815 |
| B9 | 1.08935542 |
| B10 | 1.09031499 |
| B11 | 1.08731607 |
| B12 | 1.41489565 |
| B13 | 1.41448727 |
| B14 | 1.08994292 |
| B15 | 1.50987484 |
| B16 | 1.08773159 |
| B17 | 1.08794158 |
| B18 | 1.08712803 |
| B19 | 1.40430810 |
| B20 | 1.41537129 |
| B21 | 0.96648623 |
| B22 | 1.47326744 |
| B23 | 1.09019390 |
| B24 | 1.08576079 |
| B25 | 1.09240190 |
| B26 | 1.08835905 |
| A1 | 111.88991913 |
| A2 | 138.95182348 |
| A3 | 106.30768723 |
| A4 | 103.53883411 |
| A5 | 109.73275924 |
| A6 | 77.62401049 |
| A7 | 91.15283378 |
| A8 | 109.63517539 |
| A9 | 109.88269228 |
| A10 | 110.39202284 |

| | |
|-----|---------------|
| A11 | 108.94103835 |
| A12 | 118.60327322 |
| A13 | 104.03648537 |
| A14 | 115.72136362 |
| A15 | 108.70461551 |
| A16 | 108.57754914 |
| A17 | 112.10101312 |
| A18 | 109.46492250 |
| A19 | 108.20292526 |
| A20 | 102.78595340 |
| A21 | 107.29128280 |
| A22 | 109.75145875 |
| A23 | 111.23376050 |
| A24 | 107.55495231 |
| A25 | 69.93050512 |
| D1 | 101.38891279 |
| D2 | 17.73649325 |
| D3 | 123.01717701 |
| D4 | 93.78809210 |
| D5 | 94.76092423 |
| D6 | 126.50630702 |
| D7 | 176.23490727 |
| D8 | -64.06667414 |
| D9 | 56.58135390 |
| D10 | 118.30925829 |
| D11 | 124.58816952 |
| D12 | 179.89091595 |
| D13 | 57.34317368 |
| D14 | 56.96251331 |
| D15 | 176.06997882 |
| D16 | -63.47468766 |
| D17 | -63.75198366 |
| D18 | -68.41260880 |
| D19 | 69.82063930 |
| D20 | -112.30689726 |
| D21 | 131.42236342 |
| D22 | -105.67348616 |
| D23 | 14.68929608 |
| D24 | 8.13720535 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|--------|--------|--------|---------|---------|---------|---------|---------|---------|--------|--------|
| 46.24 | 50.10 | 56.61 | 76.90 | 95.88 | 98.87 | 125.17 | 152.35 | 179.88 | 202.20 | 217.58 |
| 229.88 | 245.57 | 250.86 | 284.25 | 306.58 | 322.23 | 334.90 | 342.76 | 363.56 | 427.36 | |
| 510.02 | 555.42 | 563.09 | 587.73 | 687.32 | 850.17 | 878.51 | 893.83 | 898.88 | 902.56 | |
| 919.71 | 961.52 | 991.62 | 1056.08 | 1061.90 | 1098.41 | 1132.72 | 1138.87 | 1151.45 | | |

| | | | | | | | | |
|-------------------------------|---------|---------|-----------|-----------|-----------|---------|---------|---------|
| 1174.93 | 1179.51 | 1190.61 | 1216.20 | 1359.30 | 1371.17 | 1377.21 | 1401.20 | 1411.40 |
| 1424.99 | 1425.73 | 1432.41 | 1437.06 | 1462.95 | 1469.99 | 1484.65 | 1490.50 | 1495.87 |
| 1500.05 | 1607.85 | 1704.48 | 3056.99 | 3059.51 | 3071.95 | 3119.05 | 3126.94 | 3130.21 |
| 3143.91 | 3148.45 | 3151.70 | 3155.33 | 3168.28 | 3177.58 | 3210.21 | 3794.31 | |
| Rotational constants (B/GHZ): | | | 1.0778706 | 0.4825751 | 0.4350330 | | | |



TS4d

C

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 | 0 |
| O | 7 | B7 | 4 | A6 | 2 | D5 | 0 |
| O | 7 | B8 | 4 | A7 | 2 | D6 | 0 |
| H | 1 | B9 | 2 | A8 | 5 | D7 | 0 |
| H | 1 | B10 | 2 | A9 | 5 | D8 | 0 |
| H | 1 | B11 | 2 | A10 | 5 | D9 | 0 |
| O | 2 | B12 | 1 | A11 | 5 | D10 | 0 |
| C | 13 | B13 | 2 | A12 | 1 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 2 | D12 | 0 |
| C | 14 | B15 | 13 | A14 | 2 | D13 | 0 |
| H | 16 | B16 | 14 | A15 | 13 | D14 | 0 |
| H | 16 | B17 | 14 | A16 | 13 | D15 | 0 |
| H | 16 | B18 | 14 | A17 | 13 | D16 | 0 |
| O | 14 | B19 | 13 | A18 | 2 | D17 | 0 |
| O | 20 | B20 | 14 | A19 | 13 | D18 | 0 |
| H | 21 | B21 | 20 | A20 | 14 | D19 | 0 |
| C | 7 | B22 | 4 | A21 | 2 | D20 | 0 |
| H | 23 | B23 | 7 | A22 | 4 | D21 | 0 |
| H | 23 | B24 | 7 | A23 | 4 | D22 | 0 |
| H | 23 | B25 | 7 | A24 | 4 | D23 | 0 |
| H | 7 | B26 | 4 | A25 | 2 | D24 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51113226 |
| B2 | 1.09106878 |
| B3 | 2.27658486 |

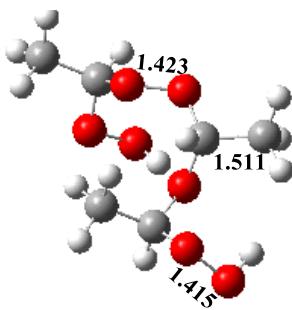
| | |
|-----|--------------|
| B4 | 1.40233705 |
| B5 | 1.13174835 |
| B6 | 2.08423609 |
| B7 | 2.17793278 |
| B8 | 1.26478990 |
| B9 | 1.08968353 |
| B10 | 1.08898223 |
| B11 | 1.08781630 |
| B12 | 1.40784866 |
| B13 | 1.41240667 |
| B14 | 1.08985931 |
| B15 | 1.51177144 |
| B16 | 1.08852348 |
| B17 | 1.08793894 |
| B18 | 1.08733343 |
| B19 | 1.40501003 |
| B20 | 1.41641966 |
| B21 | 0.96759122 |
| B22 | 1.47420366 |
| B23 | 1.09118828 |
| B24 | 1.08563478 |
| B25 | 1.08953256 |
| B26 | 1.08624902 |
| A1 | 111.63612894 |
| A2 | 141.95490742 |
| A3 | 106.14071454 |
| A4 | 93.95388048 |
| A5 | 132.15204701 |
| A6 | 68.05247230 |
| A7 | 91.20213651 |
| A8 | 109.17762042 |
| A9 | 109.59923202 |
| A10 | 110.55980123 |
| A11 | 110.39588466 |
| A12 | 117.79714561 |
| A13 | 104.06505743 |
| A14 | 115.61481159 |
| A15 | 108.97579474 |
| A16 | 108.63870620 |
| A17 | 112.33333223 |
| A18 | 109.52176804 |
| A19 | 108.08814577 |
| A20 | 102.86249331 |
| A21 | 110.66802606 |

| | |
|-----|---------------|
| A22 | 109.12435515 |
| A23 | 111.19523436 |
| A24 | 107.75276587 |
| A25 | 81.54746671 |
| D1 | 111.74224517 |
| D2 | 7.07506803 |
| D3 | 121.71009461 |
| D4 | 52.17605770 |
| D5 | 84.19564459 |
| D6 | 115.47119995 |
| D7 | 173.73856526 |
| D8 | -66.16895990 |
| D9 | 54.61408812 |
| D10 | 117.87262483 |
| D11 | 117.44944932 |
| D12 | -177.30987383 |
| D13 | 60.35047191 |
| D14 | 58.06845447 |
| D15 | 176.86817215 |
| D16 | -62.78615214 |
| D17 | -60.81570501 |
| D18 | -68.03420334 |
| D19 | 63.03925458 |
| D20 | -123.14457865 |
| D21 | 150.53793960 |
| D22 | -87.43396628 |
| D23 | 33.68050923 |
| D24 | -2.69392539 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 658.18 <i>i</i> | 34.26 | 53.14 | 67.91 | 91.27 | 100.51 | 116.33 | 142.82 | 183.09 | 203.80 | 234.78 |
| 246.53 | 271.59 | 295.63 | 303.11 | 318.58 | 349.06 | 356.13 | 399.91 | 454.44 | 481.10 | |
| 520.59 | 546.07 | 571.12 | 595.63 | 694.41 | 853.80 | 889.06 | 898.99 | 914.10 | 934.14 | |
| 966.75 | 993.98 | 1003.37 | 1054.82 | 1089.70 | 1108.44 | 1139.34 | 1148.39 | 1174.69 | | |
| 1188.52 | 1190.54 | 1200.18 | 1222.32 | 1362.93 | 1370.67 | 1372.81 | 1404.02 | 1416.11 | | |
| 1420.49 | 1431.78 | 1439.54 | 1447.59 | 1457.11 | 1470.61 | 1481.12 | 1493.25 | 1496.95 | | |
| 1503.39 | 1523.09 | 1628.03 | 1877.96 | 3060.64 | 3065.30 | 3080.68 | 3128.24 | 3134.71 | | |
| 3135.09 | 3140.36 | 3154.80 | 3161.93 | 3171.42 | 3172.85 | 3207.05 | 3772.62 | | | |

Rotational constants (B/GHZ): 1.4526259 0.4180410 0.3586741



P4d

C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| C | 1 | B1 | | | | |
| H | 2 | B2 | 1 | A1 | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 0 |
| H | 5 | B5 | 2 | A4 | 1 | D3 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 0 |
| O | 7 | B7 | 4 | A6 | 2 | D5 0 |
| O | 7 | B8 | 4 | A7 | 2 | D6 0 |
| H | 1 | B9 | 2 | A8 | 5 | D7 0 |
| H | 1 | B10 | 2 | A9 | 5 | D8 0 |
| H | 1 | B11 | 2 | A10 | 5 | D9 0 |
| O | 2 | B12 | 1 | A11 | 5 | D10 0 |
| C | 13 | B13 | 2 | A12 | 1 | D11 0 |
| H | 14 | B14 | 13 | A13 | 2 | D12 0 |
| C | 14 | B15 | 13 | A14 | 2 | D13 0 |
| H | 16 | B16 | 14 | A15 | 13 | D14 0 |
| H | 16 | B17 | 14 | A16 | 13 | D15 0 |
| H | 16 | B18 | 14 | A17 | 13 | D16 0 |
| O | 14 | B19 | 13 | A18 | 2 | D17 0 |
| O | 20 | B20 | 14 | A19 | 13 | D18 0 |
| H | 21 | B21 | 20 | A20 | 14 | D19 0 |
| C | 7 | B22 | 4 | A21 | 2 | D20 0 |
| H | 23 | B23 | 7 | A22 | 4 | D21 0 |
| H | 23 | B24 | 7 | A23 | 4 | D22 0 |
| H | 23 | B25 | 7 | A24 | 4 | D23 0 |
| H | 7 | B26 | 4 | A25 | 2 | D24 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51094944 |
| B2 | 1.09015830 |
| B3 | 2.27654943 |
| B4 | 1.39738897 |
| B5 | 2.54668381 |
| B6 | 1.41228959 |
| B7 | 2.30392621 |

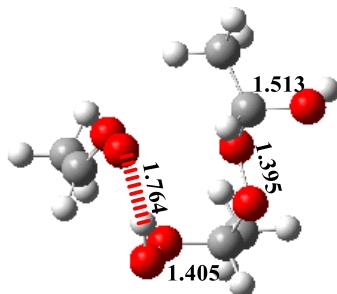
| | |
|-----|--------------|
| B8 | 1.39719820 |
| B9 | 1.08950085 |
| B10 | 1.08899092 |
| B11 | 1.08733998 |
| B12 | 1.41604970 |
| B13 | 1.41912046 |
| B14 | 1.08996381 |
| B15 | 1.51061946 |
| B16 | 1.08705922 |
| B17 | 1.08785878 |
| B18 | 1.08732663 |
| B19 | 1.40062225 |
| B20 | 1.41525997 |
| B21 | 0.96692423 |
| B22 | 1.51145596 |
| B23 | 1.08649179 |
| B24 | 1.08925210 |
| B25 | 1.08660228 |
| B26 | 1.09053277 |
| A1 | 111.76271615 |
| A2 | 141.07524901 |
| A3 | 106.04710991 |
| A4 | 80.88701993 |
| A5 | 126.64552408 |
| A6 | 106.65300592 |
| A7 | 112.60661551 |
| A8 | 109.22702497 |
| A9 | 109.76470852 |
| A10 | 110.37936152 |
| A11 | 109.89697371 |
| A12 | 117.97222871 |
| A13 | 103.93309889 |
| A14 | 115.32744007 |
| A15 | 108.59286405 |
| A16 | 108.51369423 |
| A17 | 112.24104066 |
| A18 | 109.27287591 |
| A19 | 108.28282811 |
| A20 | 102.97433461 |
| A21 | 105.24732763 |
| A22 | 109.32522277 |
| A23 | 109.74420507 |
| A24 | 109.85553198 |
| A25 | 108.93765872 |

| | |
|-----|---------------|
| D1 | 106.29855659 |
| D2 | 13.10482566 |
| D3 | 108.64749281 |
| D4 | 91.71323222 |
| D5 | 7.07985745 |
| D6 | 44.10716519 |
| D7 | 174.98865182 |
| D8 | -64.79816109 |
| D9 | 55.79812871 |
| D10 | 118.14925333 |
| D11 | 118.57633844 |
| D12 | -178.98341258 |
| D13 | 58.66364651 |
| D14 | 55.14080836 |
| D15 | 174.45668484 |
| D16 | -65.38053141 |
| D17 | -62.41151261 |
| D18 | -69.46737861 |
| D19 | 69.92706513 |
| D20 | 160.22718749 |
| D21 | 179.51000388 |
| D22 | -61.01317969 |
| D23 | 58.91156449 |
| D24 | -77.06902110 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 51.54 | 58.85 | 77.21 | 107.58 | 122.34 | 156.01 | 175.18 | 192.17 | 212.40 | 221.95 | 244.44 |
| 283.87 | 297.75 | 318.23 | 332.10 | 355.46 | 360.60 | 427.50 | 441.82 | 500.85 | 529.92 | |
| 571.69 | 584.68 | 610.26 | 636.21 | 696.37 | 852.43 | 893.01 | 904.24 | 918.44 | 937.49 | |
| 969.12 | 1057.25 | 1059.03 | 1066.99 | 1098.69 | 1120.87 | 1137.89 | 1151.68 | 1163.47 | | |
| 1178.74 | 1191.97 | 1203.33 | 1234.61 | 1359.86 | 1365.73 | 1369.53 | 1392.65 | 1405.65 | | |
| 1416.24 | 1419.73 | 1425.14 | 1436.79 | 1443.90 | 1486.34 | 1490.24 | 1492.75 | 1496.06 | | |
| 1498.24 | 1501.99 | 1511.04 | 3060.09 | 3070.00 | 3086.39 | 3124.23 | 3125.44 | 3133.10 | | |
| 3144.02 | 3152.30 | 3154.25 | 3165.66 | 3166.24 | 3185.01 | 3685.28 | 3790.98 | | | |

Rotational constants (B/GHZ): 1.2530048 0.5100976 0.4622789



IM4e

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 1 | B1 | | | | | |
| O | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 | 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 | 0 |
| C | 4 | B5 | 1 | A4 | 3 | D3 | 0 |
| O | 6 | B6 | 4 | A5 | 1 | D4 | 0 |
| O | 6 | B7 | 4 | A6 | 1 | D5 | 0 |
| C | 1 | B8 | 4 | A7 | 3 | D6 | 0 |
| H | 9 | B9 | 1 | A8 | 4 | D7 | 0 |
| H | 9 | B10 | 1 | A9 | 4 | D8 | 0 |
| H | 9 | B11 | 1 | A10 | 4 | D9 | 0 |
| O | 1 | B12 | 4 | A11 | 3 | D10 | 0 |
| C | 13 | B13 | 1 | A12 | 4 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 1 | D12 | 0 |
| C | 6 | B15 | 4 | A14 | 1 | D13 | 0 |
| H | 16 | B16 | 6 | A15 | 4 | D14 | 0 |
| H | 16 | B17 | 6 | A16 | 4 | D15 | 0 |
| H | 16 | B18 | 6 | A17 | 4 | D16 | 0 |
| H | 6 | B19 | 4 | A18 | 1 | D17 | 0 |
| O | 14 | B20 | 13 | A19 | 1 | D18 | 0 |
| C | 14 | B21 | 13 | A20 | 1 | D19 | 0 |
| H | 22 | B22 | 14 | A21 | 13 | D20 | 0 |
| H | 22 | B23 | 14 | A22 | 13 | D21 | 0 |
| H | 22 | B24 | 14 | A23 | 13 | D22 | 0 |
| O | 14 | B25 | 13 | A24 | 1 | D23 | 0 |
| H | 26 | B26 | 14 | A25 | 13 | D24 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.09220970 |
| B2 | 2.29522842 |
| B3 | 1.40492767 |
| B4 | 0.98968048 |
| B5 | 2.60386804 |
| B6 | 2.24239191 |
| B7 | 1.23643026 |
| B8 | 1.51267906 |
| B9 | 1.08755216 |
| B10 | 1.08765307 |
| B11 | 1.08749088 |
| B12 | 1.39238998 |
| B13 | 2.26405152 |
| B14 | 1.08780154 |
| B15 | 1.47358870 |
| B16 | 1.09175590 |
| B17 | 1.09062372 |

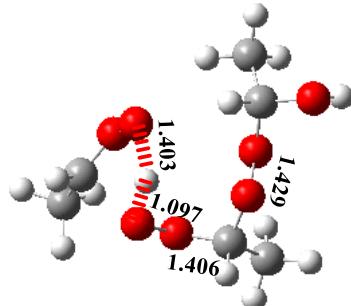
| | |
|-----|--------------|
| B18 | 1.08596931 |
| B19 | 1.08739056 |
| B20 | 1.41289320 |
| B21 | 1.51261133 |
| B22 | 1.08756319 |
| B23 | 1.09198260 |
| B24 | 1.08590923 |
| B25 | 1.39458926 |
| B26 | 0.96144134 |
| A1 | 84.80415733 |
| A2 | 35.79607281 |
| A3 | 100.70188354 |
| A4 | 138.46932268 |
| A5 | 78.38797973 |
| A6 | 91.02059383 |
| A7 | 106.13661164 |
| A8 | 109.75126776 |
| A9 | 110.22653164 |
| A10 | 109.08141611 |
| A11 | 112.45242789 |
| A12 | 143.17951957 |
| A13 | 82.72109841 |
| A14 | 106.34304468 |
| A15 | 107.64947562 |
| A16 | 109.85753602 |
| A17 | 110.99531500 |
| A18 | 71.58198198 |
| A19 | 37.45795410 |
| A20 | 141.75176202 |
| A21 | 108.63260471 |
| A22 | 110.13101323 |
| A23 | 110.39435097 |
| A24 | 94.52819455 |
| A25 | 108.59816838 |
| D1 | 133.29298164 |
| D2 | -94.01674098 |
| D3 | 110.84337941 |
| D4 | -68.24642324 |
| D5 | -37.30557012 |
| D6 | 171.89735998 |
| D7 | -64.47075845 |
| D8 | 56.30053450 |
| D9 | 175.68729752 |
| D10 | -62.51185308 |

| | |
|-----|---------------|
| D11 | -53.01133099 |
| D12 | 109.15363614 |
| D13 | 83.63928741 |
| D14 | 19.68054073 |
| D15 | 136.47363364 |
| D16 | -100.95991226 |
| D17 | -156.09248675 |
| D18 | -24.89949059 |
| D19 | -7.52021913 |
| D20 | 173.72722224 |
| D21 | -67.15204267 |
| D22 | 53.93885205 |
| D23 | -144.58242849 |
| D24 | 97.63127663 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 39.92 | 44.71 | 64.48 | 86.35 | 103.00 | 109.50 | 134.31 | 145.57 | 159.46 | 185.56 | 213.79 |
| 227.63 | 246.56 | 261.29 | 288.25 | 306.93 | 326.54 | 353.49 | 364.48 | 398.51 | 418.50 | |
| 535.81 | 567.10 | 573.87 | 586.58 | 695.12 | 779.21 | 878.66 | 890.36 | 907.02 | 909.86 | |
| 943.81 | 952.88 | 995.63 | 1014.45 | 1060.92 | 1091.25 | 1120.88 | 1133.85 | 1141.58 | | |
| 1165.51 | 1179.72 | 1183.03 | 1216.26 | 1312.53 | 1353.84 | 1377.60 | 1380.26 | 1398.46 | | |
| 1408.99 | 1419.00 | 1429.73 | 1437.59 | 1466.76 | 1467.73 | 1487.03 | 1489.41 | 1494.97 | | |
| 1502.73 | 1572.51 | 1701.18 | 3054.81 | 3063.12 | 3069.32 | 3110.08 | 3118.40 | 3138.93 | | |
| 3152.00 | 3156.53 | 3165.05 | 3174.40 | 3182.76 | 3202.08 | 3328.47 | 3882.56 | | | |

Rotational constants (B/GHZ): 0.8894646 0.6295060 0.4899185



TS4e

| C | | B1 | | A1 | | | |
|---|---|-----|---|----|---|----|---|
| H | 1 | | | | | | |
| O | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 | 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 | 0 |
| C | 3 | B5 | 1 | A4 | 4 | D3 | 0 |
| O | 6 | B6 | 3 | A5 | 1 | D4 | 0 |
| O | 6 | B7 | 3 | A6 | 1 | D5 | 0 |
| C | 1 | B8 | 4 | A7 | 3 | D6 | 0 |
| H | 9 | B9 | 1 | A8 | 4 | D7 | 0 |
| H | 9 | B10 | 1 | A9 | 4 | D8 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 9 | B11 | 1 | A10 | 4 | D9 | 0 |
| O | 1 | B12 | 4 | A11 | 3 | D10 | 0 |
| C | 13 | B13 | 1 | A12 | 4 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 1 | D12 | 0 |
| C | 6 | B15 | 3 | A14 | 1 | D13 | 0 |
| H | 16 | B16 | 6 | A15 | 3 | D14 | 0 |
| H | 16 | B17 | 6 | A16 | 3 | D15 | 0 |
| H | 16 | B18 | 6 | A17 | 3 | D16 | 0 |
| H | 6 | B19 | 3 | A18 | 1 | D17 | 0 |
| O | 14 | B20 | 13 | A19 | 1 | D18 | 0 |
| C | 14 | B21 | 13 | A20 | 1 | D19 | 0 |
| H | 22 | B22 | 14 | A21 | 13 | D20 | 0 |
| H | 22 | B23 | 14 | A22 | 13 | D21 | 0 |
| H | 22 | B24 | 14 | A23 | 13 | D22 | 0 |
| O | 14 | B25 | 13 | A24 | 1 | D23 | 0 |
| H | 26 | B26 | 14 | A25 | 13 | D24 | 0 |

Variables:

| | |
|-----|-------------|
| B1 | 1.09287817 |
| B2 | 2.28984621 |
| B3 | 1.40557360 |
| B4 | 1.09706182 |
| B5 | 2.03945879 |
| B6 | 2.17472036 |
| B7 | 1.26620599 |
| B8 | 1.51188526 |
| B9 | 1.08752614 |
| B10 | 1.08679533 |
| B11 | 1.08759252 |
| B12 | 1.39467985 |
| B13 | 2.27531668 |
| B14 | 1.08693985 |
| B15 | 1.47569140 |
| B16 | 1.08894021 |
| B17 | 1.09114703 |
| B18 | 1.08548074 |
| B19 | 1.08522402 |
| B20 | 1.41011336 |
| B21 | 1.51234598 |
| B22 | 1.08764745 |
| B23 | 1.09183501 |
| B24 | 1.08729959 |
| B25 | 1.39587460 |
| B26 | 0.96135497 |
| A1 | 85.78814742 |

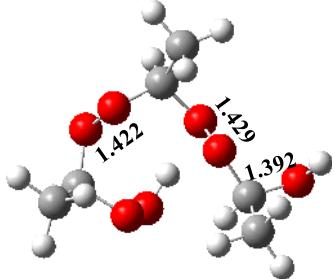
| | |
|-----|---------------|
| A2 | 35.83488413 |
| A3 | 93.25440023 |
| A4 | 130.66482395 |
| A5 | 69.73718130 |
| A6 | 93.18145956 |
| A7 | 105.91197458 |
| A8 | 109.75788025 |
| A9 | 110.10829823 |
| A10 | 108.89311895 |
| A11 | 111.94457018 |
| A12 | 142.25882840 |
| A13 | 80.47355313 |
| A14 | 108.67338487 |
| A15 | 108.19714714 |
| A16 | 109.13172173 |
| A17 | 110.61292724 |
| A18 | 83.45229567 |
| A19 | 37.02660812 |
| A20 | 139.24754252 |
| A21 | 109.03075853 |
| A22 | 110.26547268 |
| A23 | 109.63113971 |
| A24 | 98.43684239 |
| A25 | 108.51228439 |
| D1 | 132.48197594 |
| D2 | -110.57073829 |
| D3 | -37.65025627 |
| D4 | -79.42378884 |
| D5 | -48.40421172 |
| D6 | 173.36292452 |
| D7 | -66.01404221 |
| D8 | 54.53530879 |
| D9 | 174.17923200 |
| D10 | -61.40562578 |
| D11 | -51.77350181 |
| D12 | 118.01818308 |
| D13 | 73.09059040 |
| D14 | 35.64322942 |
| D15 | 153.16928567 |
| D16 | -84.99802503 |
| D17 | -165.72255577 |
| D18 | -21.91971176 |
| D19 | 5.66370608 |
| D20 | 166.79290348 |

D21 -73.65364693
 D22 46.83753809
 D23 -136.53357630
 D24 99.05969059

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 489.06 <i>i</i> | 40.44 | 59.52 | 75.62 | 87.92 | 107.34 | 117.83 | 135.76 | 162.56 | 198.51 | 221.59 |
| 232.93 | 250.26 | 291.33 | 323.63 | 336.67 | 359.75 | 388.50 | 397.95 | 434.76 | 535.10 | |
| 541.59 | 562.83 | 578.34 | 589.35 | 701.28 | 885.68 | 895.65 | 904.67 | 939.83 | 952.53 | |
| 970.13 | 1005.56 | 1015.37 | 1030.64 | 1090.97 | 1122.61 | 1131.64 | 1139.28 | 1165.45 | | |
| 1176.71 | 1184.40 | 1213.08 | 1250.71 | 1312.30 | 1354.10 | 1358.59 | 1379.70 | 1395.35 | | |
| 1411.60 | 1418.77 | 1424.46 | 1441.80 | 1453.64 | 1476.96 | 1489.37 | 1490.48 | 1496.87 | | |
| 1501.40 | 1583.38 | 1620.74 | 1932.60 | 3059.40 | 3065.43 | 3082.76 | 3107.42 | 3137.78 | | |
| 3144.80 | 3165.00 | 3165.41 | 3171.25 | 3175.56 | 3181.77 | 3208.82 | 3881.16 | | | |

Rotational constants (B/GHZ): 1.0432275 0.5769855 0.4340642



P4e

| C | | B1 | | | | | |
|---|----|----|-----|----|-----|---|-------|
| H | 1 | | B1 | | | | |
| O | 1 | | B2 | 2 | A1 | | |
| O | 1 | | B3 | 3 | A2 | 2 | D1 0 |
| H | 3 | | B4 | 1 | A3 | 4 | D2 0 |
| C | 3 | | B5 | 1 | A4 | 4 | D3 0 |
| O | 6 | | B6 | 3 | A5 | 1 | D4 0 |
| O | 6 | | B7 | 3 | A6 | 1 | D5 0 |
| C | 1 | | B8 | 4 | A7 | 3 | D6 0 |
| H | 9 | | B9 | 1 | A8 | 4 | D7 0 |
| H | 9 | | B10 | 1 | A9 | 4 | D8 0 |
| H | 9 | | B11 | 1 | A10 | 4 | D9 0 |
| O | 1 | | B12 | 4 | A11 | 3 | D10 0 |
| C | 13 | | B13 | 1 | A12 | 4 | D11 0 |
| H | 14 | | B14 | 13 | A13 | 1 | D12 0 |
| C | 6 | | B15 | 3 | A14 | 1 | D13 0 |
| H | 16 | | B16 | 6 | A15 | 3 | D14 0 |
| H | 16 | | B17 | 6 | A16 | 3 | D15 0 |
| H | 16 | | B18 | 6 | A17 | 3 | D16 0 |
| H | 6 | | B19 | 3 | A18 | 1 | D17 0 |
| O | 14 | | B20 | 13 | A19 | 1 | D18 0 |
| C | 14 | | B21 | 13 | A20 | 1 | D19 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 22 | B22 | 14 | A21 | 13 | D20 | 0 |
| H | 22 | B23 | 14 | A22 | 13 | D21 | 0 |
| H | 22 | B24 | 14 | A23 | 13 | D22 | 0 |
| O | 14 | B25 | 13 | A24 | 1 | D23 | 0 |
| H | 26 | B26 | 14 | A25 | 13 | D24 | 0 |

Variables:

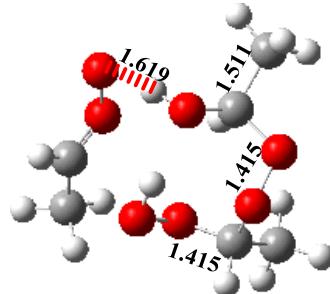
| | |
|-----|--------------|
| B1 | 1.09222826 |
| B2 | 2.27651153 |
| B3 | 1.39821153 |
| B4 | 2.58358522 |
| B5 | 1.40850208 |
| B6 | 2.27818159 |
| B7 | 1.39674139 |
| B8 | 1.51185906 |
| B9 | 1.08708121 |
| B10 | 1.08651710 |
| B11 | 1.08749742 |
| B12 | 1.40525614 |
| B13 | 2.29008779 |
| B14 | 1.08829230 |
| B15 | 1.50974902 |
| B16 | 1.08757006 |
| B17 | 1.08728053 |
| B18 | 1.08713004 |
| B19 | 1.09260914 |
| B20 | 1.41134882 |
| B21 | 1.51360235 |
| B22 | 1.08740044 |
| B23 | 1.09128742 |
| B24 | 1.08755477 |
| B25 | 1.39234294 |
| B26 | 0.96173596 |
| A1 | 81.51555155 |
| A2 | 36.54811300 |
| A3 | 73.08520154 |
| A4 | 124.02662811 |
| A5 | 93.38832111 |
| A6 | 112.00121963 |
| A7 | 106.39444339 |
| A8 | 109.36735568 |
| A9 | 110.32432812 |
| A10 | 109.09850615 |
| A11 | 112.49288735 |
| A12 | 141.80734940 |

| | |
|-----|---------------|
| A13 | 84.15830724 |
| A14 | 113.94244596 |
| A15 | 109.34093690 |
| A16 | 109.47031533 |
| A17 | 109.94902728 |
| A18 | 101.51441331 |
| A19 | 36.52675526 |
| A20 | 139.93761546 |
| A21 | 108.88744131 |
| A22 | 110.11495768 |
| A23 | 110.34682790 |
| A24 | 95.30311123 |
| A25 | 108.77755867 |
| D1 | 140.38445983 |
| D2 | -132.83480775 |
| D3 | -75.49781690 |
| D4 | -66.24791196 |
| D5 | -34.32472818 |
| D6 | 163.94405201 |
| D7 | -67.59865416 |
| D8 | 52.61630911 |
| D9 | 172.52545124 |
| D10 | -70.99255703 |
| D11 | -56.94674703 |
| D12 | 115.19566810 |
| D13 | 86.69489040 |
| D14 | 49.91622666 |
| D15 | 169.84382793 |
| D16 | -69.93059696 |
| D17 | -151.19334435 |
| D18 | -19.26833600 |
| D19 | -2.02393493 |
| D20 | 172.09428491 |
| D21 | -68.41730073 |
| D22 | 51.90940033 |
| D23 | -139.05182444 |
| D24 | 97.12413633 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 42.09 | 68.53 | 93.40 | 107.55 | 132.52 | 150.09 | 166.92 | 180.41 | 189.71 | 220.77 | 243.40 |
| 270.07 | 291.99 | 311.49 | 320.40 | 345.96 | 386.94 | 414.69 | 433.18 | 533.50 | 557.53 | |
| 578.06 | 587.16 | 593.24 | 692.01 | 700.93 | 877.34 | 890.18 | 909.80 | 932.85 | 940.13 | |
| 951.42 | 1009.12 | 1024.02 | 1060.61 | 1096.60 | 1133.22 | 1138.14 | 1142.74 | 1149.59 | | |
| 1157.83 | 1179.40 | 1203.40 | 1229.40 | 1316.79 | 1357.83 | 1359.68 | 1389.02 | 1394.15 | | |
| 1402.54 | 1416.11 | 1420.75 | 1426.22 | 1451.53 | 1467.46 | 1485.13 | 1486.12 | 1488.14 | | |

1497.03 1498.66 1504.01 3061.39 3076.06 3078.31 3112.92 3117.16 3136.27
 3160.30 3160.89 3163.48 3166.77 3169.19 3186.17 3753.02 3874.79
 Rotational constants (B/GHZ): 0.9826553 0.6317098 0.4974423



IM4f

| C | | B1 | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| O | 1 | B5 | 2 | A4 | 4 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| C | 6 | B7 | 1 | A6 | 2 | D5 | 0 |
| C | 8 | B8 | 6 | A7 | 1 | D6 | 0 |
| H | 9 | B9 | 8 | A8 | 6 | D7 | 0 |
| H | 9 | B10 | 8 | A9 | 6 | D8 | 0 |
| H | 9 | B11 | 8 | A10 | 6 | D9 | 0 |
| O | 8 | B12 | 6 | A11 | 1 | D10 | 0 |
| O | 8 | B13 | 6 | A12 | 1 | D11 | 0 |
| H | 8 | B14 | 6 | A13 | 1 | D12 | 0 |
| H | 1 | B15 | 6 | A14 | 2 | D13 | 0 |
| O | 1 | B16 | 6 | A15 | 2 | D14 | 0 |
| O | 17 | B17 | 1 | A16 | 6 | D15 | 0 |
| C | 18 | B18 | 17 | A17 | 1 | D16 | 0 |
| H | 19 | B19 | 18 | A18 | 17 | D17 | 0 |
| C | 19 | B20 | 18 | A19 | 17 | D18 | 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 | 0 |
| H | 21 | B22 | 19 | A21 | 18 | D20 | 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 | 0 |
| O | 19 | B24 | 18 | A23 | 17 | D22 | 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51142735 |
| B2 | 1.08902462 |
| B3 | 1.08806894 |
| B4 | 1.08903414 |

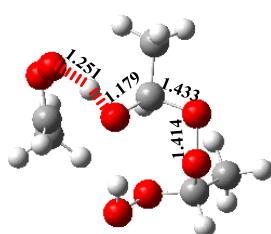
| | |
|-----|--------------|
| B5 | 1.39157906 |
| B6 | 0.99932699 |
| B7 | 3.63082891 |
| B8 | 1.47165878 |
| B9 | 1.08541214 |
| B10 | 1.08953440 |
| B11 | 1.09204001 |
| B12 | 2.23559074 |
| B13 | 1.23714932 |
| B14 | 1.08665629 |
| B15 | 1.09617765 |
| B16 | 1.42586452 |
| B17 | 1.41487055 |
| B18 | 1.39574176 |
| B19 | 1.09301048 |
| B20 | 1.50855606 |
| B21 | 1.08757429 |
| B22 | 1.08718741 |
| B23 | 1.08736669 |
| B24 | 1.41519190 |
| B25 | 1.41829273 |
| B26 | 0.98625205 |
| A1 | 108.51579916 |
| A2 | 109.20006379 |
| A3 | 110.81700105 |
| A4 | 112.79616090 |
| A5 | 106.28892428 |
| A6 | 100.58445595 |
| A7 | 130.53689279 |
| A8 | 110.89301447 |
| A9 | 108.16262133 |
| A10 | 108.80824986 |
| A11 | 45.40064927 |
| A12 | 55.07362937 |
| A13 | 84.67564192 |
| A14 | 109.54434259 |
| A15 | 109.90201139 |
| A16 | 112.39555480 |
| A17 | 112.97288203 |
| A18 | 102.11736495 |
| A19 | 115.19437005 |
| A20 | 109.68120044 |
| A21 | 110.60862035 |
| A22 | 108.95371781 |

| | |
|-----|---------------|
| A23 | 111.03437554 |
| A24 | 108.02178903 |
| A25 | 100.63840339 |
| D1 | 119.29107274 |
| D2 | -119.78178423 |
| D3 | 55.88095261 |
| D4 | 82.63220104 |
| D5 | 127.93721337 |
| D6 | 48.01327880 |
| D7 | -61.27863246 |
| D8 | 59.64803091 |
| D9 | 176.96640049 |
| D10 | -96.66967907 |
| D11 | -53.48852664 |
| D12 | 178.42627704 |
| D13 | -124.04732900 |
| D14 | 115.99935918 |
| D15 | 41.15508527 |
| D16 | 77.60846712 |
| D17 | 165.96188924 |
| D18 | 42.86467920 |
| D19 | 170.91543307 |
| D20 | -68.41380216 |
| D21 | 51.08170309 |
| D22 | -78.26159118 |
| D23 | -55.63033381 |
| D24 | 72.36844891 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 46.64 | 58.48 | 75.27 | 111.99 | 128.59 | 132.86 | 155.21 | 179.66 | 189.75 | 200.58 | 232.47 |
| 242.90 | 265.60 | 281.77 | 285.45 | 330.10 | 333.95 | 340.15 | 409.07 | 432.80 | 519.62 | |
| 561.97 | 579.23 | 615.67 | 718.30 | 740.14 | 851.70 | 885.17 | 886.67 | 895.66 | 920.56 | |
| 944.67 | 987.72 | 1017.42 | 1036.55 | 1055.32 | 1110.40 | 1120.95 | 1131.33 | 1153.68 | | |
| 1158.30 | 1182.71 | 1194.11 | 1217.91 | 1356.87 | 1368.33 | 1370.48 | 1394.52 | 1406.34 | | |
| 1421.74 | 1425.38 | 1430.64 | 1462.18 | 1468.44 | 1473.89 | 1486.93 | 1487.48 | 1492.13 | | |
| 1514.43 | 1562.63 | 1699.11 | 3043.35 | 3060.48 | 3060.98 | 3070.94 | 3075.28 | 3098.86 | | |
| 3130.07 | 3142.56 | 3154.30 | 3156.83 | 3163.14 | 3183.95 | 3218.16 | 3446.80 | | | |

Rotational constants (B/GHZ): 0.9429473 0.6563090 0.4629794



TS4f

| C | | B1 | | | | |
|---|----|-----|----|-----|----|-----|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 |
| H | 2 | B4 | 1 | A3 | 4 | D2 |
| O | 1 | B5 | 2 | A4 | 5 | D3 |
| H | 6 | B6 | 1 | A5 | 2 | D4 |
| C | 6 | B7 | 1 | A6 | 2 | D5 |
| C | 8 | B8 | 6 | A7 | 1 | D6 |
| H | 9 | B9 | 8 | A8 | 6 | D7 |
| H | 9 | B10 | 8 | A9 | 6 | D8 |
| H | 9 | B11 | 8 | A10 | 6 | D9 |
| O | 8 | B12 | 6 | A11 | 1 | D10 |
| O | 8 | B13 | 6 | A12 | 1 | D11 |
| H | 8 | B14 | 6 | A13 | 1 | D12 |
| H | 1 | B15 | 6 | A14 | 8 | D13 |
| O | 1 | B16 | 6 | A15 | 8 | D14 |
| O | 17 | B17 | 1 | A16 | 6 | D15 |
| C | 18 | B18 | 17 | A17 | 1 | D16 |
| H | 19 | B19 | 18 | A18 | 17 | D17 |
| C | 19 | B20 | 18 | A19 | 17 | D18 |
| H | 21 | B21 | 19 | A20 | 18 | D19 |
| H | 21 | B22 | 19 | A21 | 18 | D20 |
| H | 21 | B23 | 19 | A22 | 18 | D21 |
| O | 19 | B24 | 18 | A23 | 17 | D22 |
| O | 25 | B25 | 19 | A24 | 18 | D23 |
| H | 26 | B26 | 25 | A25 | 19 | D24 |

Variables:

| | |
|-----|------------|
| B1 | 1.51365507 |
| B2 | 1.08893647 |
| B3 | 1.08896139 |
| B4 | 1.08838192 |
| B5 | 1.38264951 |
| B6 | 1.17902118 |
| B7 | 2.12575719 |
| B8 | 1.46990104 |
| B9 | 1.08618478 |
| B10 | 1.09244701 |
| B11 | 1.09108271 |
| B12 | 2.18394190 |
| B13 | 1.26772206 |
| B14 | 1.08355815 |
| B15 | 1.09765692 |
| B16 | 1.43252556 |

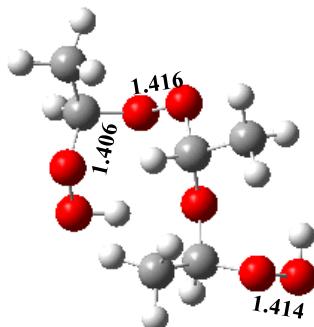
| | |
|-----|--------------|
| B17 | 1.41412955 |
| B18 | 1.40065094 |
| B19 | 1.09262656 |
| B20 | 1.50801058 |
| B21 | 1.08733642 |
| B22 | 1.08729733 |
| B23 | 1.08736733 |
| B24 | 1.41152028 |
| B25 | 1.41701412 |
| B26 | 0.97706823 |
| A1 | 109.73065520 |
| A2 | 109.45946259 |
| A3 | 110.14338221 |
| A4 | 113.87010037 |
| A5 | 114.58950205 |
| A6 | 113.94533734 |
| A7 | 113.13789462 |
| A8 | 111.19291612 |
| A9 | 107.74688520 |
| A10 | 108.89562246 |
| A11 | 66.46636284 |
| A12 | 90.90422750 |
| A13 | 79.44991169 |
| A14 | 109.13746509 |
| A15 | 111.11071122 |
| A16 | 112.34644084 |
| A17 | 113.01384575 |
| A18 | 102.05854810 |
| A19 | 115.13675530 |
| A20 | 109.51387763 |
| A21 | 110.77664955 |
| A22 | 108.99627783 |
| A23 | 110.79277701 |
| A24 | 107.99136507 |
| A25 | 100.47296530 |
| D1 | 119.55298877 |
| D2 | 120.11613669 |
| D3 | 175.09356044 |
| D4 | 8.82743511 |
| D5 | 88.83082728 |
| D6 | 44.53147236 |
| D7 | -95.62919195 |
| D8 | 26.19989302 |
| D9 | 141.99904098 |

| | |
|-----|---------------|
| D10 | -107.21991061 |
| D11 | -77.36344476 |
| D12 | 164.45529515 |
| D13 | -35.52151663 |
| D14 | -154.30952033 |
| D15 | 40.04359979 |
| D16 | 76.59132876 |
| D17 | 165.01345565 |
| D18 | 42.10947386 |
| D19 | 171.15938536 |
| D20 | -68.28513438 |
| D21 | 51.24615609 |
| D22 | -79.39084813 |
| D23 | -57.60381880 |
| D24 | 69.74750755 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 995.34 <i>i</i> | 33.90 | 71.61 | 78.57 | 128.47 | 132.22 | 149.54 | 155.72 | 174.59 | 192.72 | 227.03 |
| 260.11 | 260.30 | 290.14 | 318.24 | 321.19 | 370.28 | 382.64 | 434.49 | 492.09 | 509.78 | |
| 563.99 | 586.63 | 608.79 | 630.80 | 728.83 | 761.41 | 850.33 | 881.16 | 890.60 | 923.53 | |
| 934.88 | 976.35 | 1006.11 | 1019.45 | 1056.55 | 1113.25 | 1122.71 | 1136.68 | 1150.27 | | |
| 1164.77 | 1188.48 | 1198.36 | 1229.54 | 1351.18 | 1363.21 | 1385.37 | 1398.71 | 1415.23 | | |
| 1417.05 | 1425.46 | 1431.88 | 1449.39 | 1464.00 | 1481.18 | 1486.44 | 1491.97 | 1497.30 | | |
| 1505.45 | 1547.62 | 1608.30 | 1801.72 | 3039.05 | 3055.49 | 3062.43 | 3078.44 | 3113.02 | | |
| 3122.62 | 3146.08 | 3151.87 | 3159.32 | 3167.40 | 3169.86 | 3223.17 | 3620.99 | | | |

Rotational constants (B/GHZ): 1.1699816 0.5715202 0.4631327



P4f

| C | 1 | B1 | | | | |
|---|---|----|---|----|---|----|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 |
| H | 2 | B4 | 1 | A3 | 4 | D2 |
| O | 1 | B5 | 2 | A4 | 3 | D3 |
| H | 6 | B6 | 1 | A5 | 2 | D4 |
| C | 6 | B7 | 1 | A6 | 2 | D5 |
| C | 8 | B8 | 6 | A7 | 1 | D6 |
| | | | | | | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 9 | B9 | 8 | A8 | 6 | D7 | 0 |
| H | 9 | B10 | 8 | A9 | 6 | D8 | 0 |
| H | 9 | B11 | 8 | A10 | 6 | D9 | 0 |
| O | 8 | B12 | 6 | A11 | 1 | D10 | 0 |
| O | 8 | B13 | 6 | A12 | 1 | D11 | 0 |
| H | 8 | B14 | 6 | A13 | 1 | D12 | 0 |
| H | 1 | B15 | 6 | A14 | 8 | D13 | 0 |
| O | 1 | B16 | 6 | A15 | 8 | D14 | 0 |
| O | 17 | B17 | 1 | A16 | 6 | D15 | 0 |
| C | 18 | B18 | 17 | A17 | 1 | D16 | 0 |
| H | 19 | B19 | 18 | A18 | 17 | D17 | 0 |
| C | 19 | B20 | 18 | A19 | 17 | D18 | 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 | 0 |
| H | 21 | B22 | 19 | A21 | 18 | D20 | 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 | 0 |
| O | 19 | B24 | 18 | A23 | 17 | D22 | 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.51209329 |
| B2 | 1.08702362 |
| B3 | 1.08936431 |
| B4 | 1.08860446 |
| B5 | 1.41079284 |
| B6 | 2.40152825 |
| B7 | 1.41516231 |
| B8 | 1.51326773 |
| B9 | 1.08913324 |
| B10 | 1.08876286 |
| B11 | 1.08708082 |
| B12 | 2.28041386 |
| B13 | 1.40185680 |
| B14 | 1.09078294 |
| B15 | 1.09085298 |
| B16 | 1.41180654 |
| B17 | 1.41601692 |
| B18 | 1.40671252 |
| B19 | 1.09268617 |
| B20 | 1.50796295 |
| B21 | 1.08711592 |
| B22 | 1.08746755 |
| B23 | 1.08745735 |
| B24 | 1.40616304 |
| B25 | 1.41555893 |

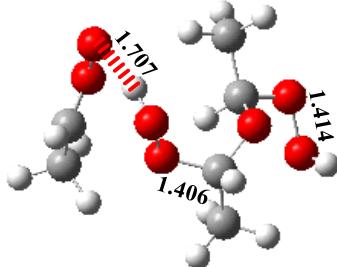
| | |
|-----|---------------|
| B26 | 0.97244740 |
| A1 | 110.12699829 |
| A2 | 109.54181221 |
| A3 | 109.59387595 |
| A4 | 113.93573669 |
| A5 | 113.08703645 |
| A6 | 118.08306445 |
| A7 | 115.68186609 |
| A8 | 111.30620261 |
| A9 | 109.76804649 |
| A10 | 108.47783422 |
| A11 | 92.93225597 |
| A12 | 110.25670321 |
| A13 | 103.95229737 |
| A14 | 108.98840206 |
| A15 | 107.69508869 |
| A16 | 112.79307307 |
| A17 | 112.86930290 |
| A18 | 101.82889840 |
| A19 | 114.95355349 |
| A20 | 109.32013123 |
| A21 | 111.00989883 |
| A22 | 109.09627925 |
| A23 | 110.49975008 |
| A24 | 107.85556957 |
| A25 | 101.43617805 |
| D1 | 120.15427817 |
| D2 | 119.42683613 |
| D3 | -65.65157791 |
| D4 | -12.74369651 |
| D5 | 73.28305853 |
| D6 | 40.38429918 |
| D7 | -72.65656306 |
| D8 | 49.02804660 |
| D9 | 168.41097603 |
| D10 | -112.81316013 |
| D11 | -80.34736991 |
| D12 | 163.32827421 |
| D13 | -52.37617768 |
| D14 | -171.63370871 |
| D15 | 47.61972724 |
| D16 | 74.85989322 |
| D17 | 164.51230186 |
| D18 | 41.93096863 |

| | |
|-----|--------------|
| D19 | 171.03441459 |
| D20 | -68.63997699 |
| D21 | 51.20616491 |
| D22 | -79.72665617 |
| D23 | -59.74850479 |
| D24 | 69.33987951 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 53.08 | 63.95 | 99.85 | 113.61 | 149.88 | 168.19 | 191.36 | 203.75 | 222.57 | 240.90 | 260.34 |
| 273.07 | 296.15 | 307.88 | 331.69 | 364.54 | 380.49 | 405.36 | 428.16 | 509.60 | 534.12 | |
| 568.88 | 588.88 | 598.83 | 690.09 | 728.85 | 841.79 | 861.93 | 902.19 | 914.12 | 936.07 | |
| 955.70 | 1021.13 | 1058.94 | 1064.19 | 1110.22 | 1135.26 | 1142.62 | 1146.95 | 1149.84 | | |
| 1182.21 | 1193.96 | 1206.25 | 1212.48 | 1362.03 | 1382.77 | 1390.85 | 1402.27 | 1419.54 | | |
| 1425.90 | 1429.31 | 1438.58 | 1449.75 | 1453.26 | 1485.97 | 1487.36 | 1490.25 | 1493.04 | | |
| 1502.05 | 1504.75 | 1511.54 | 3062.33 | 3064.11 | 3079.71 | 3112.62 | 3121.96 | 3128.35 | | |
| 3145.48 | 3148.78 | 3157.13 | 3161.22 | 3161.80 | 3167.27 | 3703.12 | 3785.57 | | | |

Rotational constants (B/GHZ): 1.3096654 0.5273363 0.4555924



IM4g

| C | | | B1 | | | | |
|---|----|--|-----|----|-----|----|-------|
| H | 1 | | | | | | |
| O | 1 | | B2 | 2 | A1 | | |
| O | 1 | | B3 | 3 | A2 | 2 | D1 0 |
| H | 3 | | B4 | 1 | A3 | 4 | D2 0 |
| C | 4 | | B5 | 1 | A4 | 3 | D3 0 |
| O | 6 | | B6 | 4 | A5 | 1 | D4 0 |
| O | 6 | | B7 | 4 | A6 | 1 | D5 0 |
| C | 1 | | B8 | 4 | A7 | 3 | D6 0 |
| H | 9 | | B9 | 1 | A8 | 4 | D7 0 |
| H | 9 | | B10 | 1 | A9 | 4 | D8 0 |
| H | 9 | | B11 | 1 | A10 | 4 | D9 0 |
| O | 1 | | B12 | 4 | A11 | 3 | D10 0 |
| C | 13 | | B13 | 1 | A12 | 4 | D11 0 |
| H | 14 | | B14 | 13 | A13 | 1 | D12 0 |
| C | 14 | | B15 | 13 | A14 | 1 | D13 0 |
| H | 16 | | B16 | 14 | A15 | 13 | D14 0 |
| H | 16 | | B17 | 14 | A16 | 13 | D15 0 |
| H | 16 | | B18 | 14 | A17 | 13 | D16 0 |
| O | 14 | | B19 | 13 | A18 | 1 | D17 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 20 | B20 | 14 | A19 | 13 | D18 | 0 |
| H | 21 | B21 | 20 | A20 | 14 | D19 | 0 |
| C | 6 | B22 | 4 | A21 | 1 | D20 | 0 |
| H | 23 | B23 | 6 | A22 | 4 | D21 | 0 |
| H | 23 | B24 | 6 | A23 | 4 | D22 | 0 |
| H | 23 | B25 | 6 | A24 | 4 | D23 | 0 |
| H | 6 | B26 | 4 | A25 | 1 | D24 | 0 |

Variables:

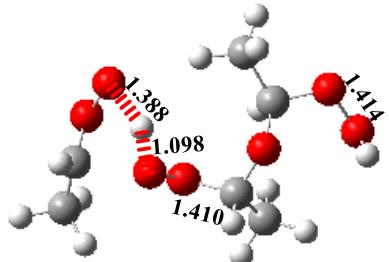
| | |
|-----|--------------|
| B1 | 1.08989225 |
| B2 | 2.29949457 |
| B3 | 1.40567969 |
| B4 | 0.99262132 |
| B5 | 2.59813611 |
| B6 | 2.23571782 |
| B7 | 1.23692891 |
| B8 | 1.51678502 |
| B9 | 1.08836639 |
| B10 | 1.08832020 |
| B11 | 1.08734580 |
| B12 | 1.40181228 |
| B13 | 1.40798287 |
| B14 | 1.09401405 |
| B15 | 1.50854856 |
| B16 | 1.08870052 |
| B17 | 1.08832000 |
| B18 | 1.08765414 |
| B19 | 1.40485863 |
| B20 | 1.41407393 |
| B21 | 0.96516271 |
| B22 | 1.47265702 |
| B23 | 1.08607334 |
| B24 | 1.09188493 |
| B25 | 1.09089266 |
| B26 | 1.08801455 |
| A1 | 80.61701396 |
| A2 | 35.88767647 |
| A3 | 118.61460704 |
| A4 | 151.10528177 |
| A5 | 79.65274847 |
| A6 | 90.50644153 |
| A7 | 105.48796101 |
| A8 | 109.24460208 |
| A9 | 111.70506268 |
| A10 | 109.40743818 |

| | |
|-----|---------------|
| A11 | 112.48098249 |
| A12 | 118.04986420 |
| A13 | 110.07398802 |
| A14 | 110.47563080 |
| A15 | 108.84796777 |
| A16 | 110.20108242 |
| A17 | 109.74513674 |
| A18 | 109.34341255 |
| A19 | 108.70507464 |
| A20 | 101.55028858 |
| A21 | 103.94932138 |
| A22 | 111.10089095 |
| A23 | 107.76094252 |
| A24 | 109.70541927 |
| A25 | 74.38022597 |
| D1 | 140.48415744 |
| D2 | -67.95223672 |
| D3 | 139.09194859 |
| D4 | -103.96836887 |
| D5 | -71.84875693 |
| D6 | 160.68689674 |
| D7 | -59.89457908 |
| D8 | 61.40228711 |
| D9 | -179.01705674 |
| D10 | -73.56617720 |
| D11 | -53.53552790 |
| D12 | -4.81315748 |
| D13 | 119.88252934 |
| D14 | 55.06037640 |
| D15 | 175.04927881 |
| D16 | -64.78934850 |
| D17 | -124.70321124 |
| D18 | 65.76088256 |
| D19 | -91.03747684 |
| D20 | 48.79600857 |
| D21 | -98.59107351 |
| D22 | 22.40915402 |
| D23 | 139.09464990 |
| D24 | 170.06310544 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|--------|--------|--------|---------|---------|---------|---------|---------|---------|--------|--------|
| 26.88 | 47.86 | 69.56 | 80.85 | 110.38 | 120.40 | 147.65 | 165.06 | 181.25 | 206.91 | 225.35 |
| 227.02 | 253.22 | 266.58 | 269.18 | 308.21 | 318.01 | 338.28 | 349.85 | 362.42 | 433.95 | |
| 514.93 | 555.45 | 566.86 | 578.57 | 679.25 | 770.53 | 856.48 | 886.80 | 895.74 | 900.49 | |
| 929.91 | 966.82 | 991.20 | 1056.06 | 1062.27 | 1102.88 | 1117.93 | 1137.76 | 1141.71 | | |

| | | | | | | | | |
|-------------------------------|---------|---------|---------|-----------|-----------|-----------|---------|---------|
| 1181.23 | 1187.44 | 1199.03 | 1219.40 | 1354.33 | 1370.00 | 1374.93 | 1408.27 | 1419.04 |
| 1420.91 | 1425.47 | 1427.11 | 1436.41 | 1467.14 | 1470.90 | 1487.34 | 1496.93 | 1501.08 |
| 1502.38 | 1614.48 | 1700.16 | 3063.96 | 3069.54 | 3074.39 | 3081.77 | 3123.57 | 3131.11 |
| 3151.19 | 3157.44 | 3158.19 | 3169.29 | 3171.15 | 3191.64 | 3221.55 | 3823.43 | |
| Rotational constants (B/GHZ): | | | | 0.9835578 | 0.5121736 | 0.4796307 | | |



TS4g

C

| | | | | | | | | |
|---|----|-----|----|-----|----|-----|---|--|
| H | 1 | B1 | | | | | | |
| O | 1 | B2 | 2 | A1 | | | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 | 0 | |
| H | 3 | B4 | 1 | A3 | 4 | D2 | 0 | |
| C | 3 | B5 | 1 | A4 | 4 | D3 | 0 | |
| O | 6 | B6 | 3 | A5 | 1 | D4 | 0 | |
| O | 6 | B7 | 3 | A6 | 1 | D5 | 0 | |
| C | 1 | B8 | 4 | A7 | 3 | D6 | 0 | |
| H | 9 | B9 | 1 | A8 | 4 | D7 | 0 | |
| H | 9 | B10 | 1 | A9 | 4 | D8 | 0 | |
| H | 9 | B11 | 1 | A10 | 4 | D9 | 0 | |
| O | 1 | B12 | 4 | A11 | 3 | D10 | 0 | |
| C | 13 | B13 | 1 | A12 | 4 | D11 | 0 | |
| H | 14 | B14 | 13 | A13 | 1 | D12 | 0 | |
| C | 14 | B15 | 13 | A14 | 1 | D13 | 0 | |
| H | 16 | B16 | 14 | A15 | 13 | D14 | 0 | |
| H | 16 | B17 | 14 | A16 | 13 | D15 | 0 | |
| H | 16 | B18 | 14 | A17 | 13 | D16 | 0 | |
| O | 14 | B19 | 13 | A18 | 1 | D17 | 0 | |
| O | 20 | B20 | 14 | A19 | 13 | D18 | 0 | |
| H | 21 | B21 | 20 | A20 | 14 | D19 | 0 | |
| C | 6 | B22 | 3 | A21 | 1 | D20 | 0 | |
| H | 23 | B23 | 6 | A22 | 3 | D21 | 0 | |
| H | 23 | B24 | 6 | A23 | 3 | D22 | 0 | |
| H | 23 | B25 | 6 | A24 | 3 | D23 | 0 | |
| H | 6 | B26 | 3 | A25 | 1 | D24 | 0 | |

Variables:

| | |
|----|------------|
| B1 | 1.09024168 |
| B2 | 2.28895762 |
| B3 | 1.41036463 |

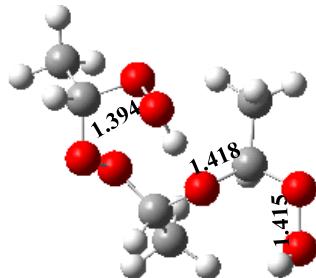
| | |
|-----|--------------|
| B4 | 1.09788771 |
| B5 | 2.04590628 |
| B6 | 2.17626749 |
| B7 | 1.26601066 |
| B8 | 1.51634779 |
| B9 | 1.08807732 |
| B10 | 1.08712510 |
| B11 | 1.08713639 |
| B12 | 1.39874285 |
| B13 | 1.41175945 |
| B14 | 1.09175802 |
| B15 | 1.50838974 |
| B16 | 1.08860773 |
| B17 | 1.08812782 |
| B18 | 1.08822610 |
| B19 | 1.40363916 |
| B20 | 1.41429717 |
| B21 | 0.96493845 |
| B22 | 1.47520435 |
| B23 | 1.08554143 |
| B24 | 1.08937415 |
| B25 | 1.09082228 |
| B26 | 1.08516786 |
| A1 | 80.81186551 |
| A2 | 36.08311069 |
| A3 | 113.60147481 |
| A4 | 136.81139745 |
| A5 | 69.22649495 |
| A6 | 92.90675000 |
| A7 | 105.52008523 |
| A8 | 109.01350230 |
| A9 | 112.01805121 |
| A10 | 109.39082940 |
| A11 | 111.86800981 |
| A12 | 118.25116172 |
| A13 | 110.18233351 |
| A14 | 110.67852053 |
| A15 | 109.22976709 |
| A16 | 109.97113199 |
| A17 | 109.64815535 |
| A18 | 108.91990231 |
| A19 | 108.50032237 |
| A20 | 101.52803244 |
| A21 | 108.93864492 |

| | |
|-----|---------------|
| A22 | 110.71040096 |
| A23 | 107.91061737 |
| A24 | 109.36440160 |
| A25 | 83.07607491 |
| D1 | 139.90143922 |
| D2 | -81.88035803 |
| D3 | 10.77072312 |
| D4 | -106.22674341 |
| D5 | -75.43454796 |
| D6 | 161.17789773 |
| D7 | -59.98461846 |
| D8 | 60.72283575 |
| D9 | -179.12579189 |
| D10 | -72.45228860 |
| D11 | -59.45402485 |
| D12 | -5.40239008 |
| D13 | 119.09214963 |
| D14 | 52.04153254 |
| D15 | 172.07606159 |
| D16 | -68.19957370 |
| D17 | -125.39754087 |
| D18 | 66.58579608 |
| D19 | -93.31387562 |
| D20 | 46.03432020 |
| D21 | -88.34484221 |
| D22 | 32.09125297 |
| D23 | 149.45874943 |
| D24 | 167.14488114 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|------------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 503.922 <i>i</i> | 20.12 | 43.73 | 73.92 | 94.65 | 105.22 | 119.78 | 133.34 | 154.39 | 180.26 | 226.15 |
| 232.55 | 257.79 | 278.22 | 309.91 | 323.95 | 347.47 | 361.81 | 409.47 | 430.05 | 508.14 | |
| 531.33 | 545.78 | 578.04 | 597.42 | 684.40 | 856.79 | 889.56 | 896.69 | 927.68 | 965.44 | |
| 975.37 | 999.85 | 1013.00 | 1059.76 | 1097.61 | 1125.54 | 1137.48 | 1140.87 | 1182.45 | | |
| 1186.16 | 197.15 | 1219.16 | 1240.43 | 1356.64 | 1363.54 | 1372.31 | 1412.04 | 1415.84 | | |
| 1421.22 | 1424.22 | 1434.24 | 1440.30 | 1452.83 | 1475.81 | 1484.11 | 1491.45 | 1493.32 | | |
| 1503.86 | 1576.19 | 1620.02 | 1926.55 | 3066.94 | 3068.49 | 3079.93 | 3117.73 | 3129.08 | | |
| 3135.18 | 3153.16 | 3158.12 | 3160.98 | 3172.13 | 3187.20 | 3200.51 | 3828.64 | | | |

Rotational constants (B/GHZ): 1.3699825 0.4366109 0.3615594



P4g

C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 0 |
| C | 3 | B5 | 1 | A4 | 4 | D3 0 |
| O | 6 | B6 | 3 | A5 | 1 | D4 0 |
| O | 6 | B7 | 3 | A6 | 1 | D5 0 |
| C | 1 | B8 | 4 | A7 | 3 | D6 0 |
| H | 9 | B9 | 1 | A8 | 4 | D7 0 |
| H | 9 | B10 | 1 | A9 | 4 | D8 0 |
| H | 9 | B11 | 1 | A10 | 4 | D9 0 |
| O | 1 | B12 | 4 | A11 | 3 | D10 0 |
| C | 13 | B13 | 1 | A12 | 4 | D11 0 |
| H | 14 | B14 | 13 | A13 | 1 | D12 0 |
| C | 14 | B15 | 13 | A14 | 1 | D13 0 |
| H | 16 | B16 | 14 | A15 | 13 | D14 0 |
| H | 16 | B17 | 14 | A16 | 13 | D15 0 |
| H | 16 | B18 | 14 | A17 | 13 | D16 0 |
| O | 14 | B19 | 13 | A18 | 1 | D17 0 |
| O | 20 | B20 | 14 | A19 | 13 | D18 0 |
| H | 21 | B21 | 20 | A20 | 14 | D19 0 |
| C | 6 | B22 | 3 | A21 | 1 | D20 0 |
| H | 23 | B23 | 6 | A22 | 3 | D21 0 |
| H | 23 | B24 | 6 | A23 | 3 | D22 0 |
| H | 23 | B25 | 6 | A24 | 3 | D23 0 |
| H | 6 | B26 | 3 | A25 | 1 | D24 0 |

Variables:

| | |
|----|------------|
| B1 | 1.08985158 |
| B2 | 2.26901670 |
| B3 | 1.40474999 |
| B4 | 2.57754897 |
| B5 | 1.40775324 |
| B6 | 2.28166469 |
| B7 | 1.39405356 |
| B8 | 1.51622451 |

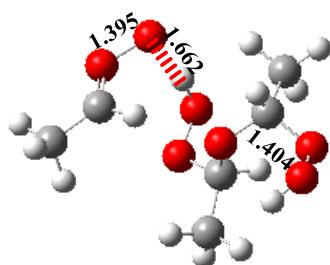
| | |
|-----|--------------|
| B9 | 1.08703337 |
| B10 | 1.08847495 |
| B11 | 1.08782495 |
| B12 | 1.41099061 |
| B13 | 1.41776867 |
| B14 | 1.08913605 |
| B15 | 1.50759213 |
| B16 | 1.08886732 |
| B17 | 1.08789395 |
| B18 | 1.08670431 |
| B19 | 1.39997740 |
| B20 | 1.41458143 |
| B21 | 0.96536910 |
| B22 | 1.51030382 |
| B23 | 1.08739045 |
| B24 | 1.08748243 |
| B25 | 1.08722838 |
| B26 | 1.09315776 |
| A1 | 77.73690322 |
| A2 | 37.01854144 |
| A3 | 70.93072060 |
| A4 | 127.64112143 |
| A5 | 92.44993805 |
| A6 | 112.04876561 |
| A7 | 105.79741176 |
| A8 | 108.13077247 |
| A9 | 111.52895514 |
| A10 | 110.26747150 |
| A11 | 111.48521801 |
| A12 | 120.42062766 |
| A13 | 109.77510499 |
| A14 | 112.19994183 |
| A15 | 110.20172979 |
| A16 | 109.49566984 |
| A17 | 109.28395458 |
| A18 | 107.50243326 |
| A19 | 108.11526033 |
| A20 | 101.75680472 |
| A21 | 113.78133568 |
| A22 | 110.03731035 |
| A23 | 109.26952836 |
| A24 | 109.61529064 |
| A25 | 101.33808511 |
| D1 | 144.19978524 |

| | |
|-----|---------------|
| D2 | -123.56769645 |
| D3 | -71.06947094 |
| D4 | -61.23705574 |
| D5 | -30.22554036 |
| D6 | 155.81622840 |
| D7 | -72.91438515 |
| D8 | 45.60455364 |
| D9 | 167.25210733 |
| D10 | -76.86288701 |
| D11 | -87.53615682 |
| D12 | -12.41258604 |
| D13 | 112.94598345 |
| D14 | 55.06824669 |
| D15 | 175.63356396 |
| D16 | -63.74585689 |
| D17 | -130.70264127 |
| D18 | 66.56541665 |
| D19 | -91.27047117 |
| D20 | 90.66866401 |
| D21 | -67.47485429 |
| D22 | 52.30525140 |
| D23 | 172.34006859 |
| D24 | -147.61887767 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 38.96 | 49.34 | 97.66 | 114.64 | 126.70 | 168.55 | 198.58 | 206.77 | 228.61 | 238.70 | 240.12 |
| 258.89 | 293.56 | 307.63 | 320.37 | 359.13 | 365.42 | 416.00 | 437.85 | 501.75 | 544.14 | |
| 576.62 | 583.29 | 597.60 | 673.59 | 703.72 | 843.35 | 879.99 | 902.95 | 920.48 | 939.40 | |
| 968.94 | 1011.39 | 1057.58 | 1063.09 | 1107.62 | 1137.69 | 1138.86 | 1148.62 | 1153.73 | | |
| 1177.02 | 1185.76 | 1216.75 | 1225.90 | 1347.01 | 1360.70 | 1377.87 | 1399.36 | 1411.39 | | |
| 1420.10 | 1424.16 | 1426.10 | 1431.23 | 1439.13 | 1478.17 | 1484.28 | 1488.17 | 1493.15 | | |
| 1495.30 | 1502.33 | 1513.27 | 3067.54 | 3070.50 | 3078.37 | 3101.23 | 3120.98 | 3132.44 | | |
| 3150.14 | 3155.17 | 3157.68 | 3161.96 | 3169.10 | 3170.95 | 3697.82 | 3817.66 | | | |

Rotational constants (B/GHZ): 1.2463103 0.5375417 0.4463805



IM4h

| | | |
|---|---|---------------|
| C | | |
| C | 1 | B1 |
| H | 2 | B2 1 A1 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| O | 7 | B7 | 5 | A6 | 2 | D5 | 0 |
| O | 7 | B8 | 5 | A7 | 2 | D6 | 0 |
| H | 1 | B9 | 2 | A8 | 5 | D7 | 0 |
| H | 1 | B10 | 2 | A9 | 5 | D8 | 0 |
| H | 1 | B11 | 2 | A10 | 5 | D9 | 0 |
| O | 2 | B12 | 1 | A11 | 5 | D10 | 0 |
| C | 13 | B13 | 2 | A12 | 1 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 2 | D12 | 0 |
| C | 14 | B15 | 13 | A14 | 2 | D13 | 0 |
| H | 16 | B16 | 14 | A15 | 13 | D14 | 0 |
| H | 16 | B17 | 14 | A16 | 13 | D15 | 0 |
| H | 16 | B18 | 14 | A17 | 13 | D16 | 0 |
| O | 14 | B19 | 13 | A18 | 2 | D17 | 0 |
| O | 20 | B20 | 14 | A19 | 13 | D18 | 0 |
| H | 21 | B21 | 20 | A20 | 14 | D19 | 0 |
| C | 7 | B22 | 5 | A21 | 2 | D20 | 0 |
| H | 23 | B23 | 7 | A22 | 5 | D21 | 0 |
| H | 23 | B24 | 7 | A23 | 5 | D22 | 0 |
| H | 23 | B25 | 7 | A24 | 5 | D23 | 0 |
| H | 7 | B26 | 5 | A25 | 2 | D24 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.51250789 |
| B2 | 1.09001999 |
| B3 | 2.29712618 |
| B4 | 1.39866631 |
| B5 | 0.99652818 |
| B6 | 2.74801161 |
| B7 | 2.22989579 |
| B8 | 1.23685783 |
| B9 | 1.08935666 |
| B10 | 1.09032332 |
| B11 | 1.08731357 |
| B12 | 1.41477750 |
| B13 | 1.41449588 |
| B14 | 1.08994561 |
| B15 | 1.50989380 |
| B16 | 1.08770720 |
| B17 | 1.08796262 |
| B18 | 1.08712253 |
| B19 | 1.40423462 |

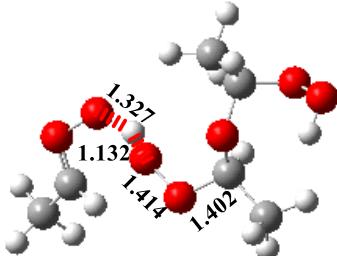
| | |
|-----|--------------|
| B20 | 1.41536296 |
| B21 | 0.96648727 |
| B22 | 1.47323096 |
| B23 | 1.09019255 |
| B24 | 1.08575402 |
| B25 | 1.09242137 |
| B26 | 1.08834197 |
| A1 | 111.88944299 |
| A2 | 138.93223725 |
| A3 | 106.30611569 |
| A4 | 103.49678822 |
| A5 | 109.75053148 |
| A6 | 77.61586504 |
| A7 | 91.11819032 |
| A8 | 109.63423583 |
| A9 | 109.88430873 |
| A10 | 110.39255344 |
| A11 | 108.94581132 |
| A12 | 118.60381164 |
| A13 | 104.03554679 |
| A14 | 115.72288898 |
| A15 | 108.70340980 |
| A16 | 108.57019001 |
| A17 | 112.10507134 |
| A18 | 109.46456417 |
| A19 | 108.20535467 |
| A20 | 102.78717962 |
| A21 | 107.25728258 |
| A22 | 109.76336014 |
| A23 | 111.23967914 |
| A24 | 107.53490663 |
| A25 | 69.99282901 |
| D1 | 101.34523386 |
| D2 | 17.76350071 |
| D3 | 123.13241061 |
| D4 | 93.82388050 |
| D5 | 94.71329763 |
| D6 | 126.47027223 |
| D7 | 176.29898494 |
| D8 | -63.99975027 |
| D9 | 56.64375032 |
| D10 | 118.30787089 |
| D11 | 124.60109674 |
| D12 | 179.87460504 |

| | |
|-----|---------------|
| D13 | 57.33552640 |
| D14 | 56.93716557 |
| D15 | 176.03712331 |
| D16 | -63.52097297 |
| D17 | -63.76356444 |
| D18 | -68.39924327 |
| D19 | 69.84639321 |
| D20 | -112.35819504 |
| D21 | 131.32852575 |
| D22 | -105.74074788 |
| D23 | 14.60561958 |
| D24 | 8.10266926 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 46.25 | 50.01 | 56.54 | 76.82 | 95.96 | 98.86 | 125.72 | 152.66 | 179.97 | 202.50 | 217.67 |
| 230.05 | 245.84 | 251.13 | 284.15 | 306.65 | 322.30 | 334.87 | 342.71 | 363.60 | 427.32 | |
| 510.02 | 555.35 | 563.05 | 587.70 | 687.29 | 850.24 | 878.90 | 893.98 | 899.20 | 902.86 | |
| 919.79 | 961.60 | 991.76 | 1056.10 | 1061.86 | 1098.54 | 1132.94 | 1138.80 | 1151.44 | | |
| 1175.01 | 1179.56 | 1190.51 | 1216.18 | 1359.20 | 1371.18 | 1377.15 | 1401.16 | 1411.40 | | |
| 1424.98 | 1425.76 | 1432.40 | 1437.10 | 1463.00 | 1470.06 | 1484.65 | 1490.53 | 1495.90 | | |
| 1500.07 | 1607.87 | 1704.35 | 3057.05 | 3059.56 | 3071.87 | 3119.07 | 3127.06 | 3130.20 | | |
| 3142.75 | 3147.99 | 3151.74 | 3154.92 | 3168.41 | 3177.72 | 3210.09 | 3794.26 | | | |

Rotational constants (B/GHZ): 1.0780273 0.4826535 0.4350768



TS4h

| C | | B1 | | | | | |
|---|----|-----|---|-----|---|-----|---|
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 | 0 |
| O | 7 | B7 | 4 | A6 | 2 | D5 | 0 |
| O | 7 | B8 | 4 | A7 | 2 | D6 | 0 |
| H | 1 | B9 | 2 | A8 | 5 | D7 | 0 |
| H | 1 | B10 | 2 | A9 | 5 | D8 | 0 |
| H | 1 | B11 | 2 | A10 | 5 | D9 | 0 |
| O | 2 | B12 | 1 | A11 | 5 | D10 | 0 |
| C | 13 | B13 | 2 | A12 | 1 | D11 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 14 | B14 | 13 | A13 | 2 | D12 | 0 |
| C | 14 | B15 | 13 | A14 | 2 | D13 | 0 |
| H | 16 | B16 | 14 | A15 | 13 | D14 | 0 |
| H | 16 | B17 | 14 | A16 | 13 | D15 | 0 |
| H | 16 | B18 | 14 | A17 | 13 | D16 | 0 |
| O | 14 | B19 | 13 | A18 | 2 | D17 | 0 |
| O | 20 | B20 | 14 | A19 | 13 | D18 | 0 |
| H | 21 | B21 | 20 | A20 | 14 | D19 | 0 |
| C | 7 | B22 | 4 | A21 | 2 | D20 | 0 |
| H | 23 | B23 | 7 | A22 | 4 | D21 | 0 |
| H | 23 | B24 | 7 | A23 | 4 | D22 | 0 |
| H | 23 | B25 | 7 | A24 | 4 | D23 | 0 |
| H | 7 | B26 | 4 | A25 | 2 | D24 | 0 |

Variables:

| | |
|-----|--------------|
| B1 | 1.51111735 |
| B2 | 1.09105838 |
| B3 | 2.27645529 |
| B4 | 1.40230789 |
| B5 | 1.13180531 |
| B6 | 2.08422088 |
| B7 | 2.17784018 |
| B8 | 1.26479641 |
| B9 | 1.08968677 |
| B10 | 1.08898829 |
| B11 | 1.08781564 |
| B12 | 1.40787769 |
| B13 | 1.41238814 |
| B14 | 1.08986656 |
| B15 | 1.51177989 |
| B16 | 1.08853822 |
| B17 | 1.08793419 |
| B18 | 1.08733194 |
| B19 | 1.40499994 |
| B20 | 1.41642665 |
| B21 | 0.96760269 |
| B22 | 1.47420472 |
| B23 | 1.09120637 |
| B24 | 1.08563402 |
| B25 | 1.08951528 |
| B26 | 1.08624575 |
| A1 | 111.63393401 |
| A2 | 141.96654623 |
| A3 | 106.15242372 |
| A4 | 93.93630395 |

| | |
|-----|---------------|
| A5 | 132.17568156 |
| A6 | 68.05685016 |
| A7 | 91.20462764 |
| A8 | 109.17059399 |
| A9 | 109.60210841 |
| A10 | 110.56148587 |
| A11 | 110.40403911 |
| A12 | 117.79727901 |
| A13 | 104.06236731 |
| A14 | 115.60328882 |
| A15 | 108.96741211 |
| A16 | 108.64539910 |
| A17 | 112.33605555 |
| A18 | 109.52344320 |
| A19 | 108.08797307 |
| A20 | 102.86301599 |
| A21 | 110.65725518 |
| A22 | 109.11616926 |
| A23 | 111.19756840 |
| A24 | 107.76019999 |
| A25 | 81.56356643 |
| D1 | 111.70436240 |
| D2 | 7.11425937 |
| D3 | 121.82731959 |
| D4 | 52.31045191 |
| D5 | 84.13396097 |
| D6 | 115.41825100 |
| D7 | 173.81278815 |
| D8 | -66.09662555 |
| D9 | 54.69059127 |
| D10 | 117.86410146 |
| D11 | 117.35404347 |
| D12 | -177.30242789 |
| D13 | 60.36650278 |
| D14 | 58.15305529 |
| D15 | 176.95982726 |
| D16 | -62.69092568 |
| D17 | -60.80584079 |
| D18 | -68.03694900 |
| D19 | 62.95635100 |
| D20 | -123.19444407 |
| D21 | 150.71284912 |
| D22 | -87.27216538 |
| D23 | 33.85671228 |

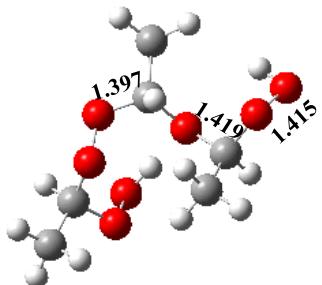
D24

-2.74069095

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 658.86 <i>i</i> | 34.38 | 53.42 | 68.01 | 91.99 | 100.45 | 118.06 | 144.55 | 183.18 | 204.13 | 234.89 |
| 246.46 | 270.97 | 295.62 | 302.86 | 318.42 | 348.45 | 356.20 | 399.73 | 454.30 | 481.18 | |
| 520.58 | 546.09 | 571.06 | 595.56 | 694.41 | 853.80 | 889.11 | 898.93 | 913.93 | 934.00 | |
| 966.68 | 993.85 | 1003.35 | 1054.79 | 1089.64 | 1108.40 | 1139.31 | 1148.40 | 1174.66 | | |
| 1188.50 | 1190.56 | 1200.10 | 1222.32 | 1362.94 | 1370.62 | 1372.83 | 1403.97 | 1416.06 | | |
| 1420.50 | 1431.74 | 1439.41 | 1447.78 | 1457.24 | 1470.75 | 1480.86 | 1493.27 | 1497.12 | | |
| 1503.46 | 1522.55 | 1627.98 | 1877.87 | 3060.70 | 3065.53 | 3080.58 | 3128.27 | 3134.93 | | |
| 3135.07 | 3140.42 | 3154.89 | 3161.79 | 3171.35 | 3173.14 | 3207.03 | 3772.52 | | | |

Rotational constants (B/GHZ): 1.4526870 0.4180504 0.3586739



P4h

C

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 | 0 |
| O | 7 | B7 | 4 | A6 | 2 | D5 | 0 |
| O | 7 | B8 | 4 | A7 | 2 | D6 | 0 |
| H | 1 | B9 | 2 | A8 | 5 | D7 | 0 |
| H | 1 | B10 | 2 | A9 | 5 | D8 | 0 |
| H | 1 | B11 | 2 | A10 | 5 | D9 | 0 |
| O | 2 | B12 | 1 | A11 | 5 | D10 | 0 |
| C | 13 | B13 | 2 | A12 | 1 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 2 | D12 | 0 |
| C | 14 | B15 | 13 | A14 | 2 | D13 | 0 |
| H | 16 | B16 | 14 | A15 | 13 | D14 | 0 |
| H | 16 | B17 | 14 | A16 | 13 | D15 | 0 |
| H | 16 | B18 | 14 | A17 | 13 | D16 | 0 |
| O | 14 | B19 | 13 | A18 | 2 | D17 | 0 |
| O | 20 | B20 | 14 | A19 | 13 | D18 | 0 |
| H | 21 | B21 | 20 | A20 | 14 | D19 | 0 |
| C | 7 | B22 | 4 | A21 | 2 | D20 | 0 |
| H | 23 | B23 | 7 | A22 | 4 | D21 | 0 |

| | | | | | | | |
|---|----|-----|---|-----|---|-----|---|
| H | 23 | B24 | 7 | A23 | 4 | D22 | 0 |
| H | 23 | B25 | 7 | A24 | 4 | D23 | 0 |
| H | 7 | B26 | 4 | A25 | 2 | D24 | 0 |

Variables:

| | |
|-----|--------------|
| B1 | 1.51095093 |
| B2 | 1.09015900 |
| B3 | 2.27655151 |
| B4 | 1.39738860 |
| B5 | 2.54666883 |
| B6 | 1.41228831 |
| B7 | 2.30393211 |
| B8 | 1.39720376 |
| B9 | 1.08950125 |
| B10 | 1.08899058 |
| B11 | 1.08734011 |
| B12 | 1.41604750 |
| B13 | 1.41912472 |
| B14 | 1.08996315 |
| B15 | 1.51062057 |
| B16 | 1.08705881 |
| B17 | 1.08785832 |
| B18 | 1.08732574 |
| B19 | 1.40062011 |
| B20 | 1.41526075 |
| B21 | 0.96692404 |
| B22 | 1.51145397 |
| B23 | 1.08649080 |
| B24 | 1.08925296 |
| B25 | 1.08660209 |
| B26 | 1.09053221 |
| A1 | 111.76215365 |
| A2 | 141.07429025 |
| A3 | 106.04628949 |
| A4 | 80.88838164 |
| A5 | 126.64507046 |
| A6 | 106.65403001 |
| A7 | 112.60652492 |
| A8 | 109.22682241 |
| A9 | 109.76470979 |
| A10 | 110.37934085 |
| A11 | 109.89654146 |
| A12 | 117.97250882 |
| A13 | 103.93314659 |
| A14 | 115.32787692 |

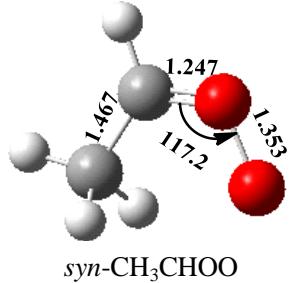
| | |
|-----|---------------|
| A15 | 108.59267295 |
| A16 | 108.51370622 |
| A17 | 112.24114827 |
| A18 | 109.27263751 |
| A19 | 108.28301023 |
| A20 | 102.97455620 |
| A21 | 105.24753377 |
| A22 | 109.32485505 |
| A23 | 109.74427763 |
| A24 | 109.85547163 |
| A25 | 108.93751579 |
| D1 | 106.29807388 |
| D2 | 13.10504939 |
| D3 | 108.64607982 |
| D4 | 91.71238897 |
| D5 | 7.07974137 |
| D6 | 44.10721597 |
| D7 | 174.98671073 |
| D8 | -64.80013914 |
| D9 | 55.79629527 |
| D10 | 118.14995971 |
| D11 | 118.57792920 |
| D12 | -178.97992775 |
| D13 | 58.66729935 |
| D14 | 55.14354213 |
| D15 | 174.45927415 |
| D16 | -65.37740815 |
| D17 | -62.40829344 |
| D18 | -69.46719065 |
| D19 | 69.92683651 |
| D20 | 160.22743689 |
| D21 | 179.50505644 |
| D22 | -61.01838330 |
| D23 | 58.90648117 |
| D24 | -77.06864978 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 51.54 | 58.86 | 77.19 | 107.58 | 122.34 | 156.01 | 175.19 | 192.17 | 212.38 | 221.94 | 244.43 |
| 283.91 | 297.76 | 318.22 | 332.10 | 355.45 | 360.58 | 427.50 | 441.83 | 500.85 | 529.92 | |
| 571.69 | 584.68 | 610.26 | 636.22 | 696.37 | 852.43 | 893.01 | 904.25 | 918.44 | 937.49 | |
| 969.12 | 1057.26 | 1059.03 | 1066.99 | 1098.69 | 1120.87 | 1137.89 | 1151.68 | 1163.47 | | |
| 1178.74 | 1191.97 | 1203.33 | 1234.61 | 1359.86 | 1365.73 | 1369.54 | 1392.65 | 1405.65 | | |
| 1416.24 | 1419.72 | 1425.14 | 1436.79 | 1443.90 | 1486.34 | 1490.24 | 1492.75 | 1496.07 | | |
| 1498.25 | 1502.00 | 1511.03 | 3060.10 | 3070.00 | 3086.40 | 3124.22 | 3125.45 | 3133.10 | | |
| 3144.02 | 3152.30 | 3154.25 | 3165.67 | 3166.25 | 3185.02 | 3685.27 | 3791.00 | | | |

Rotational constants (B/GHZ): 1.2530071 0.5100953 0.4622752

Figure S7. Optimized geometries, z-matrices and vibrational frequencies of all stationary points in the reaction of 2*syn*-CH₃CHO with HO-CH(CH₃)OO-H(Pa₂⁺ and Pb₂⁺) at the M06-2X/6-311+G(2df,2p) level of theory



| | | | | | | | |
|---|---|----|---|----|---|----|---|
| C | | | | | | | |
| O | 1 | B1 | | | | | |
| O | 2 | B2 | 1 | A1 | | | |
| H | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| C | 1 | B4 | 2 | A3 | 3 | D2 | 0 |
| H | 5 | B5 | 1 | A4 | 2 | D3 | 0 |
| H | 5 | B6 | 1 | A5 | 2 | D4 | 0 |
| H | 5 | B7 | 1 | A6 | 2 | D5 | 0 |

Variables:

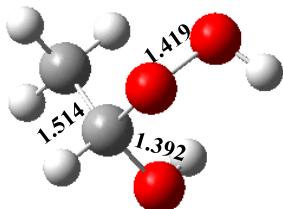
| | |
|----|--------------|
| B1 | 1.24673463 |
| B2 | 1.35257838 |
| B3 | 1.08417638 |
| B4 | 1.46657543 |
| B5 | 1.08452020 |
| B6 | 1.09346997 |
| B7 | 1.09346997 |
| A1 | 117.18473613 |
| A2 | 113.50906167 |
| A3 | 121.22148887 |
| A4 | 111.67299194 |
| A5 | 108.36774689 |
| A6 | 108.36774689 |
| D1 | 180.00000000 |
| D2 | 0.00000000 |
| D3 | 180.00000000 |
| D4 | -56.62427783 |
| D5 | 56.62427783 |

Harmonic Vibrational Frequencies (cm⁻¹):

180.02 313.30 470.29 682.06 784.99 938.95 995.40 1065.23 1108.04 1360.12

1409.89 1435.62 1462.37 1644.74 3035.96 3082.86 3172.74 3221.03

Rotational constants (B/GHZ): 17.9036510 7.2529111 5.3265305



Pa₂(syn-HO-CH(CH₃)OO-H)

C

| | | | | | | | |
|---|---|-----|---|----|---|----|---|
| O | 1 | B1 | | | | | |
| O | 2 | B2 | 1 | A1 | | | |
| H | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| O | 1 | B4 | 2 | A3 | 3 | D2 | 0 |
| H | 3 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 5 | B6 | 1 | A5 | 2 | D4 | 0 |
| C | 1 | B7 | 5 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 1 | A7 | 5 | D6 | 0 |
| H | 8 | B9 | 1 | A8 | 5 | D7 | 0 |
| H | 8 | B10 | 1 | A9 | 5 | D8 | 0 |

Variables:

| | |
|-----|---------------|
| B1 | 1.41574412 |
| B2 | 1.41909669 |
| B3 | 1.09067286 |
| B4 | 1.39184386 |
| B5 | 0.96378500 |
| B6 | 0.96073234 |
| B7 | 1.51389468 |
| B8 | 1.08824849 |
| B9 | 1.08773853 |
| B10 | 1.08994559 |
| A1 | 107.86168065 |
| A2 | 101.74558425 |
| A3 | 111.37946066 |
| A4 | 101.19029547 |
| A5 | 108.64817138 |
| A6 | 112.66192372 |
| A7 | 109.67570337 |
| A8 | 110.13170367 |
| A9 | 110.09828549 |
| D1 | 177.82956009 |
| D2 | 64.09238847 |
| D3 | -105.11788339 |
| D4 | -86.73514620 |
| D5 | 126.56282225 |
| D6 | 59.47979574 |

D7 179.80552806

D8 -60.73368006

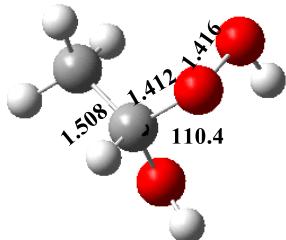
Harmonic Vibrational Frequencies (cm⁻¹):

150.83 237.33 243.85 312.28 420.17 438.32 507.63 696.96 860.78 957.79

1012.49 1090.91 1133.80 1175.40 1314.13 1389.46 1412.85 1418.37 1438.19

1493.54 1503.52 3067.74 3128.13 3149.52 3154.52 3842.07 3889.62

Rotational constants (B/GHZ): 6.9706500 4.5813473 3.6600767



P_{b2}(syn-HO-CH(CH₃)OO-H)

C

| | | | | | | | |
|---|---|-----|---|----|---|----|---|
| O | 1 | B1 | | | | | |
| O | 2 | B2 | 1 | A1 | | | |
| H | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| O | 1 | B4 | 2 | A3 | 3 | D2 | 0 |
| H | 3 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 5 | B6 | 1 | A5 | 2 | D4 | 0 |
| C | 1 | B7 | 5 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 1 | A7 | 5 | D6 | 0 |
| H | 8 | B9 | 1 | A8 | 5 | D7 | 0 |
| H | 8 | B10 | 1 | A9 | 5 | D8 | 0 |

Variables:

B1 1.41195863

B2 1.41583897

B3 1.09421397

B4 1.40063180

B5 0.96614133

B6 0.96082394

B7 1.50834430

B8 1.08789377

B9 1.08768717

B10 1.08657519

A1 109.03213737

A2 101.56077691

A3 110.37617334

A4 102.39067420

A5 109.02869039

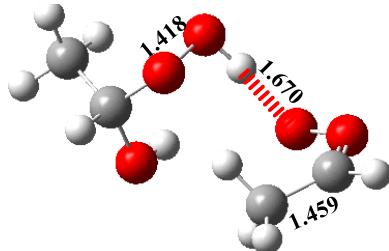
A6 108.36044040

A7 109.33838888

| | |
|----|---------------|
| A8 | 109.65383915 |
| A9 | 110.04773295 |
| D1 | -175.01638651 |
| D2 | 66.80673155 |
| D3 | -73.86249428 |
| D4 | 67.10948874 |
| D5 | 124.99768807 |
| D6 | 65.51240659 |
| D7 | -174.39368180 |
| D8 | -54.24919950 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|-------------------------------|---------|---------|---------|---------|-----------|-----------|-----------|---------|--------|
| 156.41 | 244.75 | 281.39 | 328.73 | 432.26 | 440.40 | 512.59 | 711.49 | 867.12 | 958.92 |
| 1014.22 | 1099.27 | 1144.99 | 1166.60 | 1293.62 | 1392.09 | 1403.03 | 1432.91 | 1463.23 | |
| 1493.99 | 1499.42 | 3085.44 | 3090.77 | 3164.63 | 3180.81 | 3816.10 | 3899.46 | | |
| Rotational constants (B/GHZ): | | | | | 6.9585956 | 4.6233182 | 3.6586659 | | |



IM5a

| C | | B1 | | | | | |
|---|----|-----|---|-----|---|-----|---|
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| C | 7 | B7 | 5 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 7 | A7 | 5 | D6 | 0 |
| H | 8 | B9 | 7 | A8 | 5 | D7 | 0 |
| H | 8 | B10 | 7 | A9 | 5 | D8 | 0 |
| O | 7 | B11 | 5 | A10 | 2 | D9 | 0 |
| O | 7 | B12 | 5 | A11 | 2 | D10 | 0 |
| H | 7 | B13 | 5 | A12 | 2 | D11 | 0 |
| H | 1 | B14 | 2 | A13 | 5 | D12 | 0 |
| H | 1 | B15 | 2 | A14 | 5 | D13 | 0 |
| H | 1 | B16 | 2 | A15 | 5 | D14 | 0 |
| O | 2 | B17 | 1 | A16 | 5 | D15 | 0 |
| H | 18 | B18 | 2 | A17 | 1 | D16 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51343481 |
|----|------------|

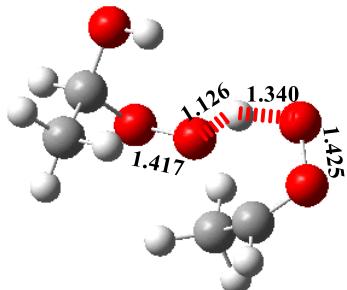
| | |
|-----|---------------|
| B2 | 1.09148326 |
| B3 | 2.30175361 |
| B4 | 1.41316732 |
| B5 | 0.99123294 |
| B6 | 3.80798980 |
| B7 | 1.45937289 |
| B8 | 1.09838575 |
| B9 | 1.09231742 |
| B10 | 1.08423902 |
| B11 | 2.22991873 |
| B12 | 1.24547630 |
| B13 | 1.08586593 |
| B14 | 1.08811022 |
| B15 | 1.08832284 |
| B16 | 1.08794594 |
| B17 | 1.39816762 |
| B18 | 0.96353069 |
| A1 | 111.24205607 |
| A2 | 90.16727392 |
| A3 | 112.49873523 |
| A4 | 101.63697870 |
| A5 | 115.38994230 |
| A6 | 58.08195389 |
| A7 | 107.93333155 |
| A8 | 109.21460269 |
| A9 | 111.35907755 |
| A10 | 58.55894465 |
| A11 | 81.34839804 |
| A12 | 136.26835627 |
| A13 | 109.13831307 |
| A14 | 110.09310841 |
| A15 | 110.30830528 |
| A16 | 112.66177549 |
| A17 | 108.75473046 |
| D1 | -142.94101934 |
| D2 | 28.61034137 |
| D3 | -133.14507035 |
| D4 | -142.77404916 |
| D5 | -42.27148165 |
| D6 | -11.40171370 |
| D7 | 101.07931270 |
| D8 | -133.95521395 |
| D9 | 69.48216489 |
| D10 | 95.63674146 |

D11 -150.77017919
 D12 -172.55267086
 D13 -52.35149091
 D14 67.44394802
 D15 -126.86212449
 D16 59.30536832

Harmonic Vibrational Frequencies (cm-1):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 37.05 | 58.37 | 65.97 | 94.23 | 124.20 | 157.77 | 224.83 | 245.64 | 273.30 | 316.45 | 333.64 |
| 381.92 | 431.45 | 474.78 | 527.19 | 677.38 | 682.12 | 789.85 | 860.29 | 916.91 | 929.88 | |
| 953.93 | 1005.27 | 1016.97 | 1083.84 | 1094.75 | 1119.42 | 1147.76 | 1165.11 | 1311.70 | | |
| 1361.67 | 1387.61 | 1411.96 | 1416.26 | 1426.39 | 1445.94 | 1471.70 | 1489.72 | 1501.46 | | |
| 1547.10 | 1667.87 | 3018.98 | 3073.84 | 3092.66 | 3108.59 | 3153.43 | 3164.72 | 3179.49 | | |
| 3207.88 | 3237.73 | 3857.81 | | | | | | | | |

Rotational constants (B/GHZ): 2.8536693 0.8515420 0.7880124



TS5a

| C | | B1 | | | | |
|---|----|-----|---|-----|---|-------|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 0 |
| O | 4 | B4 | 2 | A3 | 1 | D2 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 0 |
| C | 7 | B7 | 4 | A6 | 2 | D5 0 |
| H | 8 | B8 | 7 | A7 | 4 | D6 0 |
| H | 8 | B9 | 7 | A8 | 4 | D7 0 |
| H | 8 | B10 | 7 | A9 | 4 | D8 0 |
| O | 7 | B11 | 4 | A10 | 2 | D9 0 |
| O | 7 | B12 | 4 | A11 | 2 | D10 0 |
| H | 7 | B13 | 4 | A12 | 2 | D11 0 |
| H | 1 | B14 | 2 | A13 | 5 | D12 0 |
| H | 1 | B15 | 2 | A14 | 5 | D13 0 |
| H | 1 | B16 | 2 | A15 | 5 | D14 0 |
| O | 2 | B17 | 1 | A16 | 5 | D15 0 |
| H | 18 | B18 | 2 | A17 | 1 | D16 0 |

Variables:

B1 1.51598383

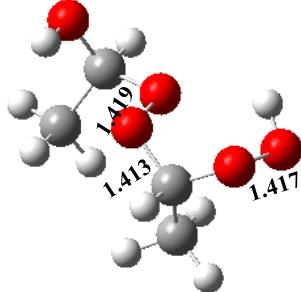
| | |
|-----|---------------|
| B2 | 1.09054669 |
| B3 | 2.27837592 |
| B4 | 1.41668873 |
| B5 | 1.12561008 |
| B6 | 2.07261490 |
| B7 | 1.47689215 |
| B8 | 1.08713872 |
| B9 | 1.08289876 |
| B10 | 1.09450647 |
| B11 | 2.20608522 |
| B12 | 1.26994802 |
| B13 | 1.08831658 |
| B14 | 1.08790940 |
| B15 | 1.08892423 |
| B16 | 1.08891949 |
| B17 | 1.38838475 |
| B18 | 0.96229392 |
| A1 | 111.44734145 |
| A2 | 92.23926399 |
| A3 | 36.53493936 |
| A4 | 122.80651359 |
| A5 | 144.16589608 |
| A6 | 95.43679993 |
| A7 | 109.64992009 |
| A8 | 111.71216658 |
| A9 | 105.85070803 |
| A10 | 67.66216296 |
| A11 | 87.96345251 |
| A12 | 106.13635289 |
| A13 | 109.25803934 |
| A14 | 110.35958281 |
| A15 | 110.26166795 |
| A16 | 112.60970163 |
| A17 | 108.07480576 |
| D1 | -145.43878710 |
| D2 | 124.80535965 |
| D3 | -169.32563500 |
| D4 | 80.18369833 |
| D5 | 35.95190351 |
| D6 | -58.12652476 |
| D7 | 64.78356427 |
| D8 | -174.84686220 |
| D9 | 129.32399617 |
| D10 | 161.74682279 |

D11 -86.07921082
 D12 -174.06269633
 D13 -54.08384737
 D14 66.28167159
 D15 -126.42300420
 D16 58.44358289

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 680.11 <i>i</i> | 25.66 | 76.01 | 99.36 | 167.75 | 194.26 | 230.33 | 246.51 | 304.66 | 347.26 | 376.51 |
| 414.12 | 435.22 | 475.71 | 523.20 | 626.52 | 688.16 | 865.24 | 874.07 | 901.31 | 940.69 | |
| 962.74 | 972.25 | 1062.79 | 1090.77 | 1119.87 | 1161.84 | 1176.19 | 1186.50 | 1322.92 | | |
| 1370.91 | 1380.75 | 1403.54 | 1410.28 | 1417.86 | 1432.11 | 1456.53 | 1479.99 | 1493.63 | | |
| 1497.45 | 1623.39 | 1942.40 | 3053.61 | 3060.51 | 3123.18 | 3142.77 | 3145.28 | 3149.84 | | |
| 3189.91 | 3208.62 | 3874.81 | | | | | | | | |

Rotational constants (B/GHZ): 2.9518200 0.8863593 0.7997626



P5a

| C | | B1 | | | | |
|---|----|-----|---|-----|---|-----|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 |
| O | 2 | B4 | 1 | A3 | 4 | D2 |
| H | 5 | B5 | 2 | A4 | 1 | D3 |
| C | 4 | B6 | 2 | A5 | 1 | D4 |
| C | 7 | B7 | 4 | A6 | 2 | D5 |
| H | 8 | B8 | 7 | A7 | 4 | D6 |
| H | 8 | B9 | 7 | A8 | 4 | D7 |
| H | 8 | B10 | 7 | A9 | 4 | D8 |
| O | 7 | B11 | 4 | A10 | 2 | D9 |
| O | 7 | B12 | 4 | A11 | 2 | D10 |
| H | 7 | B13 | 4 | A12 | 2 | D11 |
| H | 1 | B14 | 2 | A13 | 5 | D12 |
| H | 1 | B15 | 2 | A14 | 5 | D13 |
| H | 1 | B16 | 2 | A15 | 5 | D14 |
| O | 2 | B17 | 1 | A16 | 5 | D15 |
| H | 18 | B18 | 2 | A17 | 1 | D16 |

Variables:

B1 1.51494998

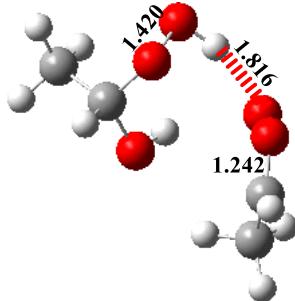
| | |
|-----|---------------|
| B2 | 1.09056339 |
| B3 | 2.28628388 |
| B4 | 1.41884962 |
| B5 | 2.25066250 |
| B6 | 1.41284327 |
| B7 | 1.51145540 |
| B8 | 1.08843979 |
| B9 | 1.08488919 |
| B10 | 1.08780553 |
| B11 | 2.31285087 |
| B12 | 1.39840684 |
| B13 | 1.09220839 |
| B14 | 1.08784746 |
| B15 | 1.08874672 |
| B16 | 1.08929913 |
| B17 | 1.38780366 |
| B18 | 0.96218586 |
| A1 | 111.28529884 |
| A2 | 92.99033146 |
| A3 | 112.03592930 |
| A4 | 158.17901614 |
| A5 | 135.07293481 |
| A6 | 113.60579390 |
| A7 | 109.13872625 |
| A8 | 111.03113365 |
| A9 | 109.00303414 |
| A10 | 103.56744328 |
| A11 | 111.32715224 |
| A12 | 101.80247766 |
| A13 | 109.06595637 |
| A14 | 110.34933562 |
| A15 | 110.50671992 |
| A16 | 112.88962011 |
| A17 | 108.49872867 |
| D1 | -145.81289978 |
| D2 | 32.38257590 |
| D3 | 134.93127510 |
| D4 | 70.46048513 |
| D5 | -27.99804965 |
| D6 | -60.00951979 |
| D7 | 60.83649868 |
| D8 | -179.32046621 |
| D9 | 66.67034906 |
| D10 | 102.56205577 |

D11 -148.39983846
 D12 -173.69098816
 D13 -53.74968015
 D14 66.76242380
 D15 -126.70718453
 D16 58.88801737

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 44.92 | 81.36 | 108.30 | 146.16 | 218.75 | 230.92 | 252.03 | 263.54 | 329.38 | 350.08 | 378.65 |
| 416.19 | 469.20 | 528.08 | 538.54 | 663.89 | 747.49 | 860.07 | 875.81 | 931.69 | 954.92 | |
| 997.17 | 1019.91 | 1088.20 | 1121.91 | 1138.50 | 1169.16 | 1178.87 | 1189.76 | 1322.30 | | |
| 1356.58 | 1374.51 | 1396.83 | 1415.38 | 1421.64 | 1427.66 | 1461.50 | 1483.73 | 1489.26 | | |
| 1499.26 | 1505.88 | 3063.50 | 3081.79 | 3121.51 | 3132.98 | 3145.54 | 3153.32 | 3155.21 | | |
| 3186.18 | 3790.70 | 3878.79 | | | | | | | | |

Rotational constants (B/GHZ): 2.9580302 1.0025194 0.9026314



IM5b

| C | | B1 | | | | | |
|---|----|-----|---|-----|---|-----|---|
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| O | 1 | B5 | 2 | A4 | 5 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 | 0 |
| C | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| C | 9 | B9 | 6 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 9 | A9 | 6 | D8 | 0 |
| H | 10 | B11 | 9 | A10 | 6 | D9 | 0 |
| H | 10 | B12 | 9 | A11 | 6 | D10 | 0 |
| O | 9 | B13 | 6 | A12 | 1 | D11 | 0 |
| O | 9 | B14 | 6 | A13 | 1 | D12 | 0 |
| H | 9 | B15 | 6 | A14 | 1 | D13 | 0 |
| H | 1 | B16 | 6 | A15 | 2 | D14 | 0 |
| O | 1 | B17 | 6 | A16 | 2 | D15 | 0 |
| H | 8 | B18 | 1 | A17 | 6 | D16 | 0 |

Variables:

B1 1.51364884

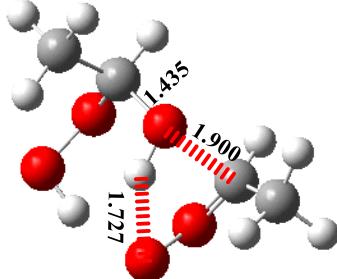
| | |
|-----|---------------|
| B2 | 1.08816420 |
| B3 | 1.08855431 |
| B4 | 1.08740114 |
| B5 | 1.40587702 |
| B6 | 0.96858792 |
| B7 | 2.30296672 |
| B8 | 3.04947260 |
| B9 | 1.46539209 |
| B10 | 1.09439214 |
| B11 | 1.09033465 |
| B12 | 1.08494745 |
| B13 | 2.23405779 |
| B14 | 1.24166790 |
| B15 | 1.08567814 |
| B16 | 1.09140892 |
| B17 | 1.40715244 |
| B18 | 0.97986526 |
| A1 | 109.12439437 |
| A2 | 110.02645515 |
| A3 | 110.38035038 |
| A4 | 112.07002288 |
| A5 | 107.89373027 |
| A6 | 98.71398587 |
| A7 | 117.33055010 |
| A8 | 79.95577098 |
| A9 | 107.57222984 |
| A10 | 108.94641969 |
| A11 | 110.87652254 |
| A12 | 62.99694955 |
| A13 | 74.42654949 |
| A14 | 118.06642015 |
| A15 | 106.19793603 |
| A16 | 111.19469227 |
| A17 | 101.38395754 |
| D1 | 120.15331873 |
| D2 | -119.83435063 |
| D3 | -57.91178541 |
| D4 | 74.92240587 |
| D5 | -92.86448434 |
| D6 | 156.88023660 |
| D7 | 176.76578507 |
| D8 | -9.25540348 |
| D9 | 106.31115695 |
| D10 | -129.56409892 |

| | |
|-----|---------------|
| D11 | -87.79694349 |
| D12 | -54.20911843 |
| D13 | 53.36969103 |
| D14 | 121.57108270 |
| D15 | -127.55684725 |
| D16 | -19.19901843 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 55.67 | 67.28 | 107.20 | 113.45 | 145.14 | 153.08 | 211.81 | 228.82 | 274.39 | 326.03 | 338.50 |
| 418.29 | 438.48 | 477.42 | 531.47 | 672.60 | 689.57 | 731.49 | 793.35 | 864.26 | 921.93 | |
| 952.05 | 995.59 | 1013.11 | 1091.13 | 1109.00 | 1129.00 | 1158.81 | 1163.40 | 1335.27 | | |
| 1365.25 | 1384.84 | 1420.63 | 1423.74 | 1428.72 | 1454.75 | 1477.72 | 1493.26 | 1503.73 | | |
| 1547.75 | 1686.43 | 3057.42 | 3074.56 | 3109.38 | 3121.07 | 3152.62 | 3166.69 | 3174.82 | | |
| 3216.31 | 3514.40 | 3751.46 | | | | | | | | |

Rotational constants (B/GHZ): 2.6720682 0.9722782 0.8326120



TS5b

| | | | | | | | | | | |
|---|----|--|-----|---|-----|----|-----|---|--|--|
| C | | | | | | | | | | |
| C | 1 | | B1 | | | | | | | |
| H | 2 | | B2 | 1 | A1 | | | | | |
| H | 2 | | B3 | 1 | A2 | 3 | D1 | 0 | | |
| H | 2 | | B4 | 1 | A3 | 4 | D2 | 0 | | |
| O | 1 | | B5 | 2 | A4 | 5 | D3 | 0 | | |
| H | 6 | | B6 | 1 | A5 | 2 | D4 | 0 | | |
| O | 1 | | B7 | 6 | A6 | 2 | D5 | 0 | | |
| C | 6 | | B8 | 1 | A7 | 2 | D6 | 0 | | |
| C | 9 | | B9 | 6 | A8 | 1 | D7 | 0 | | |
| H | 10 | | B10 | 9 | A9 | 6 | D8 | 0 | | |
| H | 10 | | B11 | 9 | A10 | 6 | D9 | 0 | | |
| H | 10 | | B12 | 9 | A11 | 6 | D10 | 0 | | |
| O | 9 | | B13 | 6 | A12 | 1 | D11 | 0 | | |
| O | 9 | | B14 | 6 | A13 | 1 | D12 | 0 | | |
| H | 9 | | B15 | 6 | A14 | 1 | D13 | 0 | | |
| H | 1 | | B16 | 6 | A15 | 9 | D14 | 0 | | |
| O | 1 | | B17 | 6 | A16 | 9 | D15 | 0 | | |
| H | 8 | | B18 | 1 | A17 | 18 | D16 | 0 | | |

Variables:

| | |
|----|------------|
| B1 | 1.51058313 |
|----|------------|

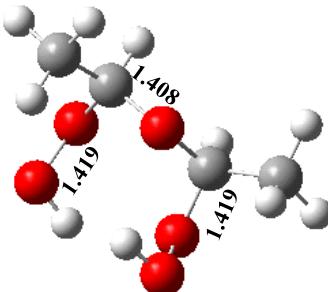
| | |
|-----|---------------|
| B2 | 1.08767122 |
| B3 | 1.08833628 |
| B4 | 1.08686159 |
| B5 | 1.43506519 |
| B6 | 1.00940126 |
| B7 | 2.29073939 |
| B8 | 1.89982191 |
| B9 | 1.48846705 |
| B10 | 1.08583226 |
| B11 | 1.08419963 |
| B12 | 1.09284477 |
| B13 | 2.22018083 |
| B14 | 1.27850834 |
| B15 | 1.08916619 |
| B16 | 1.09082927 |
| B17 | 1.38959239 |
| B18 | 0.98726281 |
| A1 | 109.60047406 |
| A2 | 109.04262334 |
| A3 | 110.38705513 |
| A4 | 109.20404196 |
| A5 | 108.91944124 |
| A6 | 96.81216209 |
| A7 | 118.32459590 |
| A8 | 95.11465779 |
| A9 | 110.34400529 |
| A10 | 111.08844855 |
| A11 | 106.19506527 |
| A12 | 76.13500039 |
| A13 | 98.44123400 |
| A14 | 103.23745252 |
| A15 | 106.02667274 |
| A16 | 111.18135760 |
| A17 | 98.91528212 |
| D1 | 119.89271416 |
| D2 | 119.39810692 |
| D3 | -59.57754442 |
| D4 | 77.75576884 |
| D5 | -93.38390795 |
| D6 | 171.51722480 |
| D7 | 166.14817545 |
| D8 | -61.52008627 |
| D9 | 62.33010397 |
| D10 | -179.41989651 |

| | |
|-----|--------------|
| D11 | -99.65418167 |
| D12 | -69.38656511 |
| D13 | 45.57358125 |
| D14 | -67.73438908 |
| D15 | 44.21969650 |
| D16 | 99.60833356 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 344.99 <i>i</i> | 57.46 | 128.76 | 147.93 | 156.17 | 194.32 | 225.34 | 270.21 | 310.14 | 312.69 |
| 345.68 | 432.33 | 469.21 | 571.75 | 642.86 | 688.91 | 749.96 | 847.11 | 877.92 | 921.99 |
| 937.35 | 979.13 | 995.25 | 1026.34 | 1106.41 | 1128.15 | 1157.78 | 1175.99 | 1193.46 | |
| 1342.95 | 1373.28 | 1390.08 | 1401.01 | 1426.99 | 1449.11 | 1465.61 | 1484.77 | 1491.52 | |
| 1503.80 | 1565.83 | 1594.73 | 2991.51 | 3059.46 | 3075.60 | 3127.97 | 3148.08 | 3156.99 | |
| 3168.61 | 3171.69 | 3197.21 | 3389.68 | | | | | | |

Rotational constants (B/GHZ): 2.5493245 1.2339589 1.0018028



P5b

| C | | B1 | | | | | |
|---|----|-----|---|-----|----|-----|---|
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| O | 1 | B5 | 2 | A4 | 5 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 | 0 |
| C | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| C | 9 | B9 | 6 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 9 | A9 | 6 | D8 | 0 |
| H | 10 | B11 | 9 | A10 | 6 | D9 | 0 |
| H | 10 | B12 | 9 | A11 | 6 | D10 | 0 |
| O | 9 | B13 | 6 | A12 | 1 | D11 | 0 |
| O | 14 | B14 | 9 | A13 | 6 | D12 | 0 |
| H | 9 | B15 | 6 | A14 | 1 | D13 | 0 |
| H | 1 | B16 | 6 | A15 | 9 | D14 | 0 |
| O | 1 | B17 | 6 | A16 | 9 | D15 | 0 |
| H | 8 | B18 | 1 | A17 | 18 | D16 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.50736917 |
|----|------------|

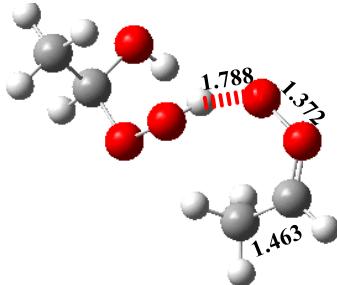
| | |
|-----|--------------|
| B2 | 1.08778753 |
| B3 | 1.08768481 |
| B4 | 1.08728320 |
| B5 | 1.40840310 |
| B6 | 2.28285434 |
| B7 | 2.30285802 |
| B8 | 1.40006779 |
| B9 | 1.50814338 |
| B10 | 1.08797238 |
| B11 | 1.08677070 |
| B12 | 1.08782637 |
| B13 | 2.30306255 |
| B14 | 1.41735620 |
| B15 | 1.09389402 |
| B16 | 1.09600419 |
| B17 | 1.40394292 |
| B18 | 0.96874445 |
| A1 | 109.74162108 |
| A2 | 109.50127609 |
| A3 | 109.64182621 |
| A4 | 107.66570361 |
| A5 | 115.32726405 |
| A6 | 94.01833524 |
| A7 | 116.36640796 |
| A8 | 108.93409449 |
| A9 | 109.39934458 |
| A10 | 110.04791650 |
| A11 | 109.68170449 |
| A12 | 89.99555915 |
| A13 | 35.72316976 |
| A14 | 111.14750837 |
| A15 | 109.77506437 |
| A16 | 112.48274600 |
| A17 | 107.86638874 |
| D1 | 120.26175310 |
| D2 | 119.80250284 |
| D3 | -60.90823506 |
| D4 | 82.51611853 |
| D5 | -94.53347428 |
| D6 | 172.30313558 |
| D7 | 150.81748658 |
| D8 | -64.86327632 |
| D9 | 54.93527223 |
| D10 | 175.08083908 |

| | |
|-----|---------------|
| D11 | -116.22201020 |
| D12 | 124.83687292 |
| D13 | 26.39322598 |
| D14 | -65.50294955 |
| D15 | 46.39340968 |
| D16 | 81.68075480 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 76.27 | 105.35 | 167.37 | 189.29 | 202.66 | 236.72 | 242.56 | 286.41 | 311.10 | 342.85 |
| 374.48 | 439.28 | 466.70 | 586.26 | 600.57 | 692.32 | 726.26 | 848.16 | 878.43 | 935.29 |
| 983.07 | 1006.20 | 1028.22 | 1124.74 | 1136.30 | 1154.32 | 1160.91 | 1178.66 | 1224.77 | |
| 1351.76 | 1370.72 | 1387.26 | 1410.41 | 1423.93 | 1434.84 | 1454.29 | 1461.83 | 1489.50 | |
| 1490.63 | 1498.00 | 1504.02 | 3071.34 | 3077.39 | 3080.58 | 3096.04 | 3157.73 | 3161.97 | |
| 3169.67 | 3171.59 | 3727.75 | 3756.69 | | | | | | |

Rotational constants (B/GHZ): 2.4323291 1.2895610 1.0352789



IM5c

| C | | B1 | | | | |
|---|----|-----|---|-----|---|-----|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 |
| O | 2 | B4 | 1 | A3 | 4 | D2 |
| H | 4 | B5 | 2 | A4 | 1 | D3 |
| C | 4 | B6 | 2 | A5 | 1 | D4 |
| C | 7 | B7 | 4 | A6 | 2 | D5 |
| H | 8 | B8 | 7 | A7 | 4 | D6 |
| H | 8 | B9 | 7 | A8 | 4 | D7 |
| H | 8 | B10 | 7 | A9 | 4 | D8 |
| O | 7 | B11 | 4 | A10 | 2 | D9 |
| O | 7 | B12 | 4 | A11 | 2 | D10 |
| H | 7 | B13 | 4 | A12 | 2 | D11 |
| H | 1 | B14 | 2 | A13 | 5 | D12 |
| H | 1 | B15 | 2 | A14 | 5 | D13 |
| H | 1 | B16 | 2 | A15 | 5 | D14 |
| O | 2 | B17 | 1 | A16 | 5 | D15 |
| H | 18 | B18 | 2 | A17 | 1 | D16 |

Variables:

| | |
|----|------------|
| B1 | 1.50822058 |
|----|------------|

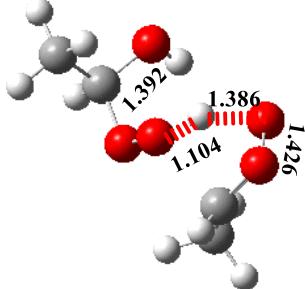
| | |
|-----|---------------|
| B2 | 1.09639410 |
| B3 | 2.31687959 |
| B4 | 1.41600147 |
| B5 | 0.98384803 |
| B6 | 3.39808882 |
| B7 | 1.46273193 |
| B8 | 1.09610288 |
| B9 | 1.09331774 |
| B10 | 1.08437269 |
| B11 | 2.23400100 |
| B12 | 1.24437625 |
| B13 | 1.08567670 |
| B14 | 1.08816799 |
| B15 | 1.08789404 |
| B16 | 1.08693034 |
| B17 | 1.39304527 |
| B18 | 0.96381004 |
| A1 | 111.43595735 |
| A2 | 93.41766811 |
| A3 | 113.11803014 |
| A4 | 90.98570155 |
| A5 | 113.71132546 |
| A6 | 79.08376626 |
| A7 | 108.75057218 |
| A8 | 108.13753614 |
| A9 | 111.20204608 |
| A10 | 53.02709793 |
| A11 | 67.05417409 |
| A12 | 126.95353408 |
| A13 | 109.38189395 |
| A14 | 109.85834780 |
| A15 | 109.51771127 |
| A16 | 108.30445783 |
| A17 | 109.39959281 |
| D1 | -143.23462844 |
| D2 | 30.13681950 |
| D3 | -124.88766027 |
| D4 | -174.74808810 |
| D5 | -37.22681026 |
| D6 | -8.03032887 |
| D7 | 106.10027942 |
| D8 | -131.02032659 |
| D9 | 60.98354346 |
| D10 | 95.89927513 |

D11 -162.37209854
 D12 -175.98880702
 D13 -55.84624496
 D14 64.48174861
 D15 -123.70231193
 D16 168.11933669

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 50.83 | 63.46 | 77.15 | 103.15 | 129.05 | 158.98 | 214.94 | 231.89 | 263.51 | 315.28 | 329.38 |
| 426.64 | 437.65 | 471.01 | 501.82 | 678.07 | 696.94 | 782.06 | 800.17 | 864.67 | 927.42 | |
| 963.82 | 1004.18 | 1011.63 | 1097.10 | 1099.24 | 1115.85 | 1149.87 | 1186.30 | 1290.66 | | |
| 1372.08 | 1381.25 | 1398.57 | 1421.62 | 1447.41 | 1459.88 | 1475.23 | 1491.99 | 1502.74 | | |
| 1561.89 | 1667.47 | 3035.97 | 3059.68 | 3084.79 | 3092.94 | 3163.67 | 3174.73 | 3179.13 | | |
| 3215.89 | 3426.07 | 3845.87 | | | | | | | | |

Rotational constants (B/GHZ): 3.0605179 0.8101218 0.7696201



TS5c

| C | | B1 | | | | | |
|---|----|-----|---|-----|---|-----|---|
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| O | 4 | B4 | 2 | A3 | 1 | D2 | 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 | 0 |
| C | 7 | B7 | 4 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 7 | A7 | 4 | D6 | 0 |
| H | 8 | B9 | 7 | A8 | 4 | D7 | 0 |
| H | 8 | B10 | 7 | A9 | 4 | D8 | 0 |
| O | 7 | B11 | 4 | A10 | 2 | D9 | 0 |
| O | 7 | B12 | 4 | A11 | 2 | D10 | 0 |
| H | 7 | B13 | 4 | A12 | 2 | D11 | 0 |
| H | 1 | B14 | 2 | A13 | 5 | D12 | 0 |
| H | 1 | B15 | 2 | A14 | 5 | D13 | 0 |
| H | 1 | B16 | 2 | A15 | 5 | D14 | 0 |
| O | 2 | B17 | 1 | A16 | 5 | D15 | 0 |
| H | 18 | B18 | 2 | A17 | 1 | D16 | 0 |

Variables:

B1 1.50825361

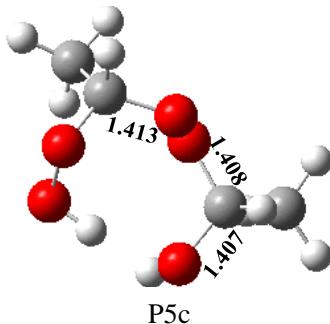
| | |
|-----|---------------|
| B2 | 1.09536218 |
| B3 | 2.29975060 |
| B4 | 1.41573133 |
| B5 | 1.10383816 |
| B6 | 2.04182005 |
| B7 | 1.47869391 |
| B8 | 1.08659193 |
| B9 | 1.08231173 |
| B10 | 1.09463960 |
| B11 | 2.20392514 |
| B12 | 1.27159971 |
| B13 | 1.08812674 |
| B14 | 1.08786440 |
| B15 | 1.08778069 |
| B16 | 1.08691236 |
| B17 | 1.39241511 |
| B18 | 0.96150557 |
| A1 | 111.64134829 |
| A2 | 92.40717945 |
| A3 | 35.79175608 |
| A4 | 92.85918452 |
| A5 | 143.51127825 |
| A6 | 97.22704675 |
| A7 | 110.17919426 |
| A8 | 111.58246078 |
| A9 | 105.51840637 |
| A10 | 68.80275494 |
| A11 | 89.29190574 |
| A12 | 104.31135699 |
| A13 | 109.35471748 |
| A14 | 109.85566715 |
| A15 | 109.65486966 |
| A16 | 108.16267677 |
| A17 | 109.63174485 |
| D1 | -143.23270839 |
| D2 | 127.94211881 |
| D3 | -123.05140418 |
| D4 | 167.30574227 |
| D5 | -15.62689755 |
| D6 | -58.34857302 |
| D7 | 65.26106208 |
| D8 | -175.16470345 |
| D9 | 77.46807520 |
| D10 | 109.80801442 |

| | |
|-----|---------------|
| D11 | -137.58274081 |
| D12 | -174.00443044 |
| D13 | -53.86315879 |
| D14 | 66.49216464 |
| D15 | -123.33252797 |
| D16 | -178.87927080 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 534.18 <i>i</i> | 47.15 | 73.54 | 125.83 | 178.38 | 217.67 | 225.67 | 255.62 | 308.96 | 376.37 | 397.81 |
| 439.84 | 444.71 | 468.72 | 501.94 | 633.41 | 712.02 | 870.34 | 874.37 | 914.79 | 951.79 | |
| 974.33 | 1000.50 | 1082.00 | 1100.75 | 1136.32 | 1171.52 | 1179.99 | 1212.08 | 1287.92 | | |
| 1369.04 | 1378.56 | 1397.39 | 1402.75 | 1447.42 | 1458.63 | 1482.15 | 1489.69 | 1498.27 | | |
| 1518.69 | 1645.65 | 1970.29 | 3059.02 | 3073.89 | 3076.61 | 3153.41 | 3157.31 | 3167.05 | | |
| 3191.87 | 3224.45 | 3886.57 | | | | | | | | |

Rotational constants (B/GHZ): 2.8979799 0.9569543 0.8847332



P5c

| C | | B1 | | | | | |
|---|----|-----|---|-----|---|-----|---|
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 | 0 |
| C | 7 | B7 | 4 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 7 | A7 | 4 | D6 | 0 |
| H | 8 | B9 | 7 | A8 | 4 | D7 | 0 |
| H | 8 | B10 | 7 | A9 | 4 | D8 | 0 |
| O | 7 | B11 | 4 | A10 | 2 | D9 | 0 |
| O | 7 | B12 | 4 | A11 | 2 | D10 | 0 |
| H | 7 | B13 | 4 | A12 | 2 | D11 | 0 |
| H | 1 | B14 | 2 | A13 | 5 | D12 | 0 |
| H | 1 | B15 | 2 | A14 | 5 | D13 | 0 |
| H | 1 | B16 | 2 | A15 | 5 | D14 | 0 |
| O | 2 | B17 | 1 | A16 | 5 | D15 | 0 |
| H | 18 | B18 | 2 | A17 | 1 | D16 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.50857757 |
| B2 | 1.09368472 |

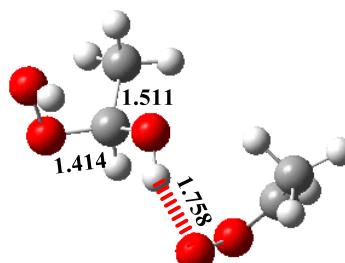
| | |
|-----|---------------|
| B3 | 2.30866532 |
| B4 | 1.40778208 |
| B5 | 2.68003297 |
| B6 | 1.41306797 |
| B7 | 1.51039244 |
| B8 | 1.08794823 |
| B9 | 1.08422436 |
| B10 | 1.08770189 |
| B11 | 2.30470002 |
| B12 | 1.40121521 |
| B13 | 1.09243481 |
| B14 | 1.08746877 |
| B15 | 1.08759745 |
| B16 | 1.08660698 |
| B17 | 1.40727618 |
| B18 | 0.96166762 |
| A1 | 111.36324113 |
| A2 | 86.58204024 |
| A3 | 114.01712663 |
| A4 | 68.45133137 |
| A5 | 131.49451198 |
| A6 | 114.17920431 |
| A7 | 109.71354245 |
| A8 | 110.85679343 |
| A9 | 108.31613779 |
| A10 | 98.92869240 |
| A11 | 111.56764351 |
| A12 | 102.55815821 |
| A13 | 109.02775270 |
| A14 | 109.89514691 |
| A15 | 110.01240315 |
| A16 | 108.17484075 |
| A17 | 108.59483488 |
| D1 | -137.22802024 |
| D2 | 23.52891190 |
| D3 | -117.19072410 |
| D4 | -152.96933011 |
| D5 | -66.75103027 |
| D6 | -50.71779327 |
| D7 | 70.01042095 |
| D8 | -170.26000691 |
| D9 | 29.85999435 |
| D10 | 64.17084107 |
| D11 | 172.44874061 |

D12 -167.69140661
 D13 -47.54578710
 D14 72.70987565
 D15 -125.28502675
 D16 -162.93415657

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 54.01 | 74.71 | 133.53 | 176.48 | 227.06 | 233.18 | 263.08 | 281.60 | 314.58 | 365.98 | 427.85 |
| 465.48 | 499.98 | 510.44 | 595.70 | 677.73 | 736.31 | 853.38 | 875.86 | 933.30 | 953.69 | |
| 991.43 | 1015.43 | 1107.55 | 1131.98 | 1145.56 | 1152.98 | 1172.61 | 1191.42 | 1293.40 | | |
| 1355.93 | 1381.92 | 1400.42 | 1416.56 | 1423.72 | 1454.87 | 1486.25 | 1488.11 | 1496.18 | | |
| 1503.63 | 1514.04 | 3077.08 | 3082.06 | 3084.78 | 3116.25 | 3158.55 | 3160.74 | 3167.53 | | |
| 3189.19 | 3734.36 | 3883.31 | | | | | | | | |

Rotational constants (B/GHZ): 2.5684054 1.1939108 1.0223523



IM5d

| | | | | | | | |
|---|----|-----|---|-----|---|-----|---|
| C | | | | | | | |
| C | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| O | 1 | B5 | 2 | A4 | 5 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 | 0 |
| C | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| C | 9 | B9 | 6 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 9 | A9 | 6 | D8 | 0 |
| H | 10 | B11 | 9 | A10 | 6 | D9 | 0 |
| H | 10 | B12 | 9 | A11 | 6 | D10 | 0 |
| O | 9 | B13 | 6 | A12 | 1 | D11 | 0 |
| O | 9 | B14 | 6 | A13 | 1 | D12 | 0 |
| H | 9 | B15 | 6 | A14 | 1 | D13 | 0 |
| H | 1 | B16 | 6 | A15 | 2 | D14 | 0 |
| O | 1 | B17 | 6 | A16 | 2 | D15 | 0 |
| H | 8 | B18 | 1 | A17 | 6 | D16 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51110581 |
| B2 | 1.08880466 |
| B3 | 1.08792822 |

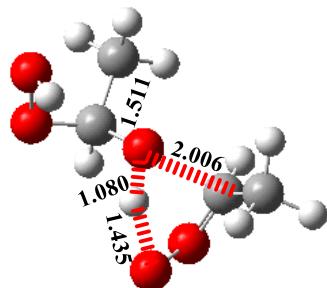
| | |
|-----|---------------|
| B4 | 1.08716364 |
| B5 | 1.39419412 |
| B6 | 0.98099156 |
| B7 | 2.29771734 |
| B8 | 3.13142443 |
| B9 | 1.46525001 |
| B10 | 1.09519879 |
| B11 | 1.09136916 |
| B12 | 1.08478390 |
| B13 | 2.23310313 |
| B14 | 1.24465627 |
| B15 | 1.08574602 |
| B16 | 1.09559886 |
| B17 | 1.41391391 |
| B18 | 0.96635319 |
| A1 | 109.62425809 |
| A2 | 110.00252393 |
| A3 | 109.83290599 |
| A4 | 109.23947589 |
| A5 | 108.64080415 |
| A6 | 92.63393522 |
| A7 | 112.12689132 |
| A8 | 78.68153770 |
| A9 | 107.85474841 |
| A10 | 108.65100472 |
| A11 | 110.96314114 |
| A12 | 57.05804571 |
| A13 | 70.17177383 |
| A14 | 123.91662718 |
| A15 | 110.92207741 |
| A16 | 110.67633843 |
| A17 | 90.08238712 |
| D1 | 120.18396948 |
| D2 | -119.70672523 |
| D3 | -54.87801516 |
| D4 | -157.04056621 |
| D5 | -92.96838461 |
| D6 | -92.80562386 |
| D7 | 167.41527413 |
| D8 | -12.64967925 |
| D9 | 102.35463689 |
| D10 | -133.70230146 |
| D11 | -95.21229285 |
| D12 | -61.02740455 |

D13 43.59511600
 D14 123.64523014
 D15 -124.64069935
 D16 -12.20718289

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 35.47 | 47.31 | 65.52 | 90.22 | 110.19 | 151.22 | 197.82 | 213.74 | 253.26 | 297.80 | 334.25 |
| 359.84 | 447.27 | 467.37 | 516.77 | 673.20 | 700.56 | 792.14 | 848.65 | 871.53 | 925.93 | |
| 963.85 | 995.59 | 1019.21 | 1093.47 | 1119.13 | 1133.63 | 1139.68 | 1174.68 | 1338.96 | | |
| 1363.83 | 1390.86 | 1407.77 | 1417.28 | 1438.51 | 1448.41 | 1470.64 | 1488.20 | 1492.51 | | |
| 1498.57 | 1665.13 | 3040.24 | 3072.90 | 3075.16 | 3100.95 | 3148.90 | 3168.72 | 3174.06 | | |
| 3208.16 | 3431.70 | 3817.63 | | | | | | | | |

Rotational constants (B/GHZ): 2.8460478 0.7209651 0.6841335



TS5d

| C | | B1 | | | | | |
|---|----|-----|---|-----|----|-----|---|
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| O | 1 | B5 | 2 | A4 | 5 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 | 0 |
| C | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| C | 9 | B9 | 6 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 9 | A9 | 6 | D8 | 0 |
| H | 10 | B11 | 9 | A10 | 6 | D9 | 0 |
| H | 10 | B12 | 9 | A11 | 6 | D10 | 0 |
| O | 9 | B13 | 6 | A12 | 1 | D11 | 0 |
| O | 9 | B14 | 6 | A13 | 1 | D12 | 0 |
| H | 9 | B15 | 6 | A14 | 1 | D13 | 0 |
| H | 1 | B16 | 6 | A15 | 9 | D14 | 0 |
| O | 1 | B17 | 6 | A16 | 9 | D15 | 0 |
| H | 8 | B18 | 1 | A17 | 18 | D16 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51062829 |
| B2 | 1.08927136 |
| B3 | 1.08792476 |

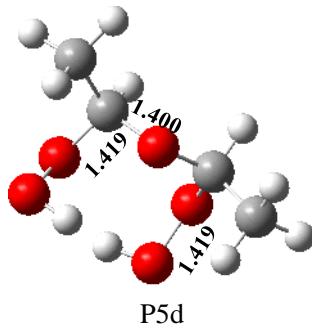
| | |
|-----|---------------|
| B4 | 1.08668999 |
| B5 | 1.40663183 |
| B6 | 1.08041040 |
| B7 | 2.29555555 |
| B8 | 2.00558029 |
| B9 | 1.48340533 |
| B10 | 1.08609956 |
| B11 | 1.08304806 |
| B12 | 1.09392478 |
| B13 | 2.19914624 |
| B14 | 1.27334179 |
| B15 | 1.08929166 |
| B16 | 1.09566361 |
| B17 | 1.40533358 |
| B18 | 0.96521403 |
| A1 | 110.09934594 |
| A2 | 109.65725917 |
| A3 | 110.09116743 |
| A4 | 110.02561777 |
| A5 | 107.43747658 |
| A6 | 93.18420134 |
| A7 | 113.31541138 |
| A8 | 93.33469697 |
| A9 | 109.75937091 |
| A10 | 111.42310478 |
| A11 | 106.17263170 |
| A12 | 70.22637961 |
| A13 | 92.95364237 |
| A14 | 106.47818263 |
| A15 | 109.93774865 |
| A16 | 109.37874886 |
| A17 | 96.59531087 |
| D1 | 119.45139911 |
| D2 | 120.13952923 |
| D3 | -54.34025832 |
| D4 | -163.38270050 |
| D5 | -92.37278002 |
| D6 | -81.45845790 |
| D7 | 167.18365888 |
| D8 | -60.34789337 |
| D9 | 63.21876756 |
| D10 | -177.49954936 |
| D11 | -98.39965615 |
| D12 | -67.68036866 |

| | |
|-----|--------------|
| D13 | 46.58430182 |
| D14 | 42.48242440 |
| D15 | 153.56172692 |
| D16 | 101.57303697 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|--------|---------|---------|---------|---------|---------|---------|--------|
| 488.52 <i>i</i> | 43.59 | 96.17 | 100.61 | 138.43 | 155.40 | 211.22 | 248.63 | 284.64 | 295.72 | 339.47 |
| 378.91 | 415.29 | 519.61 | 540.79 | 637.73 | 713.56 | 859.22 | 878.58 | 918.11 | 954.36 | |
| 972.51 | 1009.51 | 1095.22 | | 1144.96 | 1147.52 | 1155.00 | 1183.60 | 1304.44 | 1363.32 | |
| 1377.04 | 1399.35 | 1408.42 | | 1425.68 | 1431.37 | 1450.65 | 1480.85 | 1486.90 | 1499.40 | |
| 1545.86 | 1608.30 | 2045.48 | | 3053.53 | 3070.06 | 3088.81 | 3142.64 | 3144.09 | 3168.99 | |
| 3169.92 | 3198.77 | 3823.56 | | | | | | | | |

Rotational constants (B/GHZ): 2.7039816 0.9326103 0.8737853



P5d

| C | | B1 | | | | | |
|---|----|-----|---|-----|---|-----|---|
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| O | 1 | B5 | 2 | A4 | 5 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 | 0 |
| C | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| C | 9 | B9 | 6 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 9 | A9 | 6 | D8 | 0 |
| H | 10 | B11 | 9 | A10 | 6 | D9 | 0 |
| H | 10 | B12 | 9 | A11 | 6 | D10 | 0 |
| O | 9 | B13 | 6 | A12 | 1 | D11 | 0 |
| O | 9 | B14 | 6 | A13 | 1 | D12 | 0 |
| H | 9 | B15 | 6 | A14 | 1 | D13 | 0 |
| H | 1 | B16 | 6 | A15 | 9 | D14 | 0 |
| O | 8 | B17 | 1 | A16 | 6 | D15 | 0 |
| H | 8 | B18 | 1 | A17 | 6 | D16 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.50818835 |
| B2 | 1.08795330 |
| B3 | 1.08783270 |
| B4 | 1.08677247 |

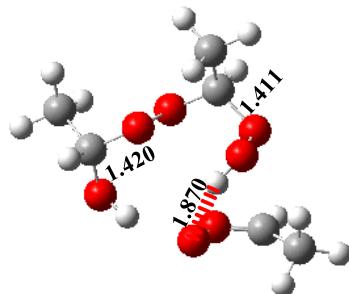
| | |
|-----|---------------|
| B5 | 1.40008457 |
| B6 | 2.86300873 |
| B7 | 2.30289480 |
| B8 | 1.40821269 |
| B9 | 1.50739267 |
| B10 | 1.08780228 |
| B11 | 1.08728782 |
| B12 | 1.08766856 |
| B13 | 2.30290612 |
| B14 | 1.40402939 |
| B15 | 1.09604673 |
| B16 | 1.09391248 |
| B17 | 1.41735732 |
| B18 | 0.97034732 |
| A1 | 109.39649757 |
| A2 | 109.68270261 |
| A3 | 110.04649901 |
| A4 | 108.92328411 |
| A5 | 77.04745371 |
| A6 | 90.02642843 |
| A7 | 116.37608360 |
| A8 | 107.67992309 |
| A9 | 109.74649478 |
| A10 | 109.63823721 |
| A11 | 109.50157912 |
| A12 | 94.02158832 |
| A13 | 112.48916455 |
| A14 | 109.78196710 |
| A15 | 111.14801185 |
| A16 | 35.71978673 |
| A17 | 86.09984124 |
| D1 | 120.06263353 |
| D2 | -119.79683665 |
| D3 | -54.80417520 |
| D4 | 147.77300240 |
| D5 | -92.95118463 |
| D6 | -150.84400215 |
| D7 | -172.28723493 |
| D8 | -59.04007568 |
| D9 | 60.88747044 |
| D10 | -179.30524038 |
| D11 | -77.75466014 |
| D12 | -46.37408592 |
| D13 | 65.51803562 |

D14 -26.43530865
 D15 -124.80010293
 D16 -7.74887022

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 76.24 | 105.26 | 166.73 | 189.33 | 202.74 | 236.79 | 242.68 | 286.36 | 311.05 | 342.93 |
| 374.60 | 439.26 | 466.79 | 586.33 | 600.22 | 692.36 | 726.28 | 848.21 | 878.52 | 935.36 |
| 983.00 | 1006.16 | 1028.20 | 1124.95 | 1136.21 | 1154.42 | 1160.83 | 1178.80 | 1224.78 | |
| 1351.84 | 1370.90 | 1387.27 | 1410.48 | 1423.88 | 1434.83 | 1454.11 | 1461.76 | 1489.36 | |
| 1490.66 | 1498.00 | 1504.03 | 3070.98 | 3077.10 | 3080.67 | 3095.91 | 3157.49 | 3162.09 | |
| 3169.41 | 3171.57 | 3728.06 | 3756.89 | | | | | | |

Rotational constants (B/GHZ): 2.4325109 1.2895706 1.0352357



IM6a

| C | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 0 |
| C | 4 | B5 | 1 | A4 | 3 | D3 0 |
| C | 6 | B6 | 4 | A5 | 1 | D4 0 |
| H | 7 | B7 | 6 | A6 | 4 | D5 0 |
| H | 7 | B8 | 6 | A7 | 4 | D6 0 |
| H | 7 | B9 | 6 | A8 | 4 | D7 0 |
| O | 6 | B10 | 4 | A9 | 1 | D8 0 |
| O | 6 | B11 | 4 | A10 | 1 | D9 0 |
| H | 6 | B12 | 4 | A11 | 1 | D10 0 |
| C | 1 | B13 | 4 | A12 | 3 | D11 0 |
| H | 14 | B14 | 1 | A13 | 4 | D12 0 |
| H | 14 | B15 | 1 | A14 | 4 | D13 0 |
| H | 14 | B16 | 1 | A15 | 4 | D14 0 |
| O | 1 | B17 | 4 | A16 | 3 | D15 0 |
| O | 18 | B18 | 1 | A17 | 4 | D16 0 |
| C | 19 | B19 | 18 | A18 | 1 | D17 0 |
| H | 20 | B20 | 19 | A19 | 18 | D18 0 |
| C | 20 | B21 | 19 | A20 | 18 | D19 0 |
| H | 22 | B22 | 20 | A21 | 19 | D20 0 |
| H | 22 | B23 | 20 | A22 | 19 | D21 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 22 | B24 | 20 | A23 | 19 | D22 | 0 |
| O | 20 | B25 | 19 | A24 | 18 | D23 | 0 |
| H | 26 | B26 | 20 | A25 | 19 | D24 | 0 |

Variables:

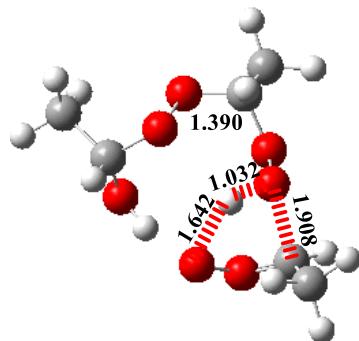
| | |
|-----|--------------|
| B1 | 1.09287536 |
| B2 | 2.32738864 |
| B3 | 1.41141271 |
| B4 | 0.98086524 |
| B5 | 2.87681419 |
| B6 | 1.46457416 |
| B7 | 1.09139947 |
| B8 | 1.08456401 |
| B9 | 1.09498544 |
| B10 | 2.23425260 |
| B11 | 1.24111813 |
| B12 | 1.08577021 |
| B13 | 1.51181071 |
| B14 | 1.08387126 |
| B15 | 1.08802231 |
| B16 | 1.08818453 |
| B17 | 1.39787059 |
| B18 | 1.43399497 |
| B19 | 1.42019190 |
| B20 | 1.09807819 |
| B21 | 1.51096727 |
| B22 | 1.08804558 |
| B23 | 1.08840268 |
| B24 | 1.08713542 |
| B25 | 1.37943248 |
| B26 | 0.97474228 |
| A1 | 136.42185312 |
| A2 | 34.85893841 |
| A3 | 97.92337524 |
| A4 | 124.86729812 |
| A5 | 87.26356072 |
| A6 | 108.54494301 |
| A7 | 110.91374758 |
| A8 | 108.04718416 |
| A9 | 74.73542775 |
| A10 | 79.91007072 |
| A11 | 103.86199850 |
| A12 | 113.19030673 |
| A13 | 110.89049875 |
| A14 | 108.99922854 |

| | |
|-----|---------------|
| A15 | 108.93288371 |
| A16 | 112.05865525 |
| A17 | 107.86499372 |
| A18 | 107.71374457 |
| A19 | 99.41269395 |
| A20 | 112.80979003 |
| A21 | 109.05980856 |
| A22 | 110.17389826 |
| A23 | 109.67839216 |
| A24 | 112.30687072 |
| A25 | 108.83043346 |
| D1 | 13.33381438 |
| D2 | -98.30229382 |
| D3 | 111.96626526 |
| D4 | -170.45647803 |
| D5 | 122.16050601 |
| D6 | -114.11398966 |
| D7 | 7.30480567 |
| D8 | -79.57699612 |
| D9 | -45.71494835 |
| D10 | 65.10500140 |
| D11 | 50.57467422 |
| D12 | -63.64245638 |
| D13 | 56.58679910 |
| D14 | 175.99623126 |
| D15 | -80.41607682 |
| D16 | 81.18760018 |
| D17 | -177.80747878 |
| D18 | -176.50369968 |
| D19 | -58.93744991 |
| D20 | -172.35662132 |
| D21 | -52.25122026 |
| D22 | 68.60096661 |
| D23 | 64.86032000 |
| D24 | 40.80129617 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 55.76 | 65.09 | 88.11 | 89.46 | 111.26 | 122.31 | 134.83 | 153.69 | 167.94 | 192.04 | 211.54 |
| 223.66 | 234.75 | 245.52 | 261.93 | 332.45 | 359.84 | 423.33 | 473.72 | 478.94 | 499.76 | |
| 518.46 | 655.36 | 669.20 | 703.68 | 734.40 | 758.43 | 800.41 | 858.64 | 882.66 | 915.80 | |
| 937.31 | 959.15 | 997.39 | 1003.38 | 1018.55 | 1102.26 | 1109.16 | 1126.71 | 1138.81 | | |
| 1145.16 | 1170.31 | 1193.31 | 1214.35 | 1335.74 | 1352.33 | 1370.60 | 1375.72 | 1397.31 | | |
| 1405.42 | 1420.06 | 1424.73 | 1455.82 | 1477.81 | 1481.35 | 1483.40 | 1494.21 | 1502.65 | | |
| 1504.07 | 1549.50 | 1687.43 | 3042.74 | 3043.87 | 3072.77 | 3079.67 | 3103.79 | 3114.80 | | |
| 3151.69 | 3154.21 | 3161.86 | 3182.58 | 3186.85 | 3206.47 | 3512.72 | 3606.66 | | | |

Rotational constants (B/GHZ): 1.0060411 0.6278635 0.4466521



TS6a

| C | | B1 | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 3 | B3 | 1 | A2 | 2 | D1 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 0 |
| C | 3 | B5 | 1 | A4 | 4 | D3 0 |
| C | 6 | B6 | 3 | A5 | 1 | D4 0 |
| H | 7 | B7 | 6 | A6 | 3 | D5 0 |
| H | 7 | B8 | 6 | A7 | 3 | D6 0 |
| H | 7 | B9 | 6 | A8 | 3 | D7 0 |
| O | 6 | B10 | 3 | A9 | 1 | D8 0 |
| O | 6 | B11 | 3 | A10 | 1 | D9 0 |
| H | 6 | B12 | 3 | A11 | 1 | D10 0 |
| C | 1 | B13 | 4 | A12 | 3 | D11 0 |
| H | 14 | B14 | 1 | A13 | 4 | D12 0 |
| H | 14 | B15 | 1 | A14 | 4 | D13 0 |
| H | 14 | B16 | 1 | A15 | 4 | D14 0 |
| O | 1 | B17 | 4 | A16 | 3 | D15 0 |
| O | 18 | B18 | 1 | A17 | 4 | D16 0 |
| C | 19 | B19 | 18 | A18 | 1 | D17 0 |
| H | 20 | B20 | 19 | A19 | 18 | D18 0 |
| C | 20 | B21 | 19 | A20 | 18 | D19 0 |
| H | 22 | B22 | 20 | A21 | 19 | D20 0 |
| H | 22 | B23 | 20 | A22 | 19 | D21 0 |
| H | 22 | B24 | 20 | A23 | 19 | D22 0 |
| O | 20 | B25 | 19 | A24 | 18 | D23 0 |
| H | 26 | B26 | 20 | A25 | 19 | D24 0 |

Variables:

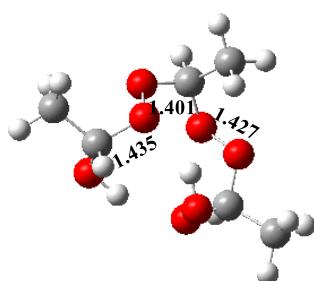
| | |
|----|------------|
| B1 | 1.09183096 |
| B2 | 2.33197421 |
| B3 | 1.41685100 |
| B4 | 1.03225747 |
| B5 | 1.90829277 |

| | |
|-----|--------------|
| B6 | 1.48722023 |
| B7 | 1.08376033 |
| B8 | 1.09310454 |
| B9 | 1.08613398 |
| B10 | 2.20188774 |
| B11 | 1.27760448 |
| B12 | 1.08826181 |
| B13 | 1.51292417 |
| B14 | 1.08523985 |
| B15 | 1.08802888 |
| B16 | 1.08766105 |
| B17 | 1.39041221 |
| B18 | 1.42921786 |
| B19 | 1.43889664 |
| B20 | 1.09755377 |
| B21 | 1.51013212 |
| B22 | 1.08784261 |
| B23 | 1.08808741 |
| B24 | 1.08750739 |
| B25 | 1.36919656 |
| B26 | 0.97956998 |
| A1 | 134.14170158 |
| A2 | 34.74394144 |
| A3 | 98.12373878 |
| A4 | 138.05780980 |
| A5 | 95.44895921 |
| A6 | 111.48993433 |
| A7 | 106.18624950 |
| A8 | 110.02139260 |
| A9 | 74.91290217 |
| A10 | 96.24918186 |
| A11 | 102.49187922 |
| A12 | 113.36023984 |
| A13 | 111.07409655 |
| A14 | 109.89352536 |
| A15 | 108.21289537 |
| A16 | 111.80764561 |
| A17 | 107.22571632 |
| A18 | 107.31414643 |
| A19 | 99.08168036 |
| A20 | 111.53136400 |
| A21 | 108.95860392 |
| A22 | 110.49601309 |
| A23 | 109.52416990 |

| | |
|-----|---------------|
| A24 | 112.49398268 |
| A25 | 107.80051948 |
| D1 | -27.76538437 |
| D2 | -104.32885156 |
| D3 | -15.01535013 |
| D4 | 173.04130624 |
| D5 | 60.13600344 |
| D6 | 178.57105549 |
| D7 | -63.92713247 |
| D8 | -93.83844414 |
| D9 | -62.23506284 |
| D10 | 52.04833222 |
| D11 | 39.63015828 |
| D12 | -70.87500489 |
| D13 | 50.17841284 |
| D14 | 169.58601900 |
| D15 | -90.53237851 |
| D16 | 67.79116729 |
| D17 | -146.75994374 |
| D18 | -175.83685933 |
| D19 | -58.37616223 |
| D20 | -170.57101551 |
| D21 | -50.24978892 |
| D22 | 70.66379801 |
| D23 | 65.21947214 |
| D24 | 62.95082382 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-------------------------------|---------|---------|---------|-----------|---------|-----------|---------|-----------|--------|--------|
| 390.07 <i>i</i> | 55.88 | 63.95 | 81.18 | 104.36 | 117.34 | 123.68 | 154.05 | 175.05 | 194.85 | 229.80 |
| 241.43 | 250.52 | 260.42 | 289.76 | 357.62 | 379.32 | 423.91 | 474.74 | 498.75 | 513.24 | |
| 543.24 | 656.42 | 674.97 | 729.85 | 844.58 | 855.83 | 867.81 | 873.85 | 930.57 | 944.54 | |
| 954.44 | 985.80 | 989.42 | 1012.65 | 1082.62 | 1101.87 | 1126.72 | 1142.10 | 1146.21 | | |
| 1165.76 | 1170.86 | 1195.89 | 1217.40 | 1351.63 | 1354.96 | 1357.57 | 1375.17 | 1400.08 | | |
| 1408.94 | 1414.16 | 1425.68 | 1452.30 | 1481.39 | 1486.55 | 1489.23 | 1496.65 | 1502.20 | | |
| 1507.31 | 1522.96 | 1577.75 | 2656.32 | 3055.17 | 3057.88 | 3073.68 | 3077.09 | 3116.16 | | |
| 3143.12 | 3150.37 | 3154.75 | 3169.13 | 3173.37 | 3187.51 | 3200.96 | 3461.22 | | | |
| Rotational constants (B/GHZ): | | | | | | | | | | |
| | | | | 1.0840814 | | 0.6088555 | | 0.4437379 | | |



P6a

| C | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 0 |
| C | 3 | B5 | 1 | A4 | 4 | D3 0 |
| C | 6 | B6 | 3 | A5 | 1 | D4 0 |
| H | 7 | B7 | 6 | A6 | 3 | D5 0 |
| H | 7 | B8 | 6 | A7 | 3 | D6 0 |
| H | 7 | B9 | 6 | A8 | 3 | D7 0 |
| O | 6 | B10 | 3 | A9 | 1 | D8 0 |
| O | 6 | B11 | 3 | A10 | 1 | D9 0 |
| H | 6 | B12 | 3 | A11 | 1 | D10 0 |
| C | 1 | B13 | 4 | A12 | 3 | D11 0 |
| H | 14 | B14 | 1 | A13 | 4 | D12 0 |
| H | 14 | B15 | 1 | A14 | 4 | D13 0 |
| H | 14 | B16 | 1 | A15 | 4 | D14 0 |
| O | 1 | B17 | 4 | A16 | 3 | D15 0 |
| O | 18 | B18 | 1 | A17 | 4 | D16 0 |
| C | 19 | B19 | 18 | A18 | 1 | D17 0 |
| H | 20 | B20 | 19 | A19 | 18 | D18 0 |
| C | 20 | B21 | 19 | A20 | 18 | D19 0 |
| H | 22 | B22 | 20 | A21 | 19 | D20 0 |
| H | 22 | B23 | 20 | A22 | 19 | D21 0 |
| H | 22 | B24 | 20 | A23 | 19 | D22 0 |
| O | 20 | B25 | 19 | A24 | 18 | D23 0 |
| H | 26 | B26 | 20 | A25 | 19 | D24 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.09232775 |
| B2 | 2.33227046 |
| B3 | 1.40996116 |
| B4 | 2.48304988 |
| B5 | 1.39609152 |
| B6 | 1.51052232 |
| B7 | 1.08672300 |
| B8 | 1.08747722 |
| B9 | 1.08717845 |
| B10 | 2.30016204 |
| B11 | 1.40984943 |
| B12 | 1.09180856 |
| B13 | 1.51263130 |
| B14 | 1.08574357 |
| B15 | 1.08745955 |
| B16 | 1.08735744 |

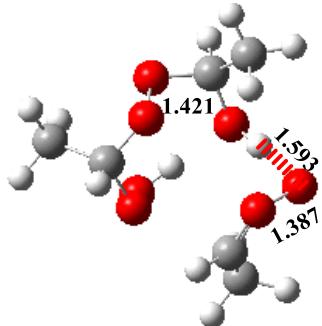
| | |
|-----|---------------|
| B17 | 1.40129954 |
| B18 | 1.42405746 |
| B19 | 1.43518760 |
| B20 | 1.09686422 |
| B21 | 1.50851575 |
| B22 | 1.08777840 |
| B23 | 1.08793578 |
| B24 | 1.08716011 |
| B25 | 1.37686178 |
| B26 | 0.96634165 |
| A1 | 130.89861590 |
| A2 | 34.96018747 |
| A3 | 84.70741739 |
| A4 | 133.32536480 |
| A5 | 106.48227027 |
| A6 | 110.23352883 |
| A7 | 108.88689193 |
| A8 | 109.62562136 |
| A9 | 91.97763633 |
| A10 | 111.25361993 |
| A11 | 110.17852313 |
| A12 | 114.33971172 |
| A13 | 111.11211706 |
| A14 | 110.04900569 |
| A15 | 108.08649059 |
| A16 | 112.07933827 |
| A17 | 109.14848862 |
| A18 | 107.12225815 |
| A19 | 99.98923234 |
| A20 | 111.88696994 |
| A21 | 109.03752352 |
| A22 | 110.20648783 |
| A23 | 109.59722007 |
| A24 | 112.03825063 |
| A25 | 108.73180053 |
| D1 | 46.54635227 |
| D2 | -116.51466728 |
| D3 | -50.42379564 |
| D4 | -170.55362763 |
| D5 | 54.59623062 |
| D6 | 174.14923184 |
| D7 | -65.96773505 |
| D8 | -77.56831130 |
| D9 | -46.89186177 |

| | |
|-----|---------------|
| D10 | 66.50660692 |
| D11 | 24.23869591 |
| D12 | -69.64380208 |
| D13 | 50.93918457 |
| D14 | 170.66503171 |
| D15 | -106.24309267 |
| D16 | 69.30988564 |
| D17 | -143.58429472 |
| D18 | -177.74184681 |
| D19 | -59.60869062 |
| D20 | -172.58315682 |
| D21 | -52.45821765 |
| D22 | 68.31886924 |
| D23 | 63.26376140 |
| D24 | 53.76675720 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 58.05 | 73.13 | 100.93 | 117.40 | 140.59 | 158.65 | 188.44 | 201.84 | 225.77 | 239.41 | 245.19 |
| 260.83 | 278.36 | 311.17 | 347.83 | 400.38 | 428.63 | 469.20 | 493.20 | 521.51 | 552.26 | |
| 575.16 | 633.04 | 680.30 | 701.42 | 716.79 | 867.54 | 872.22 | 884.62 | 936.70 | 949.90 | |
| 959.39 | 998.67 | 1011.85 | 1032.27 | 1092.68 | 1139.62 | 1141.92 | 1145.93 | 1147.71 | | |
| 162.64 | 1190.11 | 1210.18 | 1220.68 | 1331.36 | 1356.20 | 1363.53 | 1374.46 | 1391.45 | | |
| 1407.05 | 1414.22 | 1424.19 | 1425.73 | 1478.25 | 1488.79 | 1490.56 | 1491.61 | 1498.05 | | |
| 1501.13 | 1502.96 | 1505.86 | 3060.55 | 3079.20 | 3080.12 | 3083.12 | 3115.76 | 3127.66 | | |
| 3157.22 | 3159.06 | 3165.42 | 3169.59 | 3176.07 | 3178.08 | 3686.91 | 3787.18 | | | |

Rotational constants (B/GHZ): 1.1166091 0.6430181 0.4836962



IM6b

| | | | | | | | |
|---|---|----|---|----|---|----|---|
| C | | B1 | | | | | |
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| O | 1 | B5 | 2 | A4 | 5 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 | 0 |
| C | 6 | B8 | 1 | A7 | 2 | D6 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 9 | B9 | 6 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 9 | A9 | 6 | D8 | 0 |
| H | 10 | B11 | 9 | A10 | 6 | D9 | 0 |
| H | 10 | B12 | 9 | A11 | 6 | D10 | 0 |
| O | 9 | B13 | 6 | A12 | 1 | D11 | 0 |
| O | 9 | B14 | 6 | A13 | 1 | D12 | 0 |
| H | 1 | B15 | 6 | A14 | 2 | D13 | 0 |
| O | 1 | B16 | 6 | A15 | 2 | D14 | 0 |
| C | 8 | B17 | 1 | A16 | 6 | D15 | 0 |
| H | 18 | B18 | 8 | A17 | 1 | D16 | 0 |
| C | 18 | B19 | 8 | A18 | 1 | D17 | 0 |
| H | 20 | B20 | 18 | A19 | 8 | D18 | 0 |
| H | 20 | B21 | 18 | A20 | 8 | D19 | 0 |
| H | 20 | B22 | 18 | A21 | 8 | D20 | 0 |
| O | 18 | B23 | 8 | A22 | 1 | D21 | 0 |
| O | 24 | B24 | 18 | A23 | 8 | D22 | 0 |
| H | 25 | B25 | 24 | A24 | 18 | D23 | 0 |
| H | 9 | B26 | 6 | A25 | 1 | D24 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.51317426 |
| B2 | 1.08840511 |
| B3 | 1.08804452 |
| B4 | 1.08735391 |
| B5 | 1.38992697 |
| B6 | 1.00260691 |
| B7 | 2.30936846 |
| B8 | 3.50119046 |
| B9 | 1.46537993 |
| B10 | 1.09108267 |
| B11 | 1.09242474 |
| B12 | 1.08427370 |
| B13 | 2.23403508 |
| B14 | 1.24319643 |
| B15 | 1.09320907 |
| B16 | 1.42107042 |
| B17 | 1.40370076 |
| B18 | 1.09357734 |
| B19 | 1.51040113 |
| B20 | 1.08784133 |
| B21 | 1.08794685 |
| B22 | 1.08379600 |
| B23 | 1.41124339 |
| B24 | 1.41677449 |
| B25 | 0.98427302 |

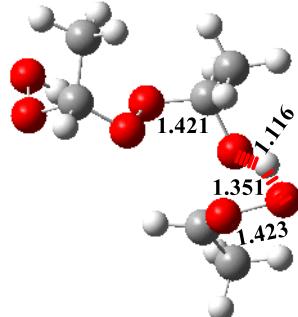
| | |
|-----|---------------|
| B26 | 1.08478801 |
| A1 | 109.42188671 |
| A2 | 109.58543282 |
| A3 | 110.50917541 |
| A4 | 112.95366151 |
| A5 | 111.58769451 |
| A6 | 95.86864899 |
| A7 | 117.97673452 |
| A8 | 81.23215186 |
| A9 | 108.90925358 |
| A10 | 108.14001914 |
| A11 | 110.80712111 |
| A12 | 47.68340738 |
| A13 | 62.46799949 |
| A14 | 108.59419711 |
| A15 | 110.73243326 |
| A16 | 125.89146972 |
| A17 | 102.03480640 |
| A18 | 114.05795790 |
| A19 | 109.04087900 |
| A20 | 108.86854776 |
| A21 | 110.81228817 |
| A22 | 112.25030447 |
| A23 | 111.48351364 |
| A24 | 101.35621500 |
| A25 | 131.26928206 |
| D1 | 120.00218236 |
| D2 | -119.30539364 |
| D3 | -58.76953185 |
| D4 | 16.46870264 |
| D5 | -93.43476402 |
| D6 | 63.78321017 |
| D7 | 168.13713478 |
| D8 | -11.40965599 |
| D9 | 103.86552760 |
| D10 | -132.76709815 |
| D11 | -94.71724775 |
| D12 | -57.05316559 |
| D13 | 123.89810973 |
| D14 | -127.08452562 |
| D15 | -44.86921973 |
| D16 | 156.56772324 |
| D17 | -83.10845370 |
| D18 | -174.38975763 |

| | |
|-----|--------------|
| D19 | -54.82769480 |
| D20 | 65.44514466 |
| D21 | 47.70671429 |
| D22 | -83.32124957 |
| D23 | 79.18160109 |
| D24 | 40.38019172 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 31.79 | 45.34 | 71.63 | 91.34 | 119.93 | 132.08 | 140.86 | 152.71 | 167.70 | 211.75 | 217.09 |
| 237.67 | 261.64 | 275.15 | 287.50 | 332.28 | 335.39 | 436.93 | 471.20 | 504.59 | 509.92 | |
| 527.62 | 672.74 | 680.10 | 737.88 | 799.94 | 823.86 | 851.51 | 868.41 | 906.46 | 932.23 | |
| 954.67 | 991.32 | 1003.98 | 1021.43 | 1046.01 | 1099.33 | 1111.87 | 1120.23 | 1142.33 | | |
| 1148.34 | 1163.65 | 1194.50 | 1200.62 | 1355.09 | 1358.69 | 1365.28 | 1379.20 | 1409.46 | | |
| 1413.78 | 1421.14 | 1425.82 | 1444.08 | 1462.90 | 1488.55 | 1490.85 | 1491.21 | 1502.08 | | |
| 1506.06 | 1549.07 | 1680.30 | 2966.53 | 3060.74 | 3075.03 | 3086.23 | 3100.24 | 3105.57 | | |
| 3120.26 | 3152.80 | 3160.95 | 3172.54 | 3185.71 | 3195.50 | 3203.23 | 3404.80 | | | |

Rotational constants (B/GHZ): 0.9289166 0.7259506 0.5181123



TS6b

| C | | B1 | | | | | |
|---|----|-----|---|-----|---|-----|---|
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| O | 1 | B5 | 2 | A4 | 5 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 | 0 |
| C | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| C | 9 | B9 | 6 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 9 | A9 | 6 | D8 | 0 |
| H | 10 | B11 | 9 | A10 | 6 | D9 | 0 |
| H | 10 | B12 | 9 | A11 | 6 | D10 | 0 |
| O | 9 | B13 | 6 | A12 | 1 | D11 | 0 |
| O | 9 | B14 | 6 | A13 | 1 | D12 | 0 |
| H | 1 | B15 | 6 | A14 | 9 | D13 | 0 |
| O | 1 | B16 | 6 | A15 | 9 | D14 | 0 |
| C | 8 | B17 | 1 | A16 | 6 | D15 | 0 |
| H | 18 | B18 | 8 | A17 | 1 | D16 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 18 | B19 | 8 | A18 | 1 | D17 | 0 |
| H | 20 | B20 | 18 | A19 | 8 | D18 | 0 |
| H | 20 | B21 | 18 | A20 | 8 | D19 | 0 |
| H | 20 | B22 | 18 | A21 | 8 | D20 | 0 |
| O | 18 | B23 | 8 | A22 | 1 | D21 | 0 |
| O | 24 | B24 | 18 | A23 | 8 | D22 | 0 |
| H | 25 | B25 | 24 | A24 | 18 | D23 | 0 |
| H | 9 | B26 | 6 | A25 | 1 | D24 | 0 |

Variables:

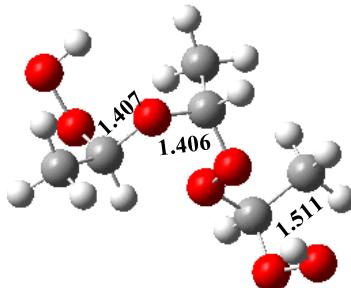
| | |
|-----|--------------|
| B1 | 1.51399662 |
| B2 | 1.08895147 |
| B3 | 1.08833497 |
| B4 | 1.08755876 |
| B5 | 1.39235250 |
| B6 | 1.11559127 |
| B7 | 2.32878812 |
| B8 | 2.02765906 |
| B9 | 1.48228714 |
| B10 | 1.08572901 |
| B11 | 1.08276327 |
| B12 | 1.09466229 |
| B13 | 2.20037070 |
| B14 | 1.27565320 |
| B15 | 1.09461200 |
| B16 | 1.42052603 |
| B17 | 1.41330311 |
| B18 | 1.09225917 |
| B19 | 1.51061594 |
| B20 | 1.08781882 |
| B21 | 1.08816878 |
| B22 | 1.08523799 |
| B23 | 1.40006795 |
| B24 | 1.41704229 |
| B25 | 0.96681096 |
| B26 | 1.08727512 |
| A1 | 108.80132582 |
| A2 | 110.03866314 |
| A3 | 110.71951449 |
| A4 | 112.87207872 |
| A5 | 113.06415763 |
| A6 | 99.44642741 |
| A7 | 121.08602261 |
| A8 | 91.92531681 |
| A9 | 109.72791230 |

| | |
|-----|---------------|
| A10 | 111.86206078 |
| A11 | 105.72621397 |
| A12 | 68.76500782 |
| A13 | 92.83081702 |
| A14 | 107.86541923 |
| A15 | 110.96154713 |
| A16 | 132.55427674 |
| A17 | 101.65079116 |
| A18 | 113.69161859 |
| A19 | 109.03699467 |
| A20 | 108.92685577 |
| A21 | 111.16905132 |
| A22 | 111.12891098 |
| A23 | 110.65766449 |
| A24 | 102.29726169 |
| A25 | 106.95266913 |
| D1 | 119.14264472 |
| D2 | -118.96687882 |
| D3 | -59.29506347 |
| D4 | 3.43441022 |
| D5 | -93.29438901 |
| D6 | 88.69964630 |
| D7 | 159.20467327 |
| D8 | -62.39200400 |
| D9 | 61.39615006 |
| D10 | -179.22084156 |
| D11 | -105.77070651 |
| D12 | -76.20195743 |
| D13 | -148.13872073 |
| D14 | -39.33985431 |
| D15 | -168.56812700 |
| D16 | -151.12819780 |
| D17 | -30.98163922 |
| D18 | 179.32994131 |
| D19 | -61.37434680 |
| D20 | 59.50000732 |
| D21 | 99.63857868 |
| D22 | -86.08386313 |
| D23 | 77.60741106 |
| D24 | 37.93221196 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|--------|--------|--------|--------|--------|--------|--------|--------|--------|--------|
| 649.03 <i>i</i> | 34.87 | 38.63 | 78.35 | 89.77 | 108.76 | 134.84 | 150.52 | 202.51 | 219.08 | 225.14 |
| 241.54 | 250.41 | 269.29 | 310.63 | 337.99 | 369.04 | 385.81 | 441.02 | 462.22 | 507.90 | |
| 527.72 | 541.14 | 631.79 | 681.62 | 745.41 | 850.70 | 858.54 | 871.53 | 921.26 | 931.32 | |

| | | | | | | | | |
|-------------------------------|---------|---------|---------|-----------|-----------|-----------|---------|---------|
| 950.42 | 967.28 | 989.51 | 1020.35 | 1043.65 | 1108.15 | 1127.14 | 1153.28 | 1156.78 |
| 1162.01 | 1172.00 | 1192.23 | 1219.97 | 1353.63 | 1359.10 | 1367.23 | 1376.86 | 1397.56 |
| 1403.48 | 1418.70 | 1422.21 | 1448.00 | 1461.21 | 1479.48 | 1483.75 | 1485.54 | 1494.72 |
| 1499.80 | 1504.78 | 1597.72 | 1880.60 | 3048.09 | 3071.46 | 3076.57 | 3086.11 | 3117.90 |
| 3146.56 | 3151.49 | 3157.05 | 3168.14 | 3183.75 | 3203.26 | 3216.63 | 3802.54 | |
| Rotational constants (B/GHZ): | | | | 1.3397503 | 0.4587138 | 0.4208758 | | |



P6b

C

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| O | 1 | B5 | 2 | A4 | 5 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 | 0 |
| C | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| C | 9 | B9 | 6 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 9 | A9 | 6 | D8 | 0 |
| H | 10 | B11 | 9 | A10 | 6 | D9 | 0 |
| H | 10 | B12 | 9 | A11 | 6 | D10 | 0 |
| O | 9 | B13 | 6 | A12 | 1 | D11 | 0 |
| O | 9 | B14 | 6 | A13 | 1 | D12 | 0 |
| H | 1 | B15 | 6 | A14 | 9 | D13 | 0 |
| O | 1 | B16 | 6 | A15 | 9 | D14 | 0 |
| C | 8 | B17 | 1 | A16 | 6 | D15 | 0 |
| H | 18 | B18 | 8 | A17 | 1 | D16 | 0 |
| C | 18 | B19 | 8 | A18 | 1 | D17 | 0 |
| H | 20 | B20 | 18 | A19 | 8 | D18 | 0 |
| H | 20 | B21 | 18 | A20 | 8 | D19 | 0 |
| H | 20 | B22 | 18 | A21 | 8 | D20 | 0 |
| O | 18 | B23 | 8 | A22 | 1 | D21 | 0 |
| O | 24 | B24 | 18 | A23 | 8 | D22 | 0 |
| H | 25 | B25 | 24 | A24 | 18 | D23 | 0 |
| H | 9 | B26 | 6 | A25 | 1 | D24 | 0 |

Variables:

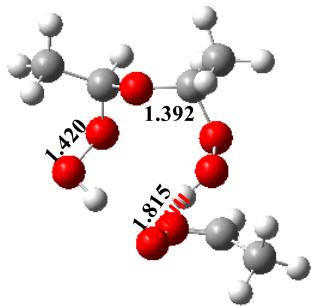
| | |
|----|------------|
| B1 | 1.51553945 |
|----|------------|

| | |
|-----|--------------|
| B2 | 1.08984968 |
| B3 | 1.08885590 |
| B4 | 1.08551591 |
| B5 | 1.40627607 |
| B6 | 2.53388302 |
| B7 | 2.32936067 |
| B8 | 1.40726816 |
| B9 | 1.50880351 |
| B10 | 1.08758529 |
| B11 | 1.08657176 |
| B12 | 1.08792037 |
| B13 | 2.30452359 |
| B14 | 1.41067256 |
| B15 | 1.09121741 |
| B16 | 1.41131701 |
| B17 | 1.41405674 |
| B18 | 1.09201683 |
| B19 | 1.51134044 |
| B20 | 1.08776333 |
| B21 | 1.08829637 |
| B22 | 1.08523736 |
| B23 | 1.39868601 |
| B24 | 1.41689016 |
| B25 | 0.96652364 |
| B26 | 1.09072761 |
| A1 | 108.25187425 |
| A2 | 109.55325584 |
| A3 | 111.44597072 |
| A4 | 113.70779610 |
| A5 | 102.43054855 |
| A6 | 106.41497271 |
| A7 | 118.98820491 |
| A8 | 107.45004050 |
| A9 | 109.34452298 |
| A10 | 110.27344214 |
| A11 | 109.39723970 |
| A12 | 94.42182086 |
| A13 | 111.43212349 |
| A14 | 104.10005531 |
| A15 | 112.27363653 |
| A16 | 133.19787457 |
| A17 | 101.43222052 |
| A18 | 113.56912065 |
| A19 | 109.08606719 |

| | |
|-----|---------------|
| A20 | 109.00075566 |
| A21 | 111.14940638 |
| A22 | 111.34154654 |
| A23 | 110.63066598 |
| A24 | 102.20651625 |
| A25 | 110.69356374 |
| D1 | 117.81243089 |
| D2 | -120.87017488 |
| D3 | -61.82055000 |
| D4 | -0.61021759 |
| D5 | -93.46094095 |
| D6 | 78.80582207 |
| D7 | 165.49149803 |
| D8 | -65.26258622 |
| D9 | 54.72699941 |
| D10 | 174.84159232 |
| D11 | -101.93468293 |
| D12 | -69.86832660 |
| D13 | -161.11388746 |
| D14 | -51.53678302 |
| D15 | -157.70696352 |
| D16 | -153.08035543 |
| D17 | -32.97466576 |
| D18 | 177.75671975 |
| D19 | -63.01711282 |
| D20 | 57.99206491 |
| D21 | 97.69601128 |
| D22 | -86.36157161 |
| D23 | 81.26654545 |
| D24 | 42.89362777 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-------------------------------|---------|---------|-----------|---------|-----------|---------|-----------|---------|--------|--------|
| 33.62 | 39.08 | 76.83 | 106.68 | 118.57 | 142.98 | 157.94 | 192.04 | 217.34 | 235.13 | 252.07 |
| 260.02 | 271.41 | 280.07 | 309.82 | 333.64 | 365.68 | 409.64 | 420.99 | 471.69 | 516.58 | |
| 533.92 | 569.67 | 694.26 | 715.89 | 750.79 | 832.71 | 859.64 | 884.65 | 928.20 | 938.84 | |
| 965.31 | 999.30 | 1018.52 | 1021.78 | 1109.58 | 1123.29 | 1134.17 | 1154.59 | 1161.22 | | |
| 1171.66 | 1189.62 | 1198.40 | 1207.70 | 1355.15 | 1368.38 | 1389.01 | 1391.57 | 1397.95 | | |
| 1415.93 | 1419.68 | 1423.57 | 1432.71 | 1441.88 | 1463.52 | 1486.50 | 1487.32 | 1497.82 | | |
| 1499.27 | 1505.46 | 1509.63 | 3073.49 | 3078.38 | 3082.97 | 3116.06 | 3121.12 | 3134.99 | | |
| 3145.00 | 3156.03 | 3159.83 | 3174.81 | 3177.69 | 3181.48 | 3801.67 | 3807.53 | | | |
| Rotational constants (B/GHZ): | | | 1.4677668 | | 0.4281024 | | 0.3978915 | | | |



IM6c

C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 0 |
| C | 4 | B5 | 1 | A4 | 3 | D3 0 |
| C | 6 | B6 | 4 | A5 | 1 | D4 0 |
| H | 7 | B7 | 6 | A6 | 4 | D5 0 |
| H | 7 | B8 | 6 | A7 | 4 | D6 0 |
| H | 7 | B9 | 6 | A8 | 4 | D7 0 |
| O | 6 | B10 | 4 | A9 | 1 | D8 0 |
| O | 6 | B11 | 4 | A10 | 1 | D9 0 |
| H | 6 | B12 | 4 | A11 | 1 | D10 0 |
| C | 1 | B13 | 4 | A12 | 3 | D11 0 |
| H | 14 | B14 | 1 | A13 | 4 | D12 0 |
| H | 14 | B15 | 1 | A14 | 4 | D13 0 |
| H | 14 | B16 | 1 | A15 | 4 | D14 0 |
| O | 1 | B17 | 4 | A16 | 3 | D15 0 |
| C | 18 | B18 | 1 | A17 | 4 | D16 0 |
| H | 19 | B19 | 18 | A18 | 1 | D17 0 |
| C | 19 | B20 | 18 | A19 | 1 | D18 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 0 |
| H | 21 | B22 | 19 | A21 | 18 | D20 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 0 |
| O | 19 | B24 | 18 | A23 | 1 | D22 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 0 |

Variables:

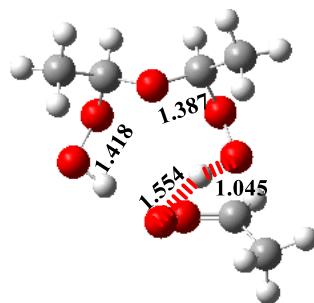
| | |
|----|------------|
| B1 | 1.09650175 |
| B2 | 2.30179254 |
| B3 | 1.41453735 |
| B4 | 0.97964335 |
| B5 | 2.94886439 |
| B6 | 1.46425930 |
| B7 | 1.09594559 |

| | |
|-----|--------------|
| B8 | 1.09065092 |
| B9 | 1.08489577 |
| B10 | 2.24067000 |
| B11 | 1.24079340 |
| B12 | 1.08600075 |
| B13 | 1.51133505 |
| B14 | 1.08647719 |
| B15 | 1.08823950 |
| B16 | 1.08801093 |
| B17 | 1.39202231 |
| B18 | 1.40582526 |
| B19 | 1.09666390 |
| B20 | 1.51029084 |
| B21 | 1.08787763 |
| B22 | 1.08787867 |
| B23 | 1.08597582 |
| B24 | 1.40028495 |
| B25 | 1.41993919 |
| B26 | 0.97995523 |
| A1 | 136.91681269 |
| A2 | 35.81821623 |
| A3 | 109.04099850 |
| A4 | 149.12756122 |
| A5 | 87.08318793 |
| A6 | 108.02883607 |
| A7 | 108.85771576 |
| A8 | 110.69713747 |
| A9 | 70.15959267 |
| A10 | 76.27577065 |
| A11 | 107.84299396 |
| A12 | 112.06685850 |
| A13 | 109.54178283 |
| A14 | 110.01101320 |
| A15 | 109.39349454 |
| A16 | 112.82288332 |
| A17 | 117.23965535 |
| A18 | 109.32499149 |
| A19 | 107.68783209 |
| A20 | 109.38197883 |
| A21 | 109.60946229 |
| A22 | 109.73779621 |
| A23 | 113.17953961 |
| A24 | 109.35492588 |
| A25 | 101.53680931 |

| | |
|-----|---------------|
| D1 | 8.84239083 |
| D2 | -80.28448049 |
| D3 | 128.46518964 |
| D4 | -175.73656659 |
| D5 | -2.20194272 |
| D6 | 112.88956557 |
| D7 | -123.19168972 |
| D8 | -83.71249864 |
| D9 | -49.68536053 |
| D10 | 59.55993818 |
| D11 | 54.61077001 |
| D12 | -70.77160758 |
| D13 | 49.39287064 |
| D14 | 169.75200314 |
| D15 | -68.04515670 |
| D16 | -86.02278392 |
| D17 | -36.77210248 |
| D18 | -157.94433911 |
| D19 | 64.92634414 |
| D20 | -174.76620843 |
| D21 | -54.97892285 |
| D22 | 75.81330475 |
| D23 | 75.86746711 |
| D24 | -112.39108021 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-------------------------------|---------|---------|---------|-----------|---------|-----------|---------|-----------|--------|--------|
| 41.59 | 52.23 | 66.76 | 76.77 | 105.50 | 115.07 | 126.87 | 167.32 | 195.36 | 203.01 | 210.89 |
| 219.93 | 225.47 | 278.17 | 307.74 | 325.32 | 355.89 | 363.10 | 411.33 | 469.88 | 473.97 | |
| 604.50 | 628.96 | 688.59 | 692.77 | 695.87 | 744.74 | 797.03 | 858.46 | 883.02 | 918.39 | |
| 941.61 | 977.79 | 997.95 | 1007.84 | 1033.73 | 1100.23 | 1127.20 | 1129.20 | 1148.75 | | |
| 1149.72 | 1172.74 | 1184.32 | 1227.72 | 1357.87 | 1371.97 | 1379.03 | 1384.69 | 1420.28 | | |
| 1422.21 | 1424.75 | 1438.88 | 1448.34 | 1475.82 | 1485.56 | 1487.54 | 1497.98 | 1501.65 | | |
| 1528.45 | 1560.95 | 1689.23 | 3042.06 | 3056.41 | 3066.13 | 3076.11 | 3080.49 | 3108.03 | | |
| 3152.38 | 3158.55 | 3173.81 | 3177.62 | 3178.03 | 3201.31 | 3474.02 | 3520.41 | | | |
| Rotational constants (B/GHZ): | | | | 1.0047034 | | 0.6105839 | | 0.4315045 | | |



TS6c

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 3 | B3 | 1 | A2 | 2 | D1 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 0 |
| C | 3 | B5 | 1 | A4 | 4 | D3 0 |
| C | 6 | B6 | 3 | A5 | 1 | D4 0 |
| H | 7 | B7 | 6 | A6 | 3 | D5 0 |
| H | 7 | B8 | 6 | A7 | 3 | D6 0 |
| H | 7 | B9 | 6 | A8 | 3 | D7 0 |
| O | 6 | B10 | 3 | A9 | 1 | D8 0 |
| O | 6 | B11 | 3 | A10 | 1 | D9 0 |
| H | 6 | B12 | 3 | A11 | 1 | D10 0 |
| C | 1 | B13 | 4 | A12 | 3 | D11 0 |
| H | 14 | B14 | 1 | A13 | 4 | D12 0 |
| H | 14 | B15 | 1 | A14 | 4 | D13 0 |
| H | 14 | B16 | 1 | A15 | 4 | D14 0 |
| O | 1 | B17 | 4 | A16 | 3 | D15 0 |
| C | 18 | B18 | 1 | A17 | 4 | D16 0 |
| H | 19 | B19 | 18 | A18 | 1 | D17 0 |
| C | 19 | B20 | 18 | A19 | 1 | D18 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 0 |
| H | 21 | B22 | 19 | A21 | 18 | D20 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 0 |
| O | 19 | B24 | 18 | A23 | 1 | D22 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.09560305 |
| B2 | 2.30839318 |
| B3 | 1.41617842 |
| B4 | 1.04539627 |
| B5 | 1.95997817 |
| B6 | 1.48498009 |
| B7 | 1.08606556 |
| B8 | 1.08371614 |
| B9 | 1.09355793 |
| B10 | 2.19649820 |
| B11 | 1.27452426 |
| B12 | 1.08822872 |
| B13 | 1.51094667 |
| B14 | 1.08693765 |
| B15 | 1.08796712 |
| B16 | 1.08769980 |
| B17 | 1.38673477 |

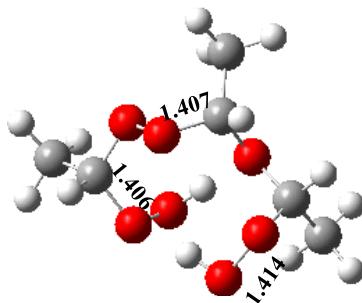
| | |
|-----|---------------|
| B18 | 1.42111594 |
| B19 | 1.09565670 |
| B20 | 1.50956776 |
| B21 | 1.08799222 |
| B22 | 1.08771933 |
| B23 | 1.08578961 |
| B24 | 1.39299349 |
| B25 | 1.41766508 |
| B26 | 0.98815607 |
| A1 | 135.54577515 |
| A2 | 35.66324411 |
| A3 | 93.73332142 |
| A4 | 135.42228298 |
| A5 | 94.27126028 |
| A6 | 109.81765237 |
| A7 | 111.76301824 |
| A8 | 106.13299266 |
| A9 | 72.77118657 |
| A10 | 94.53080764 |
| A11 | 103.71321433 |
| A12 | 112.40696130 |
| A13 | 110.08740590 |
| A14 | 110.05435080 |
| A15 | 109.09340442 |
| A16 | 112.12762378 |
| A17 | 116.62498801 |
| A18 | 108.35438876 |
| A19 | 107.43097642 |
| A20 | 109.43471243 |
| A21 | 109.43148005 |
| A22 | 109.96117251 |
| A23 | 112.84731686 |
| A24 | 110.15139079 |
| A25 | 102.18386441 |
| D1 | -9.83351858 |
| D2 | -109.49752362 |
| D3 | -29.98164606 |
| D4 | -176.60310847 |
| D5 | -64.99738758 |
| D6 | 59.04856676 |
| D7 | 177.69111408 |
| D8 | -83.10280409 |
| D9 | -51.69233105 |
| D10 | 62.24696079 |

| | |
|-----|---------------|
| D11 | 54.05361962 |
| D12 | -72.19055229 |
| D13 | 48.45181171 |
| D14 | 168.59807193 |
| D15 | -69.01443359 |
| D16 | -83.35116427 |
| D17 | -34.51863604 |
| D18 | -155.14899755 |
| D19 | 66.17774461 |
| D20 | -173.51433802 |
| D21 | -54.01061254 |
| D22 | 78.14497887 |
| D23 | 80.99908896 |
| D24 | -98.42616155 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 403.46 <i>i</i> | 36.31 | 60.01 | 99.28 | 103.33 | 110.63 | 136.01 | 171.60 | 205.98 | 215.67 | 225.41 |
| 246.79 | 272.11 | 294.39 | 324.05 | 342.94 | 361.43 | 390.97 | 409.34 | 470.25 | 529.34 | |
| 612.03 | 656.44 | 691.37 | 705.35 | 841.27 | 853.86 | 866.47 | 886.11 | 931.43 | 939.51 | |
| 974.81 | 984.53 | 1009.07 | 1024.51 | 1102.46 | 1107.29 | 1136.69 | 1154.76 | 1166.02 | | |
| 1169.36 | 1189.50 | 1223.64 | 1235.10 | 1361.52 | 1363.17 | 1375.15 | 1385.17 | 1406.35 | | |
| 1419.49 | 1426.61 | 1440.23 | 1452.28 | 1483.57 | 1484.85 | 1491.81 | 1496.58 | 1500.20 | | |
| 1531.40 | 1577.95 | 1593.57 | 2419.50 | 3057.41 | 3061.05 | 3073.19 | 3075.05 | 3078.23 | | |
| 3146.63 | 3155.24 | 3157.98 | 3163.52 | 3176.89 | 3191.06 | 3204.87 | 3313.33 | | | |

Rotational constants (B/GHZ): 1.0795508 0.6078223 0.4384923



P6c

| C | | B1 | | | | |
|---|---|-----|---|----|---|----|
| H | 1 | | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 |
| H | 3 | B4 | 1 | A3 | 4 | D2 |
| C | 3 | B5 | 1 | A4 | 4 | D3 |
| C | 6 | B6 | 3 | A5 | 1 | D4 |
| H | 7 | B7 | 6 | A6 | 3 | D5 |
| H | 7 | B8 | 6 | A7 | 3 | D6 |
| H | 7 | B9 | 6 | A8 | 3 | D7 |
| O | 6 | B10 | 3 | A9 | 1 | D8 |
| | | | | | | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 6 | B11 | 3 | A10 | 1 | D9 | 0 |
| H | 6 | B12 | 3 | A11 | 1 | D10 | 0 |
| C | 1 | B13 | 4 | A12 | 3 | D11 | 0 |
| H | 14 | B14 | 1 | A13 | 4 | D12 | 0 |
| H | 14 | B15 | 1 | A14 | 4 | D13 | 0 |
| H | 14 | B16 | 1 | A15 | 4 | D14 | 0 |
| O | 1 | B17 | 4 | A16 | 3 | D15 | 0 |
| C | 18 | B18 | 1 | A17 | 4 | D16 | 0 |
| H | 19 | B19 | 18 | A18 | 1 | D17 | 0 |
| C | 19 | B20 | 18 | A19 | 1 | D18 | 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 | 0 |
| H | 21 | B22 | 19 | A21 | 18 | D20 | 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 | 0 |
| O | 19 | B24 | 18 | A23 | 1 | D22 | 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 | 0 |

Variables:

| | |
|-----|--------------|
| B1 | 1.09273088 |
| B2 | 2.28740838 |
| B3 | 1.40696920 |
| B4 | 2.56874799 |
| B5 | 1.39918914 |
| B6 | 1.50921907 |
| B7 | 1.08730077 |
| B8 | 1.08662650 |
| B9 | 1.08742368 |
| B10 | 2.30678677 |
| B11 | 1.40628023 |
| B12 | 1.09307671 |
| B13 | 1.51063899 |
| B14 | 1.08670125 |
| B15 | 1.08794822 |
| B16 | 1.08811017 |
| B17 | 1.41036536 |
| B18 | 1.42028898 |
| B19 | 1.09502309 |
| B20 | 1.50767938 |
| B21 | 1.08785486 |
| B22 | 1.08768175 |
| B23 | 1.08721096 |
| B24 | 1.39569974 |
| B25 | 1.41445596 |
| B26 | 0.97305997 |
| A1 | 137.30810966 |

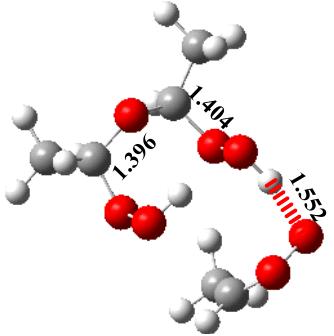
| | |
|-----|---------------|
| A2 | 36.43005647 |
| A3 | 70.60121784 |
| A4 | 128.00014020 |
| A5 | 106.30772153 |
| A6 | 109.76475307 |
| A7 | 110.01577235 |
| A8 | 108.85466392 |
| A9 | 92.47933884 |
| A10 | 111.35743826 |
| A11 | 110.12416798 |
| A12 | 113.18789801 |
| A13 | 110.13348802 |
| A14 | 109.95900869 |
| A15 | 109.11935873 |
| A16 | 110.99215647 |
| A17 | 115.08242248 |
| A18 | 108.78984752 |
| A19 | 107.84130622 |
| A20 | 109.48121501 |
| A21 | 109.22750324 |
| A22 | 110.34159116 |
| A23 | 111.25869432 |
| A24 | 109.84724950 |
| A25 | 103.57464406 |
| D1 | 14.68520550 |
| D2 | -117.54770524 |
| D3 | -64.69409610 |
| D4 | -153.95981456 |
| D5 | -62.86161353 |
| D6 | 57.80515453 |
| D7 | 177.32837852 |
| D8 | -60.28517621 |
| D9 | -29.65000167 |
| D10 | 83.30823960 |
| D11 | 49.61555489 |
| D12 | -70.91875593 |
| D13 | 49.50076651 |
| D14 | 169.53654836 |
| D15 | -73.45359452 |
| D16 | -100.80677439 |
| D17 | -54.50741795 |
| D18 | -175.96447441 |
| D19 | 63.96254126 |
| D20 | -176.13392732 |

D21 -56.63482353
 D22 57.34958293
 D23 74.46854615
 D24 -78.10017539

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 58.79 | 61.10 | 88.01 | 114.04 | 127.09 | 186.28 | 190.42 | 202.70 | 213.21 | 228.67 | 243.02 |
| 273.80 | 298.93 | 314.12 | 333.40 | 358.99 | 417.64 | 437.84 | 477.66 | 544.05 | 566.01 | |
| 600.03 | 650.14 | 675.04 | 713.43 | 716.85 | 855.66 | 882.27 | 895.10 | 937.04 | 947.40 | |
| 985.00 | 1006.64 | 1019.43 | 1030.65 | 1112.93 | 1137.22 | 1148.31 | 1151.46 | 1155.31 | | |
| 1170.88 | 1174.29 | 1207.08 | 1230.17 | 1358.28 | 1365.23 | 1377.85 | 1393.12 | 1397.83 | | |
| 1423.20 | 1426.45 | 1431.17 | 1439.14 | 1469.40 | 1486.61 | 1488.37 | 1489.62 | 1498.20 | | |
| 1500.55 | 1504.32 | 1525.04 | 3070.84 | 3074.94 | 3077.90 | 3085.63 | 3111.48 | 3113.14 | | |
| 3151.75 | 3157.42 | 3163.48 | 3164.89 | 3166.72 | 3178.23 | 3638.72 | 3670.88 | | | |

Rotational constants (B/GHZ): 1.0948628 0.6441370 0.5157937



IM6d

| C | | B1 | | | | |
|---|----|-----|----|-----|---|-------|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 0 |
| C | 7 | B7 | 4 | A6 | 2 | D5 0 |
| H | 8 | B8 | 7 | A7 | 4 | D6 0 |
| H | 8 | B9 | 7 | A8 | 4 | D7 0 |
| H | 8 | B10 | 7 | A9 | 4 | D8 0 |
| O | 7 | B11 | 4 | A10 | 2 | D9 0 |
| O | 7 | B12 | 4 | A11 | 2 | D10 0 |
| H | 7 | B13 | 4 | A12 | 2 | D11 0 |
| H | 1 | B14 | 2 | A13 | 5 | D12 0 |
| H | 1 | B15 | 2 | A14 | 5 | D13 0 |
| H | 1 | B16 | 2 | A15 | 5 | D14 0 |
| O | 2 | B17 | 1 | A16 | 5 | D15 0 |
| C | 18 | B18 | 2 | A17 | 1 | D16 0 |
| H | 19 | B19 | 18 | A18 | 2 | D17 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 19 | B20 | 18 | A19 | 2 | D18 | 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 | 0 |
| H | 21 | B22 | 19 | A21 | 18 | D20 | 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 | 0 |
| O | 19 | B24 | 18 | A23 | 2 | D22 | 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 | 0 |

Variables:

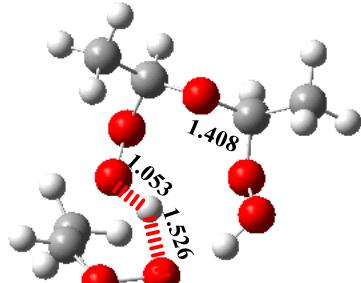
| | |
|-----|--------------|
| B1 | 1.50883558 |
| B2 | 1.09683531 |
| B3 | 2.30787589 |
| B4 | 1.41436008 |
| B5 | 0.98233289 |
| B6 | 2.71166631 |
| B7 | 1.46305750 |
| B8 | 1.08420925 |
| B9 | 1.09412241 |
| B10 | 1.09252422 |
| B11 | 2.23817668 |
| B12 | 1.24494459 |
| B13 | 1.08483049 |
| B14 | 1.08787215 |
| B15 | 1.08784783 |
| B16 | 1.08706289 |
| B17 | 1.39581588 |
| B18 | 1.40366970 |
| B19 | 1.09658736 |
| B20 | 1.50975114 |
| B21 | 1.08680085 |
| B22 | 1.08775367 |
| B23 | 1.08784975 |
| B24 | 1.40424412 |
| B25 | 1.43018309 |
| B26 | 1.01699850 |
| A1 | 112.24477788 |
| A2 | 94.37895421 |
| A3 | 112.70249004 |
| A4 | 88.95372624 |
| A5 | 131.26610268 |
| A6 | 92.24612677 |
| A7 | 110.80109742 |
| A8 | 108.54013441 |
| A9 | 108.09481748 |
| A10 | 102.01112923 |

| | |
|-----|---------------|
| A11 | 99.98296411 |
| A12 | 79.19718589 |
| A13 | 109.72255156 |
| A14 | 109.60287937 |
| A15 | 109.52339801 |
| A16 | 107.83041070 |
| A17 | 117.68983924 |
| A18 | 110.24835709 |
| A19 | 107.46269876 |
| A20 | 109.53708665 |
| A21 | 109.52809085 |
| A22 | 109.67567938 |
| A23 | 112.35624463 |
| A24 | 107.45316983 |
| A25 | 100.67548806 |
| D1 | -145.30840338 |
| D2 | 31.44383795 |
| D3 | -122.87810130 |
| D4 | 157.75549865 |
| D5 | -11.07745960 |
| D6 | -80.03721913 |
| D7 | 41.21230412 |
| D8 | 156.29332843 |
| D9 | 78.64090632 |
| D10 | 113.10301314 |
| D11 | -135.32194067 |
| D12 | -175.06089681 |
| D13 | -54.77773879 |
| D14 | 65.18785358 |
| D15 | -123.80948064 |
| D16 | -170.27215656 |
| D17 | 43.55529549 |
| D18 | 166.07880420 |
| D19 | 57.11286296 |
| D20 | 176.90132728 |
| D21 | -62.78861218 |
| D22 | -69.22357802 |
| D23 | -60.14993763 |
| D24 | -176.30702421 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|--------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 54.05 | 71.85 | 78.02 | 99.69 | 130.53 | 144.54 | 159.61 | 165.45 | 197.67 | 208.30 | 221.24 |
| 228.95 | 243.26 | 266.73 | 318.41 | 337.96 | 358.29 | 389.73 | 425.93 | 457.69 | 481.80 | |
| 589.03 | 672.99 | 688.47 | 723.52 | 742.18 | 812.34 | 848.75 | 881.26 | 903.86 | 938.19 | |
| 977.43 | 1005.25 | 1008.37 | 1032.37 | 1081.35 | 1113.59 | 1115.33 | 1128.53 | 1145.83 | | |

| | | | | | | | | |
|-------------------------------|---------|---------|---------|-----------|-----------|-----------|---------|---------|
| 1152.57 | 1162.50 | 1184.04 | 1226.50 | 1344.23 | 1374.35 | 1376.11 | 1380.63 | 1404.76 |
| 1418.88 | 1423.34 | 1433.79 | 1447.90 | 1470.87 | 1484.49 | 1489.87 | 1495.94 | 1499.79 |
| 1549.36 | 1589.55 | 1674.11 | 2819.93 | 3051.44 | 3063.37 | 3068.07 | 3075.24 | 3081.39 |
| 3108.77 | 3154.28 | 3163.47 | 3168.85 | 3169.82 | 3189.82 | 3227.91 | 3493.60 | |
| Rotational constants (B/GHZ): | | | | 1.0734553 | 0.5800376 | 0.4342363 | | |



TS6d

| C | | B1 | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| O | 4 | B4 | 2 | A3 | 1 | D2 | 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 | 0 |
| C | 7 | B7 | 4 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 7 | A7 | 4 | D6 | 0 |
| H | 8 | B9 | 7 | A8 | 4 | D7 | 0 |
| H | 8 | B10 | 7 | A9 | 4 | D8 | 0 |
| O | 7 | B11 | 4 | A10 | 2 | D9 | 0 |
| O | 7 | B12 | 4 | A11 | 2 | D10 | 0 |
| H | 7 | B13 | 4 | A12 | 2 | D11 | 0 |
| H | 1 | B14 | 2 | A13 | 5 | D12 | 0 |
| H | 1 | B15 | 2 | A14 | 5 | D13 | 0 |
| H | 1 | B16 | 2 | A15 | 5 | D14 | 0 |
| O | 2 | B17 | 1 | A16 | 5 | D15 | 0 |
| C | 18 | B18 | 2 | A17 | 1 | D16 | 0 |
| H | 19 | B19 | 18 | A18 | 2 | D17 | 0 |
| C | 19 | B20 | 18 | A19 | 2 | D18 | 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 | 0 |
| H | 21 | B22 | 19 | A21 | 18 | D20 | 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 | 0 |
| O | 19 | B24 | 18 | A23 | 2 | D22 | 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.50839397 |
| B2 | 1.09719255 |

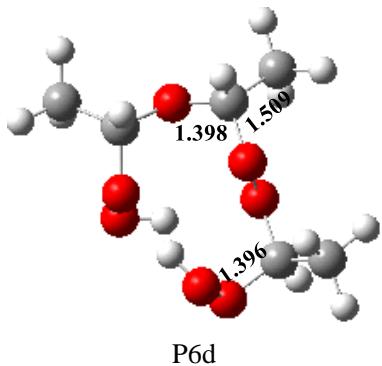
| | |
|-----|--------------|
| B3 | 2.28406222 |
| B4 | 1.41130140 |
| B5 | 1.05315022 |
| B6 | 1.92383542 |
| B7 | 1.48290641 |
| B8 | 1.08699841 |
| B9 | 1.08348453 |
| B10 | 1.09338908 |
| B11 | 2.20204570 |
| B12 | 1.27990917 |
| B13 | 1.08788709 |
| B14 | 1.08770950 |
| B15 | 1.08799062 |
| B16 | 1.08720911 |
| B17 | 1.38586199 |
| B18 | 1.40810983 |
| B19 | 1.09588545 |
| B20 | 1.50976011 |
| B21 | 1.08651033 |
| B22 | 1.08776729 |
| B23 | 1.08791112 |
| B24 | 1.40043149 |
| B25 | 1.42707712 |
| B26 | 0.97649954 |
| A1 | 112.15192248 |
| A2 | 93.82407211 |
| A3 | 36.58030946 |
| A4 | 110.40718635 |
| A5 | 152.78790389 |
| A6 | 99.02652254 |
| A7 | 109.71624911 |
| A8 | 111.28395758 |
| A9 | 106.24330698 |
| A10 | 72.36040169 |
| A11 | 91.06677679 |
| A12 | 102.95371257 |
| A13 | 109.43254337 |
| A14 | 109.89444761 |
| A15 | 109.53560393 |
| A16 | 108.17515987 |
| A17 | 116.72666586 |
| A18 | 109.63170151 |
| A19 | 107.82243457 |
| A20 | 109.57902232 |

| | |
|-----|---------------|
| A21 | 109.75853446 |
| A22 | 109.46014058 |
| A23 | 112.33310134 |
| A24 | 108.78557965 |
| A25 | 99.76687610 |
| D1 | -144.26126527 |
| D2 | 123.87044182 |
| D3 | -151.13014962 |
| D4 | 98.53689642 |
| D5 | 31.69711412 |
| D6 | -60.71470285 |
| D7 | 62.43724641 |
| D8 | -177.95594559 |
| D9 | 123.41311238 |
| D10 | 156.99532730 |
| D11 | -90.42540012 |
| D12 | -173.41606828 |
| D13 | -53.33632886 |
| D14 | 67.31302039 |
| D15 | -124.66633078 |
| D16 | -176.91329625 |
| D17 | 30.99592584 |
| D18 | 153.16270568 |
| D19 | 54.32265761 |
| D20 | 174.18087020 |
| D21 | -65.40617257 |
| D22 | -81.36602023 |
| D23 | -73.79236609 |
| D24 | 140.04765813 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 391.32 <i>i</i> | 46.77 | 75.30 | 97.28 | 116.64 | 125.59 | 162.72 | 174.58 | 180.83 | 206.66 | 213.96 |
| 222.93 | 257.32 | 311.80 | 325.55 | 357.85 | 379.03 | 391.70 | 446.35 | 460.05 | 478.57 | |
| 588.94 | 591.70 | 650.00 | 682.88 | 724.33 | 851.98 | 879.79 | 881.21 | 924.93 | 937.48 | |
| 963.35 | 985.64 | 1006.91 | 1024.81 | 1099.87 | 1115.33 | 1145.70 | 1155.65 | 1166.09 | | |
| 1169.89 | 1189.12 | 1206.04 | 1231.18 | 1352.75 | 1360.21 | 1374.64 | 1387.08 | 1398.67 | | |
| 1415.42 | 1422.97 | 1439.56 | 1445.18 | 1482.74 | 1485.83 | 1487.43 | 1496.09 | 1498.45 | | |
| 1503.29 | 531.05 | 1611.38 | 2389.51 | 3061.83 | 3063.08 | 3070.70 | 3073.93 | 3080.34 | | |
| 3146.43 | 3152.59 | 3161.10 | 3168.71 | 3171.24 | 3188.00 | 3203.11 | 3591.36 | | | |

Rotational constants (B/GHZ): 1.0821220 0.6035619 0.4460361



P6d

C

| | | | | | | |
|---|----|-----|----|-----|----|-----|
| C | 1 | B1 | | | | |
| H | 2 | B2 | 1 | A1 | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 |
| O | 2 | B4 | 1 | A3 | 4 | D2 |
| H | 5 | B5 | 2 | A4 | 1 | D3 |
| C | 4 | B6 | 2 | A5 | 1 | D4 |
| C | 7 | B7 | 4 | A6 | 2 | D5 |
| H | 8 | B8 | 7 | A7 | 4 | D6 |
| H | 8 | B9 | 7 | A8 | 4 | D7 |
| H | 8 | B10 | 7 | A9 | 4 | D8 |
| O | 7 | B11 | 4 | A10 | 2 | D9 |
| O | 7 | B12 | 4 | A11 | 2 | D10 |
| H | 7 | B13 | 4 | A12 | 2 | D11 |
| H | 1 | B14 | 2 | A13 | 5 | D12 |
| H | 1 | B15 | 2 | A14 | 5 | D13 |
| H | 1 | B16 | 2 | A15 | 5 | D14 |
| O | 2 | B17 | 1 | A16 | 5 | D15 |
| C | 18 | B18 | 2 | A17 | 1 | D16 |
| H | 19 | B19 | 18 | A18 | 2 | D17 |
| C | 19 | B20 | 18 | A19 | 2 | D18 |
| H | 21 | B21 | 19 | A20 | 18 | D19 |
| H | 21 | B22 | 19 | A21 | 18 | D20 |
| H | 21 | B23 | 19 | A22 | 18 | D21 |
| O | 19 | B24 | 18 | A23 | 2 | D22 |
| O | 25 | B25 | 19 | A24 | 18 | D23 |
| H | 26 | B26 | 25 | A25 | 19 | D24 |
| | | | | | | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.50947108 |
| B2 | 1.09679183 |
| B3 | 2.28260436 |
| B4 | 1.40640036 |
| B5 | 2.60660857 |
| B6 | 1.41662598 |
| B7 | 1.51027904 |

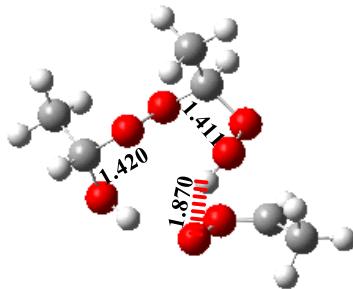
| | |
|-----|--------------|
| B8 | 1.08811475 |
| B9 | 1.08391221 |
| B10 | 1.08781694 |
| B11 | 2.30907153 |
| B12 | 1.39638624 |
| B13 | 1.09261305 |
| B14 | 1.08755105 |
| B15 | 1.08794282 |
| B16 | 1.08669604 |
| B17 | 1.39775918 |
| B18 | 1.39632479 |
| B19 | 1.09630606 |
| B20 | 1.50812598 |
| B21 | 1.08683182 |
| B22 | 1.08766693 |
| B23 | 1.08781224 |
| B24 | 1.41666974 |
| B25 | 1.41370485 |
| B26 | 0.97021768 |
| A1 | 111.85104021 |
| A2 | 91.63217525 |
| A3 | 113.53447511 |
| A4 | 124.66877705 |
| A5 | 144.53920220 |
| A6 | 113.70068633 |
| A7 | 109.40964512 |
| A8 | 110.89444772 |
| A9 | 108.45100280 |
| A10 | 101.56303140 |
| A11 | 111.21727278 |
| A12 | 101.88446815 |
| A13 | 109.37695782 |
| A14 | 109.62762129 |
| A15 | 109.94632273 |
| A16 | 107.83405836 |
| A17 | 116.79100298 |
| A18 | 110.71093623 |
| A19 | 108.31700104 |
| A20 | 109.49136672 |
| A21 | 109.64596124 |
| A22 | 109.60332892 |
| A23 | 111.62590618 |
| A24 | 109.24664608 |
| A25 | 101.02347492 |

| | |
|-----|---------------|
| D1 | -143.88141956 |
| D2 | 30.64823415 |
| D3 | -150.57376211 |
| D4 | 127.73533205 |
| D5 | -44.51099162 |
| D6 | -51.91847630 |
| D7 | 69.00163962 |
| D8 | -171.20951740 |
| D9 | 51.08012199 |
| D10 | 86.41666343 |
| D11 | -164.82966596 |
| D12 | -171.32052970 |
| D13 | -51.30914384 |
| D14 | 69.05524015 |
| D15 | -125.24244864 |
| D16 | -175.34928977 |
| D17 | 34.72063409 |
| D18 | 158.32180059 |
| D19 | 57.03748031 |
| D20 | 176.95388041 |
| D21 | -62.75901516 |
| D22 | -77.88235106 |
| D23 | -60.76022825 |
| D24 | 90.02412158 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 59.11 | 68.03 | 83.83 | 122.13 | 149.81 | 170.16 | 188.28 | 192.54 | 195.04 | 227.24 | 245.63 |
| 255.36 | 262.46 | 308.38 | 317.68 | 361.07 | 400.56 | 414.89 | 463.80 | 488.19 | 513.15 | |
| 553.55 | 595.05 | 674.22 | 711.99 | 746.59 | 858.96 | 865.48 | 894.38 | 937.59 | 947.32 | |
| 973.90 | 1001.32 | 1012.66 | 1031.09 | 1126.10 | 1130.99 | 1140.60 | 1153.71 | 1162.99 | | |
| 1172.05 | 1190.87 | 1197.35 | 1234.37 | 1353.57 | 1359.54 | 1375.34 | 1380.33 | 1399.09 | | |
| 1417.45 | 1421.51 | 1429.78 | 1437.92 | 1483.96 | 1484.80 | 1485.99 | 1489.94 | 1498.94 | | |
| 1503.33 | 1507.75 | 1520.96 | 3069.13 | 3070.49 | 3075.54 | 3076.95 | 3082.97 | 3109.12 | | |
| 3149.32 | 3153.30 | 3157.17 | 3169.02 | 3174.87 | 3194.10 | 3700.96 | 3738.65 | | | |

Rotational constants (B/GHZ): 1.1154876 0.6590922 0.4770579



IM6e

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| O | 1 | B4 | 3 | A3 | 4 | D2 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 0 |
| C | 5 | B6 | 1 | A5 | 3 | D4 0 |
| C | 7 | B7 | 5 | A6 | 1 | D5 0 |
| H | 8 | B8 | 7 | A7 | 5 | D6 0 |
| H | 8 | B9 | 7 | A8 | 5 | D7 0 |
| H | 8 | B10 | 7 | A9 | 5 | D8 0 |
| O | 7 | B11 | 5 | A10 | 1 | D9 0 |
| O | 7 | B12 | 5 | A11 | 1 | D10 0 |
| C | 1 | B13 | 5 | A12 | 4 | D11 0 |
| H | 14 | B14 | 1 | A13 | 5 | D12 0 |
| H | 14 | B15 | 1 | A14 | 5 | D13 0 |
| H | 14 | B16 | 1 | A15 | 5 | D14 0 |
| O | 1 | B17 | 5 | A16 | 4 | D15 0 |
| C | 3 | B18 | 1 | A17 | 18 | D16 0 |
| H | 19 | B19 | 3 | A18 | 1 | D17 0 |
| C | 19 | B20 | 3 | A19 | 1 | D18 0 |
| H | 21 | B21 | 19 | A20 | 3 | D19 0 |
| H | 21 | B22 | 19 | A21 | 3 | D20 0 |
| H | 7 | B23 | 5 | A22 | 1 | D21 0 |
| O | 19 | B24 | 3 | A23 | 1 | D22 0 |
| H | 25 | B25 | 19 | A24 | 3 | D23 0 |
| H | 21 | B26 | 19 | A25 | 3 | D24 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.09287805 |
| B2 | 2.28915411 |
| B3 | 2.32740991 |
| B4 | 1.41138799 |
| B5 | 0.98085436 |
| B6 | 2.87648149 |
| B7 | 1.46458523 |
| B8 | 1.08457584 |
| B9 | 1.09497181 |
| B10 | 1.09138771 |
| B11 | 2.23423975 |
| B12 | 1.24111140 |
| B13 | 1.51181664 |
| B14 | 1.08802348 |
| B15 | 1.08818186 |
| B16 | 1.08386829 |
| B17 | 1.39787734 |

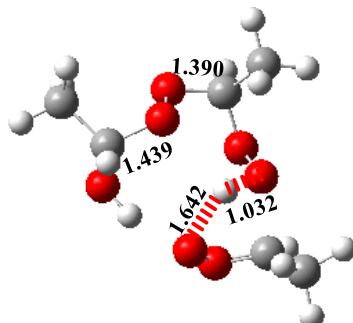
| | |
|-----|---------------|
| B18 | 1.42017120 |
| B19 | 1.09808565 |
| B20 | 1.51097194 |
| B21 | 1.08804482 |
| B22 | 1.08840600 |
| B23 | 1.08576690 |
| B24 | 1.37941385 |
| B25 | 0.97477546 |
| B26 | 1.08713730 |
| A1 | 138.23943266 |
| A2 | 76.81222823 |
| A3 | 102.52179905 |
| A4 | 97.91624670 |
| A5 | 124.87937302 |
| A6 | 87.26993561 |
| A7 | 110.90914727 |
| A8 | 108.04866820 |
| A9 | 108.54877600 |
| A10 | 74.73980576 |
| A11 | 79.90645347 |
| A12 | 113.19224751 |
| A13 | 108.99781975 |
| A14 | 108.93335565 |
| A15 | 110.89142838 |
| A16 | 112.05822455 |
| A17 | 143.20635398 |
| A18 | 99.41235488 |
| A19 | 112.81032356 |
| A20 | 109.06092411 |
| A21 | 110.17331390 |
| A22 | 103.84913444 |
| A23 | 112.30557741 |
| A24 | 108.82945756 |
| A25 | 109.67777597 |
| D1 | -148.72937625 |
| D2 | 23.74068541 |
| D3 | -98.32040905 |
| D4 | 68.66932830 |
| D5 | -170.43838057 |
| D6 | -114.14597933 |
| D7 | 7.26863570 |
| D8 | 122.13040617 |
| D9 | -79.55602163 |
| D10 | -45.69525160 |

| | |
|-----|---------------|
| D11 | 50.56670670 |
| D12 | 56.60101880 |
| D13 | 176.00920156 |
| D14 | -63.62836613 |
| D15 | -80.42537295 |
| D16 | 3.49026964 |
| D17 | -178.62272138 |
| D18 | -61.05797990 |
| D19 | -172.32074051 |
| D20 | -52.21439342 |
| D21 | 65.12697841 |
| D22 | 62.73877793 |
| D23 | 40.79450012 |
| D24 | 68.63581139 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 55.79 | 65.10 | 88.11 | 89.50 | 111.28 | 122.32 | 134.82 | 153.70 | 167.93 | 192.02 | 211.17 |
| 223.37 | 234.73 | 245.50 | 261.91 | 332.51 | 359.85 | 423.37 | 473.69 | 478.96 | 499.79 | |
| 518.47 | 655.38 | 669.19 | 703.62 | 734.43 | 758.68 | 800.42 | 858.65 | 882.68 | 915.94 | |
| 937.31 | 959.16 | 997.41 | 1003.37 | 1018.54 | 1102.23 | 1109.21 | 1126.75 | 1138.82 | | |
| 1145.18 | 1170.30 | 1193.31 | 1214.36 | 1335.81 | 1352.34 | 1370.61 | 1375.75 | 1397.35 | | |
| 1405.43 | 1420.05 | 1424.76 | 1455.80 | 1477.79 | 1481.39 | 1483.41 | 1494.20 | 1502.68 | | |
| 1504.06 | 1549.39 | 1687.48 | 3042.67 | 3043.96 | 3072.79 | 3079.64 | 3103.77 | 3114.91 | | |
| 3151.69 | 3154.18 | 3161.92 | 3182.46 | 3186.89 | 3206.54 | 3512.81 | 3605.99 | | | |

Rotational constants (B/GHZ): 1.0061122 0.6279030 0.4466782



TS6e

| C | | | | | | | |
|---|---|-----|---|----|---|----|---|
| H | 1 | B1 | | | | | |
| O | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 | 0 |
| O | 4 | B4 | 1 | A3 | 3 | D2 | 0 |
| H | 4 | B5 | 1 | A4 | 5 | D3 | 0 |
| C | 4 | B6 | 1 | A5 | 5 | D4 | 0 |
| C | 7 | B7 | 4 | A6 | 1 | D5 | 0 |
| H | 8 | B8 | 7 | A7 | 4 | D6 | 0 |
| H | 8 | B9 | 7 | A8 | 4 | D7 | 0 |
| H | 8 | B10 | 7 | A9 | 4 | D8 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 7 | B11 | 4 | A10 | 1 | D9 | 0 |
| O | 7 | B12 | 4 | A11 | 1 | D10 | 0 |
| C | 1 | B13 | 5 | A12 | 4 | D11 | 0 |
| H | 14 | B14 | 1 | A13 | 5 | D12 | 0 |
| H | 14 | B15 | 1 | A14 | 5 | D13 | 0 |
| H | 14 | B16 | 1 | A15 | 5 | D14 | 0 |
| O | 1 | B17 | 5 | A16 | 4 | D15 | 0 |
| C | 3 | B18 | 1 | A17 | 18 | D16 | 0 |
| H | 19 | B19 | 3 | A18 | 1 | D17 | 0 |
| C | 19 | B20 | 3 | A19 | 1 | D18 | 0 |
| H | 21 | B21 | 19 | A20 | 3 | D19 | 0 |
| H | 21 | B22 | 19 | A21 | 3 | D20 | 0 |
| H | 7 | B23 | 4 | A22 | 1 | D21 | 0 |
| O | 19 | B24 | 3 | A23 | 1 | D22 | 0 |
| H | 25 | B25 | 19 | A24 | 3 | D23 | 0 |
| H | 21 | B26 | 19 | A25 | 3 | D24 | 0 |

Variables:

| | |
|-----|--------------|
| B1 | 1.09183070 |
| B2 | 2.26999537 |
| B3 | 2.33197891 |
| B4 | 1.41685183 |
| B5 | 1.03224466 |
| B6 | 1.90818318 |
| B7 | 1.48722239 |
| B8 | 1.09310614 |
| B9 | 1.08613474 |
| B10 | 1.08375985 |
| B11 | 2.20193964 |
| B12 | 1.27761968 |
| B13 | 1.51292091 |
| B14 | 1.08802857 |
| B15 | 1.08766103 |
| B16 | 1.08524035 |
| B17 | 1.39039750 |
| B18 | 1.43889897 |
| B19 | 1.09755246 |
| B20 | 1.51013037 |
| B21 | 1.08784287 |
| B22 | 1.08808821 |
| B23 | 1.08826251 |
| B24 | 1.36921798 |
| B25 | 0.97957115 |
| B26 | 1.08750752 |
| A1 | 139.81935457 |

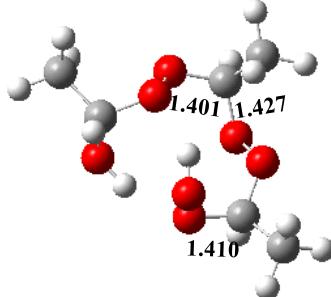
| | |
|-----|---------------|
| A2 | 76.01155374 |
| A3 | 34.74418965 |
| A4 | 98.12505653 |
| A5 | 138.06187380 |
| A6 | 95.45304451 |
| A7 | 106.18788181 |
| A8 | 110.02291507 |
| A9 | 111.48452389 |
| A10 | 74.91215455 |
| A11 | 96.25130706 |
| A12 | 113.36024645 |
| A13 | 109.89326068 |
| A14 | 108.21221162 |
| A15 | 111.07468780 |
| A16 | 111.80704618 |
| A17 | 135.10857019 |
| A18 | 99.08335894 |
| A19 | 111.53133892 |
| A20 | 108.95878301 |
| A21 | 110.49619002 |
| A22 | 102.49513806 |
| A23 | 112.49228921 |
| A24 | 107.79815945 |
| A25 | 109.52383848 |
| D1 | -144.82571474 |
| D2 | 121.04252153 |
| D3 | -104.33502524 |
| D4 | -15.01210457 |
| D5 | 173.03637959 |
| D6 | 178.65666916 |
| D7 | -63.84379342 |
| D8 | 60.21832646 |
| D9 | -93.84030288 |
| D10 | -62.24022103 |
| D11 | 39.63074085 |
| D12 | 50.20746535 |
| D13 | 169.61471534 |
| D14 | -70.84640905 |
| D15 | -90.53230189 |
| D16 | 47.86679090 |
| D17 | 157.13107380 |
| D18 | -85.40563862 |
| D19 | -170.56550065 |
| D20 | -50.24430015 |

| | |
|-----|-------------|
| D21 | 52.04420862 |
| D22 | 38.18753161 |
| D23 | 62.95688675 |
| D24 | 70.66917103 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 390.13 <i>i</i> | 55.81 | 63.88 | 80.65 | 104.18 | 117.33 | 123.57 | 154.04 | 174.96 | 195.08 | 229.81 |
| 241.72 | 250.56 | 260.43 | 289.76 | 357.67 | 379.30 | 423.92 | 474.76 | 498.76 | 513.25 | |
| 543.20 | 656.37 | 674.97 | 729.89 | 844.59 | 855.83 | 867.82 | 873.86 | 930.52 | 944.55 | |
| 954.44 | 985.73 | 989.41 | 1012.64 | 1082.59 | 1101.85 | 1126.71 | 1142.11 | 1146.17 | | |
| 1165.80 | 1170.90 | 1195.94 | 1217.34 | 1351.64 | 1354.95 | 1357.54 | 1375.16 | 1399.99 | | |
| 1408.94 | 1414.18 | 1425.70 | 1452.22 | 1481.34 | 1486.59 | 1489.22 | 1496.76 | 1502.19 | | |
| 1507.28 | 1522.96 | 1577.71 | 2656.54 | 3055.18 | 3057.91 | 3073.70 | 3077.09 | 3116.16 | | |
| 3143.01 | 3150.37 | 3154.75 | 3169.13 | 3173.39 | 3187.44 | 3200.90 | 3461.20 | | | |

Rotational constants (B/GHZ): 1.0841080 0.6088603 0.4437443



P6e

| C | | | | | | | |
|---|----|-----|---|-----|----|-----|---|
| H | 1 | B1 | | | | | |
| O | 1 | B2 | 2 | A1 | | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 | 0 |
| O | 1 | B4 | 3 | A3 | 4 | D2 | 0 |
| H | 3 | B5 | 1 | A4 | 5 | D3 | 0 |
| C | 4 | B6 | 1 | A5 | 5 | D4 | 0 |
| C | 7 | B7 | 4 | A6 | 1 | D5 | 0 |
| H | 8 | B8 | 7 | A7 | 4 | D6 | 0 |
| H | 8 | B9 | 7 | A8 | 4 | D7 | 0 |
| H | 8 | B10 | 7 | A9 | 4 | D8 | 0 |
| O | 7 | B11 | 4 | A10 | 1 | D9 | 0 |
| O | 7 | B12 | 4 | A11 | 1 | D10 | 0 |
| C | 1 | B13 | 5 | A12 | 4 | D11 | 0 |
| H | 14 | B14 | 1 | A13 | 5 | D12 | 0 |
| H | 14 | B15 | 1 | A14 | 5 | D13 | 0 |
| H | 14 | B16 | 1 | A15 | 5 | D14 | 0 |
| O | 1 | B17 | 5 | A16 | 4 | D15 | 0 |
| C | 3 | B18 | 1 | A17 | 18 | D16 | 0 |
| H | 19 | B19 | 3 | A18 | 1 | D17 | 0 |
| C | 19 | B20 | 3 | A19 | 1 | D18 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|---|-----|---|
| H | 21 | B21 | 19 | A20 | 3 | D19 | 0 |
| H | 21 | B22 | 19 | A21 | 3 | D20 | 0 |
| H | 7 | B23 | 4 | A22 | 1 | D21 | 0 |
| O | 19 | B24 | 3 | A23 | 1 | D22 | 0 |
| H | 25 | B25 | 19 | A24 | 3 | D23 | 0 |
| H | 21 | B26 | 19 | A25 | 3 | D24 | 0 |

Variables:

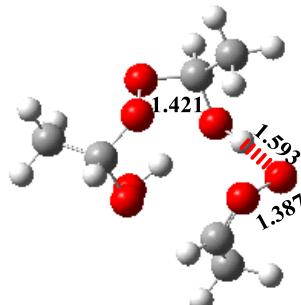
| | |
|-----|--------------|
| B1 | 1.09232763 |
| B2 | 2.30233071 |
| B3 | 2.33228700 |
| B4 | 1.40996525 |
| B5 | 1.97306172 |
| B6 | 1.39610042 |
| B7 | 1.51052173 |
| B8 | 1.08747823 |
| B9 | 1.08717823 |
| B10 | 1.08672329 |
| B11 | 2.30015912 |
| B12 | 1.40984273 |
| B13 | 1.51263265 |
| B14 | 1.08746020 |
| B15 | 1.08735704 |
| B16 | 1.08574228 |
| B17 | 1.40129841 |
| B18 | 1.43517979 |
| B19 | 1.09686337 |
| B20 | 1.50851603 |
| B21 | 1.08777716 |
| B22 | 1.08793676 |
| B23 | 1.09180806 |
| B24 | 1.37686715 |
| B25 | 0.96634036 |
| B26 | 1.08716126 |
| A1 | 136.74781942 |
| A2 | 85.72663493 |
| A3 | 96.53163235 |
| A4 | 98.49830547 |
| A5 | 133.32416850 |
| A6 | 106.48182653 |
| A7 | 108.88720199 |
| A8 | 109.62554151 |
| A9 | 110.23350803 |
| A10 | 91.97734485 |
| A11 | 111.25353859 |

| | |
|-----|---------------|
| A12 | 114.34047917 |
| A13 | 110.04882641 |
| A14 | 108.08655297 |
| A15 | 111.11239609 |
| A16 | 112.07936758 |
| A17 | 133.08536765 |
| A18 | 99.98939102 |
| A19 | 111.88729009 |
| A20 | 109.03755764 |
| A21 | 110.20663278 |
| A22 | 110.17779251 |
| A23 | 112.03845032 |
| A24 | 108.73204654 |
| A25 | 109.59702317 |
| D1 | -151.48933084 |
| D2 | 33.30427955 |
| D3 | 44.35298943 |
| D4 | -50.42518604 |
| D5 | -170.55331049 |
| D6 | 174.14782924 |
| D7 | -65.96897981 |
| D8 | 54.59466690 |
| D9 | -77.56696189 |
| D10 | -46.89074661 |
| D11 | 24.23946572 |
| D12 | 50.93900595 |
| D13 | 170.66480832 |
| D14 | -69.64377409 |
| D15 | -106.24356188 |
| D16 | 50.96499844 |
| D17 | 154.39545515 |
| D18 | -87.47126171 |
| D19 | -172.58558718 |
| D20 | -52.46034473 |
| D21 | 66.50759224 |
| D22 | 35.40109965 |
| D23 | 53.76696301 |
| D24 | 68.31648381 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 58.04 | 73.13 | 100.93 | 117.40 | 140.57 | 158.65 | 188.44 | 201.84 | 225.77 | 239.40 | 245.18 |
| 260.82 | 278.30 | 311.16 | 347.81 | 400.38 | 428.62 | 469.19 | 493.20 | 521.50 | 552.25 | |
| 575.13 | 633.00 | 680.29 | 701.42 | 716.79 | 867.54 | 872.22 | 884.62 | 936.70 | 949.90 | |
| 959.39 | 998.67 | 1011.85 | 1032.27 | 1092.68 | 1139.62 | 1141.92 | 1145.92 | 1147.70 | | |
| 1162.63 | 1190.10 | 1210.17 | 1220.67 | 1331.35 | 1356.20 | 1363.53 | 1374.46 | 1391.45 | | |

| | | | | | | | | |
|-------------------------------|---------|---------|---------|-----------|-----------|-----------|---------|---------|
| 1407.05 | 1414.22 | 1424.19 | 1425.73 | 1478.25 | 1488.78 | 1490.57 | 1491.61 | 1498.05 |
| 1501.13 | 1502.96 | 1505.85 | 3060.55 | 3079.21 | 3080.12 | 3083.12 | 3115.76 | 3127.66 |
| 3157.22 | 3159.07 | 3165.42 | 3169.59 | 3176.07 | 3178.08 | 3686.93 | 3787.22 | |
| Rotational constants (B/GHZ): | | | | 1.1166072 | 0.6430101 | 0.4836910 | | |



IM6f

C

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| O | 1 | B5 | 2 | A4 | 5 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 | 0 |
| C | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| C | 9 | B9 | 6 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 9 | A9 | 6 | D8 | 0 |
| H | 10 | B11 | 9 | A10 | 6 | D9 | 0 |
| H | 10 | B12 | 9 | A11 | 6 | D10 | 0 |
| O | 9 | B13 | 6 | A12 | 1 | D11 | 0 |
| O | 9 | B14 | 6 | A13 | 1 | D12 | 0 |
| H | 1 | B15 | 6 | A14 | 2 | D13 | 0 |
| O | 1 | B16 | 6 | A15 | 2 | D14 | 0 |
| C | 8 | B17 | 1 | A16 | 6 | D15 | 0 |
| H | 18 | B18 | 8 | A17 | 1 | D16 | 0 |
| C | 18 | B19 | 8 | A18 | 1 | D17 | 0 |
| H | 20 | B20 | 18 | A19 | 8 | D18 | 0 |
| H | 20 | B21 | 18 | A20 | 8 | D19 | 0 |
| H | 20 | B22 | 18 | A21 | 8 | D20 | 0 |
| O | 18 | B23 | 8 | A22 | 1 | D21 | 0 |
| O | 24 | B24 | 18 | A23 | 8 | D22 | 0 |
| H | 25 | B25 | 24 | A24 | 18 | D23 | 0 |
| H | 9 | B26 | 6 | A25 | 1 | D24 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51317946 |
| B2 | 1.08840665 |
| B3 | 1.08804456 |

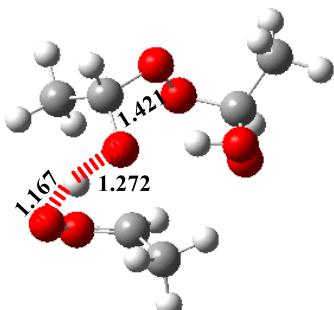
| | |
|-----|--------------|
| B4 | 1.08735218 |
| B5 | 1.38994699 |
| B6 | 1.00266894 |
| B7 | 2.30937866 |
| B8 | 3.50139576 |
| B9 | 1.46538382 |
| B10 | 1.08427247 |
| B11 | 1.09107278 |
| B12 | 1.09243110 |
| B13 | 2.23403837 |
| B14 | 1.24319194 |
| B15 | 1.09320928 |
| B16 | 1.42104172 |
| B17 | 1.40372630 |
| B18 | 1.09357910 |
| B19 | 1.51040284 |
| B20 | 1.08794535 |
| B21 | 1.08379688 |
| B22 | 1.08784128 |
| B23 | 1.41121193 |
| B24 | 1.41678031 |
| B25 | 0.98432789 |
| B26 | 1.08479251 |
| A1 | 109.42012466 |
| A2 | 109.58667469 |
| A3 | 110.50885470 |
| A4 | 112.95115304 |
| A5 | 111.58793350 |
| A6 | 95.87010109 |
| A7 | 117.96084043 |
| A8 | 81.24858666 |
| A9 | 110.80469456 |
| A10 | 108.91235270 |
| A11 | 108.13867789 |
| A12 | 47.67376362 |
| A13 | 62.45409136 |
| A14 | 108.59445287 |
| A15 | 110.73259313 |
| A16 | 125.88854598 |
| A17 | 102.03442601 |
| A18 | 114.05630846 |
| A19 | 108.86826981 |
| A20 | 110.81123173 |
| A21 | 109.04144873 |

| | |
|-----|---------------|
| A22 | 112.25120391 |
| A23 | 111.48540253 |
| A24 | 101.35633255 |
| A25 | 131.26879988 |
| D1 | 120.00122761 |
| D2 | -119.30453605 |
| D3 | -58.76844478 |
| D4 | 16.46728057 |
| D5 | -93.43469368 |
| D6 | 63.78291555 |
| D7 | 168.12873958 |
| D8 | -132.77243000 |
| D9 | -11.41230641 |
| D10 | 103.86967944 |
| D11 | -94.73610220 |
| D12 | -57.06143004 |
| D13 | 123.89699981 |
| D14 | -127.08462855 |
| D15 | -44.86832325 |
| D16 | 156.57329203 |
| D17 | -83.10359704 |
| D18 | -54.80076772 |
| D19 | 65.47253030 |
| D20 | -174.36245236 |
| D21 | 47.71259707 |
| D22 | -83.31110651 |
| D23 | 79.17719125 |
| D24 | 40.35781894 |

Harmonic Vibrational Frequencies (cm-1):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 31.57 | 45.37 | 71.60 | 91.32 | 119.94 | 132.05 | 140.87 | 152.61 | 167.69 | 211.71 | 217.06 |
| 237.67 | 261.70 | 275.17 | 287.55 | 332.27 | 335.39 | 436.93 | 471.19 | 504.60 | 509.93 | |
| 527.62 | 672.72 | 680.11 | 737.88 | 800.04 | 824.14 | 851.52 | 868.43 | 906.39 | 932.22 | |
| 954.67 | 991.31 | 1003.97 | 1021.41 | 1046.37 | 1099.36 | 1111.88 | 1120.26 | 1142.34 | | |
| 1148.36 | 1163.63 | 1194.48 | 1200.61 | 1355.07 | 1358.66 | 1365.24 | 1379.19 | 1409.44 | | |
| 1413.75 | 1421.13 | 1425.81 | 1444.10 | 1462.90 | 1488.54 | 1490.84 | 1491.18 | 1502.12 | | |
| 1506.04 | 1549.23 | 1680.31 | 2965.70 | 3060.73 | 3075.03 | 3086.22 | 3100.16 | 3105.55 | | |
| 3120.29 | 3152.80 | 3160.94 | 3172.49 | 3185.69 | 3195.49 | 3203.18 | 3403.81 | | | |

Rotational constants (B/GHZ): 0.9289128 0.7260303 0.5181500



TS6f

C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| C | 1 | B1 | | | | |
| H | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| H | 2 | B4 | 1 | A3 | 4 | D2 0 |
| O | 1 | B5 | 2 | A4 | 5 | D3 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 0 |
| C | 6 | B8 | 1 | A7 | 2 | D6 0 |
| C | 9 | B9 | 6 | A8 | 1 | D7 0 |
| H | 10 | B10 | 9 | A9 | 6 | D8 0 |
| H | 10 | B11 | 9 | A10 | 6 | D9 0 |
| H | 10 | B12 | 9 | A11 | 6 | D10 0 |
| O | 9 | B13 | 6 | A12 | 1 | D11 0 |
| O | 9 | B14 | 6 | A13 | 1 | D12 0 |
| H | 1 | B15 | 6 | A14 | 9 | D13 0 |
| O | 1 | B16 | 6 | A15 | 9 | D14 0 |
| C | 8 | B17 | 1 | A16 | 6 | D15 0 |
| H | 18 | B18 | 8 | A17 | 1 | D16 0 |
| C | 18 | B19 | 8 | A18 | 1 | D17 0 |
| H | 20 | B20 | 18 | A19 | 8 | D18 0 |
| H | 20 | B21 | 18 | A20 | 8 | D19 0 |
| H | 20 | B22 | 18 | A21 | 8 | D20 0 |
| O | 18 | B23 | 8 | A22 | 1 | D21 0 |
| O | 24 | B24 | 18 | A23 | 8 | D22 0 |
| H | 25 | B25 | 24 | A24 | 18 | D23 0 |
| H | 9 | B26 | 6 | A25 | 1 | D24 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51945669 |
| B2 | 1.08871207 |
| B3 | 1.08825121 |
| B4 | 1.08724659 |
| B5 | 1.38433286 |
| B6 | 1.27173805 |
| B7 | 2.31297405 |

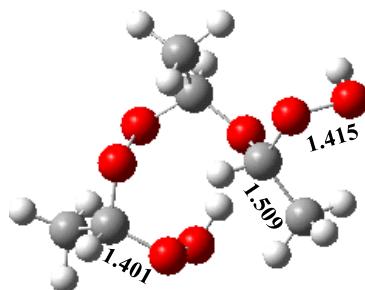
| | |
|-----|--------------|
| B8 | 2.23404085 |
| B9 | 1.47195852 |
| B10 | 1.08465653 |
| B11 | 1.08190763 |
| B12 | 1.09769797 |
| B13 | 2.20525129 |
| B14 | 1.26934601 |
| B15 | 1.09796198 |
| B16 | 1.42132035 |
| B17 | 1.40701808 |
| B18 | 1.09332762 |
| B19 | 1.51059492 |
| B20 | 1.08803203 |
| B21 | 1.08383621 |
| B22 | 1.08799779 |
| B23 | 1.40563187 |
| B24 | 1.41980350 |
| B25 | 0.98322305 |
| B26 | 1.08735213 |
| A1 | 110.12805894 |
| A2 | 109.15654378 |
| A3 | 110.84255920 |
| A4 | 114.56556539 |
| A5 | 112.12305452 |
| A6 | 95.26985871 |
| A7 | 122.34605065 |
| A8 | 89.75025650 |
| A9 | 110.18982712 |
| A10 | 112.80553914 |
| A11 | 104.16801365 |
| A12 | 64.93465324 |
| A13 | 87.42144854 |
| A14 | 109.66080751 |
| A15 | 110.76579092 |
| A16 | 125.50177285 |
| A17 | 102.09134642 |
| A18 | 113.77903694 |
| A19 | 108.92196209 |
| A20 | 110.87364085 |
| A21 | 108.99880677 |
| A22 | 111.85415920 |
| A23 | 111.01367568 |
| A24 | 101.28615866 |
| A25 | 110.65362431 |

| | |
|-----|---------------|
| D1 | 119.90813905 |
| D2 | 119.68581317 |
| D3 | -63.24791476 |
| D4 | -36.20712732 |
| D5 | -93.37049852 |
| D6 | 41.49089783 |
| D7 | 164.87945943 |
| D8 | -70.88968758 |
| D9 | 55.03284894 |
| D10 | 173.55409655 |
| D11 | -100.12047293 |
| D12 | -69.72227892 |
| D13 | 165.58164355 |
| D14 | -85.17236538 |
| D15 | -47.02257099 |
| D16 | 153.79254788 |
| D17 | -86.04426095 |
| D18 | -56.21825952 |
| D19 | 64.21943886 |
| D20 | -175.71883353 |
| D21 | 44.70039168 |
| D22 | -83.43709024 |
| D23 | 81.82184920 |
| D24 | 43.06193513 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 882.91 <i>i</i> | 46.69 | 81.47 | 100.00 | 117.51 | 130.39 | 151.83 | 178.27 | 197.68 | 220.54 | 236.66 |
| 255.13 | 271.32 | 277.10 | 303.64 | 337.33 | 350.07 | 413.46 | 470.57 | 511.11 | 520.60 | |
| 527.14 | 636.46 | 671.42 | 733.70 | 745.21 | 823.76 | 854.05 | 855.17 | 876.30 | 928.49 | |
| 941.54 | 954.04 | 957.34 | 988.74 | 1018.19 | 1083.42 | 1110.58 | 1138.97 | 1154.51 | 1160.30 | |
| 1175.91 | 1193.14 | 1218.87 | 1353.17 | 1360.83 | 1370.43 | 1377.26 | 1397.77 | 1407.20 | | |
| 1414.33 | 1422.65 | 1429.22 | 1459.43 | 1473.93 | 1484.98 | 1492.23 | 1499.79 | 1502.47 | | |
| 1540.53 | 1607.43 | 1868.10 | 3026.72 | 3046.64 | 3065.13 | 3091.33 | 3103.64 | 3141.75 | | |
| 3154.29 | 3155.10 | 3167.30 | 3195.89 | 3204.14 | 3217.29 | 3443.30 | | | | |

Rotational constants (B/GHZ): 1.2463340 0.5375475 0.4463976



P6f

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| O | 1 | B5 | 2 | A4 | 5 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| O | 1 | B7 | 6 | A6 | 2 | D5 | 0 |
| C | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| C | 9 | B9 | 6 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 9 | A9 | 6 | D8 | 0 |
| H | 10 | B11 | 9 | A10 | 6 | D9 | 0 |
| H | 10 | B12 | 9 | A11 | 6 | D10 | 0 |
| O | 9 | B13 | 6 | A12 | 1 | D11 | 0 |
| O | 9 | B14 | 6 | A13 | 1 | D12 | 0 |
| H | 1 | B15 | 6 | A14 | 9 | D13 | 0 |
| O | 1 | B16 | 6 | A15 | 9 | D14 | 0 |
| C | 8 | B17 | 1 | A16 | 17 | D15 | 0 |
| H | 18 | B18 | 8 | A17 | 1 | D16 | 0 |
| C | 18 | B19 | 8 | A18 | 1 | D17 | 0 |
| H | 20 | B20 | 18 | A19 | 8 | D18 | 0 |
| H | 20 | B21 | 18 | A20 | 8 | D19 | 0 |
| H | 20 | B22 | 18 | A21 | 8 | D20 | 0 |
| O | 18 | B23 | 8 | A22 | 1 | D21 | 0 |
| O | 24 | B24 | 18 | A23 | 8 | D22 | 0 |
| H | 25 | B25 | 24 | A24 | 18 | D23 | 0 |
| H | 9 | B26 | 6 | A25 | 1 | D24 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.51498467 |
| B2 | 1.08677924 |
| B3 | 1.08813882 |
| B4 | 1.08591682 |
| B5 | 1.41325137 |
| B6 | 2.54139921 |
| B7 | 2.29632938 |
| B8 | 1.41992540 |
| B9 | 1.50924210 |
| B10 | 1.08633924 |
| B11 | 1.08689815 |
| B12 | 1.08801150 |
| B13 | 2.30376784 |
| B14 | 1.40671765 |
| B15 | 1.09163490 |
| B16 | 1.40697681 |
| B17 | 1.41292654 |

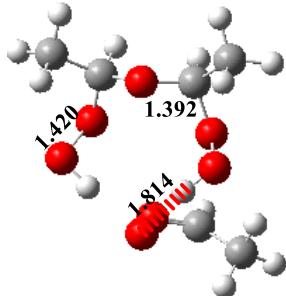
| | |
|-----|--------------|
| B18 | 1.09260695 |
| B19 | 1.51009170 |
| B20 | 1.08780868 |
| B21 | 1.08428702 |
| B22 | 1.08786834 |
| B23 | 1.40133909 |
| B24 | 1.41747588 |
| B25 | 0.97125762 |
| B26 | 1.09065905 |
| A1 | 110.44914362 |
| A2 | 107.61534911 |
| A3 | 112.10535128 |
| A4 | 116.15703638 |
| A5 | 107.46767446 |
| A6 | 97.83374265 |
| A7 | 120.22645770 |
| A8 | 107.89479500 |
| A9 | 109.90235176 |
| A10 | 110.14843666 |
| A11 | 108.84722506 |
| A12 | 94.55060324 |
| A13 | 110.24273645 |
| A14 | 104.95547753 |
| A15 | 110.74457370 |
| A16 | 126.48827666 |
| A17 | 101.59393520 |
| A18 | 113.28349727 |
| A19 | 108.83538156 |
| A20 | 110.97051647 |
| A21 | 109.10482545 |
| A22 | 111.74171429 |
| A23 | 111.31502611 |
| A24 | 101.52659488 |
| A25 | 110.63759257 |
| D1 | 119.36553687 |
| D2 | 119.50005045 |
| D3 | -60.99070410 |
| D4 | -50.06901703 |
| D5 | -94.65585259 |
| D6 | 31.99955658 |
| D7 | 162.08059276 |
| D8 | -70.76436575 |
| D9 | 50.22145138 |
| D10 | 169.50567890 |

| | |
|-----|---------------|
| D11 | -106.66555970 |
| D12 | -74.04722996 |
| D13 | 154.12231247 |
| D14 | -97.66508603 |
| D15 | 68.78299630 |
| D16 | 149.83347403 |
| D17 | -90.17335955 |
| D18 | -58.82538710 |
| D19 | 61.67673085 |
| D20 | -178.31895720 |
| D21 | 40.68965694 |
| D22 | -87.70985558 |
| D23 | 88.47478270 |
| D24 | 39.13642512 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 58.10 | 82.69 | 105.54 | 109.39 | 127.57 | 169.58 | 182.65 | 195.56 | 211.34 | 229.97 | 249.58 |
| 256.12 | 265.10 | 281.63 | 333.86 | 339.31 | 374.63 | 407.05 | 463.47 | 506.86 | 528.11 | |
| 590.16 | 594.78 | 691.50 | 721.56 | 739.99 | 824.01 | 855.76 | 891.31 | 931.29 | 932.58 | |
| 959.08 | 993.29 | 1016.89 | 1020.75 | 1101.81 | 1128.74 | 1140.24 | 1148.83 | 1157.81 | | |
| 1159.86 | 1187.26 | 1195.81 | 1213.31 | 1363.16 | 1368.24 | 1374.19 | 1384.75 | 1388.43 | | |
| 1415.10 | 1424.94 | 1428.32 | 1431.03 | 1437.76 | 1478.95 | 1486.30 | 1487.54 | 1494.99 | | |
| 1500.56 | 1506.00 | 1507.20 | 3078.88 | 3081.84 | 3082.56 | 3106.83 | 3112.98 | 3143.83 | | |
| 3157.01 | 3159.00 | 3160.18 | 3174.23 | 3175.68 | 3195.44 | 3700.26 | 3805.64 | | | |

Rotational constants (B/GHZ): 1.3417004 0.5635910 0.4565588



IM6g

| C | | | | | | | |
|---|---|--|-----|---|----|---|----|
| H | 1 | | B1 | | | | |
| O | 1 | | B2 | 2 | A1 | | |
| O | 1 | | B3 | 3 | A2 | 2 | D1 |
| H | 3 | | B4 | 1 | A3 | 4 | D2 |
| C | 4 | | B5 | 1 | A4 | 3 | D3 |
| C | 6 | | B6 | 4 | A5 | 1 | D4 |
| H | 7 | | B7 | 6 | A6 | 4 | D5 |
| H | 7 | | B8 | 6 | A7 | 4 | D6 |
| H | 7 | | B9 | 6 | A8 | 4 | D7 |
| O | 6 | | B10 | 4 | A9 | 1 | D8 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 6 | B11 | 4 | A10 | 1 | D9 | 0 |
| H | 6 | B12 | 4 | A11 | 1 | D10 | 0 |
| C | 1 | B13 | 4 | A12 | 3 | D11 | 0 |
| H | 14 | B14 | 1 | A13 | 4 | D12 | 0 |
| H | 14 | B15 | 1 | A14 | 4 | D13 | 0 |
| H | 14 | B16 | 1 | A15 | 4 | D14 | 0 |
| O | 1 | B17 | 4 | A16 | 3 | D15 | 0 |
| C | 18 | B18 | 1 | A17 | 4 | D16 | 0 |
| H | 19 | B19 | 18 | A18 | 1 | D17 | 0 |
| C | 19 | B20 | 18 | A19 | 1 | D18 | 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 | 0 |
| H | 21 | B22 | 19 | A21 | 18 | D20 | 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 | 0 |
| O | 19 | B24 | 18 | A23 | 1 | D22 | 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 | 0 |

Variables:

| | |
|-----|--------------|
| B1 | 1.09649557 |
| B2 | 2.30176060 |
| B3 | 1.41453505 |
| B4 | 0.97965383 |
| B5 | 2.94837541 |
| B6 | 1.46426993 |
| B7 | 1.09593887 |
| B8 | 1.09064721 |
| B9 | 1.08489583 |
| B10 | 2.24069886 |
| B11 | 1.24078167 |
| B12 | 1.08600085 |
| B13 | 1.51133996 |
| B14 | 1.08647652 |
| B15 | 1.08824007 |
| B16 | 1.08801230 |
| B17 | 1.39203470 |
| B18 | 1.40582584 |
| B19 | 1.09666383 |
| B20 | 1.51028999 |
| B21 | 1.08787731 |
| B22 | 1.08787791 |
| B23 | 1.08597768 |
| B24 | 1.40027257 |
| B25 | 1.41993205 |
| B26 | 0.97994335 |
| A1 | 136.91515798 |

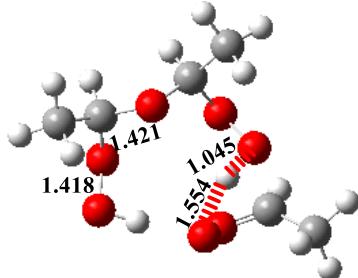
| | |
|-----|---------------|
| A2 | 35.81860431 |
| A3 | 109.03741938 |
| A4 | 149.11004085 |
| A5 | 87.07937420 |
| A6 | 108.02682625 |
| A7 | 108.86201020 |
| A8 | 110.69569445 |
| A9 | 70.16420026 |
| A10 | 76.28002436 |
| A11 | 107.84233799 |
| A12 | 112.06744738 |
| A13 | 109.54137976 |
| A14 | 110.01138457 |
| A15 | 109.39349606 |
| A16 | 112.82265571 |
| A17 | 117.23992274 |
| A18 | 109.32557199 |
| A19 | 107.68837284 |
| A20 | 109.38144684 |
| A21 | 109.60996170 |
| A22 | 109.73842838 |
| A23 | 113.17843915 |
| A24 | 109.35286247 |
| A25 | 101.53919946 |
| D1 | 8.84543864 |
| D2 | -80.28135318 |
| D3 | 128.46414001 |
| D4 | -175.75043141 |
| D5 | -2.18580904 |
| D6 | 112.91139840 |
| D7 | -123.17636861 |
| D8 | -83.72229657 |
| D9 | -49.69669308 |
| D10 | 59.54977740 |
| D11 | 54.60925713 |
| D12 | -70.77187038 |
| D13 | 49.39208897 |
| D14 | 169.75182556 |
| D15 | -68.04913608 |
| D16 | -86.03575549 |
| D17 | -36.76989291 |
| D18 | -157.94346289 |
| D19 | 64.92834302 |
| D20 | -174.76444587 |

D21 -54.97628096
 D22 75.81412038
 D23 75.87758265
 D24 -112.35655170

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 41.54 | 52.20 | 66.76 | 76.75 | 105.46 | 115.11 | 126.84 | 167.24 | 195.35 | 203.03 | 210.81 |
| 219.95 | 225.44 | 278.17 | 307.79 | 325.31 | 355.86 | 363.10 | 411.34 | 469.87 | 473.96 | |
| 604.52 | 629.02 | 688.61 | 692.78 | 695.87 | 744.64 | 797.06 | 858.46 | 883.04 | 918.35 | |
| 941.62 | 977.80 | 997.95 | 1007.87 | 1033.74 | 1100.26 | 1127.16 | 1129.21 | 1148.76 | | |
| 1149.72 | 1172.76 | 1184.31 | 1227.71 | 1357.87 | 1371.98 | 1379.03 | 1384.71 | 1420.28 | | |
| 1422.21 | 1424.76 | 1438.88 | 1448.34 | 1475.82 | 1485.57 | 1487.55 | 1497.98 | 1501.67 | | |
| 1528.55 | 1560.93 | 1689.25 | 3042.11 | 3056.43 | 3066.18 | 3076.12 | 3080.49 | 3108.10 | | |
| 3152.40 | 3158.55 | 3173.82 | 3177.62 | 3178.01 | 3201.20 | 3474.26 | 3520.29 | | | |

Rotational constants (B/GHZ): 1.0046496 0.6106915 0.4315555



TS6g

| C | | B1 | | A1 | | D1 | 0 |
|---|----|-----|----|-----|----|-----|---|
| H | 1 | | | | | | |
| O | 1 | B2 | 2 | A1 | | | |
| O | 3 | B3 | 1 | A2 | 2 | D1 | 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 | 0 |
| C | 3 | B5 | 1 | A4 | 4 | D3 | 0 |
| C | 6 | B6 | 3 | A5 | 1 | D4 | 0 |
| H | 7 | B7 | 6 | A6 | 3 | D5 | 0 |
| H | 7 | B8 | 6 | A7 | 3 | D6 | 0 |
| H | 7 | B9 | 6 | A8 | 3 | D7 | 0 |
| O | 6 | B10 | 3 | A9 | 1 | D8 | 0 |
| O | 6 | B11 | 3 | A10 | 1 | D9 | 0 |
| H | 6 | B12 | 3 | A11 | 1 | D10 | 0 |
| C | 1 | B13 | 4 | A12 | 3 | D11 | 0 |
| H | 14 | B14 | 1 | A13 | 4 | D12 | 0 |
| H | 14 | B15 | 1 | A14 | 4 | D13 | 0 |
| H | 14 | B16 | 1 | A15 | 4 | D14 | 0 |
| O | 1 | B17 | 4 | A16 | 3 | D15 | 0 |
| C | 18 | B18 | 1 | A17 | 4 | D16 | 0 |
| H | 19 | B19 | 18 | A18 | 1 | D17 | 0 |
| C | 19 | B20 | 18 | A19 | 1 | D18 | 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 21 | B22 | 19 | A21 | 18 | D20 | 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 | 0 |
| O | 19 | B24 | 18 | A23 | 1 | D22 | 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 | 0 |

Variables:

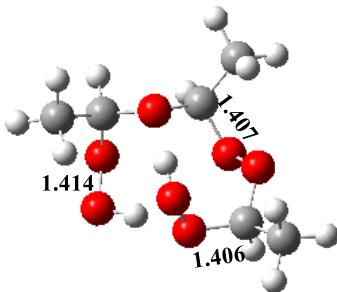
| | |
|-----|--------------|
| B1 | 1.09558379 |
| B2 | 2.30796796 |
| B3 | 1.41624099 |
| B4 | 1.04545092 |
| B5 | 1.96121400 |
| B6 | 1.48480472 |
| B7 | 1.08615362 |
| B8 | 1.08368897 |
| B9 | 1.09358542 |
| B10 | 2.19697740 |
| B11 | 1.27454258 |
| B12 | 1.08825276 |
| B13 | 1.51099404 |
| B14 | 1.08695007 |
| B15 | 1.08799000 |
| B16 | 1.08772184 |
| B17 | 1.38680325 |
| B18 | 1.42092907 |
| B19 | 1.09567571 |
| B20 | 1.50948031 |
| B21 | 1.08799187 |
| B22 | 1.08769635 |
| B23 | 1.08577049 |
| B24 | 1.39307310 |
| B25 | 1.41760896 |
| B26 | 0.98796329 |
| A1 | 135.60381856 |
| A2 | 35.67478130 |
| A3 | 93.99629685 |
| A4 | 135.37052302 |
| A5 | 94.34337851 |
| A6 | 109.84282567 |
| A7 | 111.69150850 |
| A8 | 106.12902690 |
| A9 | 72.71747248 |
| A10 | 94.47102183 |
| A11 | 103.66268779 |
| A12 | 112.38231554 |

| | |
|-----|---------------|
| A13 | 110.08276496 |
| A14 | 110.04809704 |
| A15 | 109.10279454 |
| A16 | 112.09808856 |
| A17 | 116.62889146 |
| A18 | 108.35592337 |
| A19 | 107.42426989 |
| A20 | 109.41511823 |
| A21 | 109.44260825 |
| A22 | 109.97403183 |
| A23 | 112.84578596 |
| A24 | 110.16137251 |
| A25 | 102.25998450 |
| D1 | -9.47406200 |
| D2 | -108.93240908 |
| D3 | -29.16992006 |
| D4 | -176.85975883 |
| D5 | -63.05998865 |
| D6 | 60.97143546 |
| D7 | 179.73342166 |
| D8 | -83.31089340 |
| D9 | -51.92061995 |
| D10 | 61.99639917 |
| D11 | 54.31287876 |
| D12 | -72.15875547 |
| D13 | 48.48361470 |
| D14 | 168.62095373 |
| D15 | -68.74251223 |
| D16 | -83.94308661 |
| D17 | -35.01363359 |
| D18 | -155.63381734 |
| D19 | 66.18719670 |
| D20 | -173.50716202 |
| D21 | -53.98103850 |
| D22 | 77.62520806 |
| D23 | 81.02996891 |
| D24 | -98.32368841 |

Harmonic Vibrational Frequencies (cm^{-1}):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 404.04 <i>i</i> | 36.43 | 55.87 | 95.70 | 98.60 | 107.87 | 128.39 | 170.73 | 207.70 | 215.25 | 226.02 |
| 248.43 | 271.88 | 293.59 | 323.78 | 343.24 | 361.16 | 390.24 | 409.53 | 470.41 | 528.15 | |
| 612.01 | 654.34 | 691.52 | 705.18 | 837.23 | 853.64 | 867.22 | 886.34 | 930.84 | 939.07 | |
| 974.31 | 982.41 | 1009.47 | 1024.95 | 1101.98 | 1107.28 | 1137.13 | 1154.80 | 1166.03 | | |
| 1169.31 | 1189.09 | 1223.81 | 1235.29 | 1361.27 | 1363.44 | 1375.56 | 1385.34 | 1403.76 | | |
| 1419.71 | 1426.41 | 1440.41 | 1450.74 | 1480.56 | 1485.20 | 1492.34 | 1496.61 | 1500.10 | | |

1532.60 1576.80 1593.34 2421.59 3056.46 3061.53 3073.11 3075.71 3078.02
 3144.22 3155.11 3158.64 3164.44 3175.57 3189.05 3202.26 3318.08
 Rotational constants (B/GHZ): 1.0803045 0.6061730 0.4378650



P6g

C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| H | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| O | 1 | B3 | 3 | A2 | 2 | D1 0 |
| H | 3 | B4 | 1 | A3 | 4 | D2 0 |
| C | 3 | B5 | 1 | A4 | 4 | D3 0 |
| C | 6 | B6 | 3 | A5 | 1 | D4 0 |
| H | 7 | B7 | 6 | A6 | 3 | D5 0 |
| H | 7 | B8 | 6 | A7 | 3 | D6 0 |
| H | 7 | B9 | 6 | A8 | 3 | D7 0 |
| O | 6 | B10 | 3 | A9 | 1 | D8 0 |
| O | 6 | B11 | 3 | A10 | 1 | D9 0 |
| H | 6 | B12 | 3 | A11 | 1 | D10 0 |
| C | 1 | B13 | 4 | A12 | 3 | D11 0 |
| H | 14 | B14 | 1 | A13 | 4 | D12 0 |
| H | 14 | B15 | 1 | A14 | 4 | D13 0 |
| H | 14 | B16 | 1 | A15 | 4 | D14 0 |
| O | 1 | B17 | 4 | A16 | 3 | D15 0 |
| C | 18 | B18 | 1 | A17 | 4 | D16 0 |
| H | 19 | B19 | 18 | A18 | 1 | D17 0 |
| C | 19 | B20 | 18 | A19 | 1 | D18 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 0 |
| H | 21 | B22 | 19 | A21 | 18 | D20 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 0 |
| O | 19 | B24 | 18 | A23 | 1 | D22 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 0 |

Variables:

| | |
|----|------------|
| B1 | 1.09272989 |
| B2 | 2.28738625 |
| B3 | 1.40698772 |
| B4 | 2.56868194 |

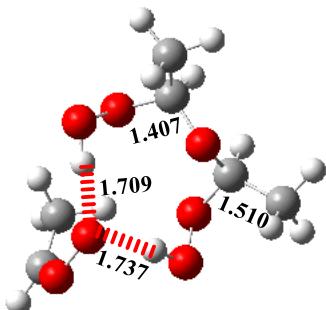
| | |
|-----|--------------|
| B5 | 1.39920313 |
| B6 | 1.50922735 |
| B7 | 1.08729649 |
| B8 | 1.08662671 |
| B9 | 1.08742064 |
| B10 | 2.30679945 |
| B11 | 1.40625469 |
| B12 | 1.09308523 |
| B13 | 1.51066940 |
| B14 | 1.08670114 |
| B15 | 1.08794873 |
| B16 | 1.08810724 |
| B17 | 1.41032996 |
| B18 | 1.42039824 |
| B19 | 1.09502270 |
| B20 | 1.50769118 |
| B21 | 1.08784406 |
| B22 | 1.08768902 |
| B23 | 1.08721152 |
| B24 | 1.39559400 |
| B25 | 1.41447171 |
| B26 | 0.97305510 |
| A1 | 137.30409043 |
| A2 | 36.42963001 |
| A3 | 70.59886783 |
| A4 | 128.01426630 |
| A5 | 106.30743081 |
| A6 | 109.76497702 |
| A7 | 110.01312293 |
| A8 | 108.85366188 |
| A9 | 92.47243809 |
| A10 | 111.35642264 |
| A11 | 110.12693569 |
| A12 | 113.19243272 |
| A13 | 110.12627757 |
| A14 | 109.96080372 |
| A15 | 109.12403297 |
| A16 | 110.99214774 |
| A17 | 115.07829102 |
| A18 | 108.77957929 |
| A19 | 107.84048318 |
| A20 | 109.48365548 |
| A21 | 109.22706388 |
| A22 | 110.34010596 |

| | |
|-----|---------------|
| A23 | 111.25560139 |
| A24 | 109.85096152 |
| A25 | 103.58561194 |
| D1 | 14.72094049 |
| D2 | -117.51504677 |
| D3 | -64.67283429 |
| D4 | -153.95826857 |
| D5 | -62.83847293 |
| D6 | 57.82885392 |
| D7 | 177.35162269 |
| D8 | -60.27776248 |
| D9 | -29.64754197 |
| D10 | 83.30881855 |
| D11 | 49.58616740 |
| D12 | -70.97191214 |
| D13 | 49.44352532 |
| D14 | 169.48585131 |
| D15 | -73.48106921 |
| D16 | -100.75914071 |
| D17 | -54.50400627 |
| D18 | -175.95925180 |
| D19 | 63.95504164 |
| D20 | -176.14085651 |
| D21 | -56.64373524 |
| D22 | 57.34956199 |
| D23 | 74.46974902 |
| D24 | -78.09749349 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 58.79 | 61.00 | 87.94 | 114.19 | 127.06 | 186.32 | 190.49 | 202.63 | 213.19 | 228.44 | 242.95 |
| 273.71 | 298.91 | 314.06 | 333.40 | 358.97 | 417.66 | 437.76 | 477.66 | 544.22 | 566.07 | |
| 600.08 | 650.53 | 675.06 | 713.46 | 716.82 | 855.60 | 882.30 | 895.10 | 937.09 | 947.39 | |
| 984.96 | 1006.66 | 1019.40 | 1030.68 | 1112.84 | 1137.19 | 1148.33 | 1151.44 | 1155.35 | | |
| 1170.86 | 1174.26 | 1207.09 | 1230.16 | 1358.25 | 1365.23 | 1377.82 | 1393.18 | 1397.86 | | |
| 1423.19 | 1426.42 | 1431.17 | 1439.11 | 1469.19 | 1486.57 | 1488.32 | 1489.63 | 1498.17 | | |
| 1500.52 | 1504.34 | 1525.22 | 3070.83 | 3074.95 | 3078.01 | 3085.72 | 3111.40 | 3113.12 | | |
| 3151.75 | 3157.51 | 3163.49 | 3164.74 | 3166.85 | 3178.31 | 3638.68 | 3670.62 | | | |

Rotational constants (B/GHZ): 1.0949408 0.6441656 0.5157917



IM6h

C

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 | 0 |
| C | 7 | B7 | 4 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 7 | A7 | 4 | D6 | 0 |
| H | 8 | B9 | 7 | A8 | 4 | D7 | 0 |
| H | 8 | B10 | 7 | A9 | 4 | D8 | 0 |
| O | 7 | B11 | 4 | A10 | 2 | D9 | 0 |
| O | 7 | B12 | 4 | A11 | 2 | D10 | 0 |
| H | 7 | B13 | 4 | A12 | 2 | D11 | 0 |
| H | 1 | B14 | 2 | A13 | 5 | D12 | 0 |
| H | 1 | B15 | 2 | A14 | 5 | D13 | 0 |
| H | 1 | B16 | 2 | A15 | 5 | D14 | 0 |
| O | 2 | B17 | 1 | A16 | 5 | D15 | 0 |
| C | 18 | B18 | 2 | A17 | 1 | D16 | 0 |
| H | 19 | B19 | 18 | A18 | 2 | D17 | 0 |
| C | 19 | B20 | 18 | A19 | 2 | D18 | 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 | 0 |
| H | 21 | B22 | 19 | A21 | 18 | D20 | 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 | 0 |
| O | 19 | B24 | 18 | A23 | 2 | D22 | 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 | 0 |

Variables:

| | |
|----|------------|
| B1 | 1.50975000 |
| B2 | 1.09578514 |
| B3 | 2.31556026 |
| B4 | 1.40714344 |
| B5 | 0.98046850 |
| B6 | 3.84902584 |
| B7 | 1.46004358 |

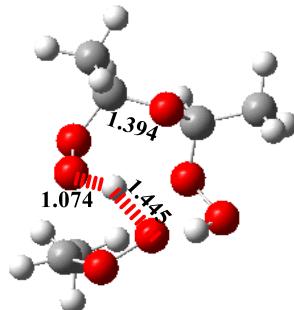
| | |
|-----|--------------|
| B8 | 1.09613712 |
| B9 | 1.08441359 |
| B10 | 1.09536997 |
| B11 | 2.24965885 |
| B12 | 1.24497071 |
| B13 | 1.08677102 |
| B14 | 1.08784423 |
| B15 | 1.08785481 |
| B16 | 1.08598230 |
| B17 | 1.40372857 |
| B18 | 1.40174794 |
| B19 | 1.09569412 |
| B20 | 1.51006130 |
| B21 | 1.08601017 |
| B22 | 1.08777135 |
| B23 | 1.08798779 |
| B24 | 1.40888036 |
| B25 | 1.41666391 |
| B26 | 0.98632258 |
| A1 | 111.47914265 |
| A2 | 87.20621932 |
| A3 | 113.37602806 |
| A4 | 101.76816920 |
| A5 | 110.08448304 |
| A6 | 54.09431372 |
| A7 | 109.81958089 |
| A8 | 110.62382869 |
| A9 | 109.05808642 |
| A10 | 43.84357246 |
| A11 | 73.64872672 |
| A12 | 160.46698622 |
| A13 | 109.11806410 |
| A14 | 109.79882643 |
| A15 | 110.02064874 |
| A16 | 108.18372035 |
| A17 | 116.67332246 |
| A18 | 109.72891903 |
| A19 | 108.33921583 |
| A20 | 110.01420189 |
| A21 | 109.86706400 |
| A22 | 109.12058949 |
| A23 | 112.39082847 |
| A24 | 110.12173364 |
| A25 | 102.83429012 |

| | |
|-----|---------------|
| D1 | -137.88357664 |
| D2 | 24.02516668 |
| D3 | -124.96201807 |
| D4 | -160.42948440 |
| D5 | -62.15702076 |
| D6 | 76.86485999 |
| D7 | -159.71094327 |
| D8 | -37.74059032 |
| D9 | 82.16844064 |
| D10 | 98.41233760 |
| D11 | -152.67672306 |
| D12 | -168.01053792 |
| D13 | -47.77990806 |
| D14 | 72.26079348 |
| D15 | -125.75078509 |
| D16 | -153.46155662 |
| D17 | 28.74718576 |
| D18 | 150.78401800 |
| D19 | 52.46523804 |
| D20 | 172.55061740 |
| D21 | -67.17284529 |
| D22 | -83.51553832 |
| D23 | -76.53769192 |
| D24 | 84.38735404 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 49.51 | 52.20 | 63.12 | 93.31 | 106.23 | 123.38 | 143.01 | 158.59 | 200.34 | 221.82 | 231.79 |
| 252.37 | 273.79 | 283.41 | 319.64 | 320.30 | 347.07 | 367.26 | 403.37 | 469.31 | 481.55 | |
| 612.63 | 671.81 | 692.28 | 697.52 | 781.71 | 791.90 | 840.29 | 861.50 | 882.18 | 925.44 | |
| 935.95 | 978.28 | 1006.60 | 1012.84 | 1031.58 | 1104.32 | 1124.07 | 1135.40 | 1137.77 | | |
| 1151.14 | 1176.15 | 1181.08 | 1225.24 | 1365.19 | 1368.48 | 1383.49 | 1385.92 | 1419.69 | | |
| 1422.68 | 1425.85 | 1441.41 | 1454.32 | 1476.87 | 1483.27 | 1489.06 | 1494.36 | 1499.00 | | |
| 1501.98 | 1543.75 | 1669.83 | 3031.59 | 3060.22 | 3071.40 | 3073.86 | 3076.41 | 3080.82 | | |
| 3151.18 | 3155.59 | 3169.31 | 3169.47 | 3171.81 | 3202.77 | 3344.91 | 3471.92 | | | |

Rotational constants (B/GHZ): 0.9334877 0.6165261 0.4455141



TS6h

C

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| O | 4 | B4 | 2 | A3 | 1 | D2 | 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 | 0 |
| C | 7 | B7 | 4 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 7 | A7 | 4 | D6 | 0 |
| H | 8 | B9 | 7 | A8 | 4 | D7 | 0 |
| H | 8 | B10 | 7 | A9 | 4 | D8 | 0 |
| O | 7 | B11 | 4 | A10 | 2 | D9 | 0 |
| O | 7 | B12 | 4 | A11 | 2 | D10 | 0 |
| H | 7 | B13 | 4 | A12 | 2 | D11 | 0 |
| H | 1 | B14 | 2 | A13 | 5 | D12 | 0 |
| H | 1 | B15 | 2 | A14 | 5 | D13 | 0 |
| H | 1 | B16 | 2 | A15 | 5 | D14 | 0 |
| O | 2 | B17 | 1 | A16 | 5 | D15 | 0 |
| C | 18 | B18 | 2 | A17 | 1 | D16 | 0 |
| H | 19 | B19 | 18 | A18 | 2 | D17 | 0 |
| C | 19 | B20 | 18 | A19 | 2 | D18 | 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 | 0 |
| H | 21 | B22 | 19 | A21 | 18 | D20 | 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 | 0 |
| O | 19 | B24 | 18 | A23 | 2 | D22 | 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.51034559 |
| B2 | 1.09571987 |
| B3 | 2.30216649 |
| B4 | 1.41423500 |
| B5 | 1.07363063 |
| B6 | 2.01050930 |
| B7 | 1.47655379 |
| B8 | 1.08274644 |
| B9 | 1.09528129 |
| B10 | 1.08694291 |
| B11 | 2.21912884 |
| B12 | 1.27771680 |
| B13 | 1.08854666 |
| B14 | 1.08769019 |
| B15 | 1.08789183 |
| B16 | 1.08685170 |
| B17 | 1.39354251 |

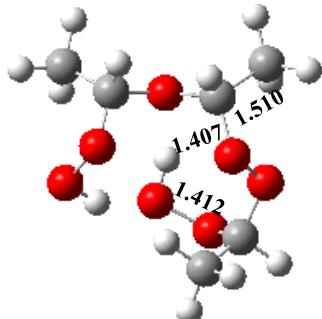
| | |
|-----|---------------|
| B18 | 1.41275009 |
| B19 | 1.09530639 |
| B20 | 1.50905551 |
| B21 | 1.08599086 |
| B22 | 1.08755708 |
| B23 | 1.08785043 |
| B24 | 1.40230223 |
| B25 | 1.41779428 |
| B26 | 0.98293214 |
| A1 | 111.83499594 |
| A2 | 90.04794310 |
| A3 | 35.68923185 |
| A4 | 87.50780907 |
| A5 | 139.11483110 |
| A6 | 98.08424818 |
| A7 | 113.89605568 |
| A8 | 104.96896989 |
| A9 | 109.50771547 |
| A10 | 69.53201868 |
| A11 | 90.47267619 |
| A12 | 103.94417710 |
| A13 | 109.16640977 |
| A14 | 109.82711519 |
| A15 | 110.16764572 |
| A16 | 108.50816372 |
| A17 | 116.98750431 |
| A18 | 108.86956507 |
| A19 | 107.79568017 |
| A20 | 109.90009319 |
| A21 | 109.82971510 |
| A22 | 109.13321806 |
| A23 | 112.70700612 |
| A24 | 110.93510190 |
| A25 | 102.70336293 |
| D1 | -141.13776596 |
| D2 | 131.50485285 |
| D3 | -108.04711094 |
| D4 | -176.05789065 |
| D5 | -19.50159002 |
| D6 | 60.13630365 |
| D7 | -179.36443635 |
| D8 | -63.33773162 |
| D9 | 76.08803625 |
| D10 | 107.13442832 |

| | |
|-----|---------------|
| D11 | -140.99067049 |
| D12 | -169.40750779 |
| D13 | -49.23037514 |
| D14 | 71.18698642 |
| D15 | -124.55334350 |
| D16 | -156.25993115 |
| D17 | 30.19507669 |
| D18 | 151.55435296 |
| D19 | 53.23911619 |
| D20 | 173.14420229 |
| D21 | -66.49153684 |
| D22 | -82.16434402 |
| D23 | -81.85434054 |
| D24 | 94.31677646 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 423.44 <i>i</i> | 48.52 | 89.87 | 103.52 | 127.85 | 140.36 | 173.14 | 192.53 | 202.53 | 220.15 | 223.59 |
| 252.89 | 281.91 | 311.41 | 328.67 | 359.16 | 378.05 | 402.72 | 425.73 | 458.58 | 480.07 | |
| 610.03 | 640.66 | 688.28 | 710.89 | 791.92 | 858.23 | 867.39 | 883.83 | 932.32 | 937.52 | |
| 960.78 | 984.04 | 1012.17 | 1028.15 | 1097.01 | 1112.67 | 1143.00 | 1149.36 | 1167.28 | | |
| 1176.96 | 1184.37 | 1224.15 | 1270.11 | 1361.04 | 1366.23 | 1377.76 | 1384.93 | 1411.29 | | |
| 1422.92 | 1425.97 | 1439.61 | 1444.02 | 1478.06 | 1487.02 | 1489.58 | 1494.93 | 1501.19 | | |
| 1514.53 | 1542.76 | 1643.10 | 2148.77 | 3039.48 | 3069.92 | 3076.68 | 3081.09 | 3081.93 | | |
| 3137.71 | 3157.61 | 3160.76 | 3167.47 | 3173.90 | 3187.96 | 3226.86 | 3427.04 | | | |

Rotational constants (B/GHZ): 0.9709020 0.6823635 0.4977185



P6h

| C | | B1 | | | | | |
|---|---|-----|---|----|---|----|---|
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| O | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| H | 4 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 4 | B6 | 2 | A5 | 1 | D4 | 0 |
| C | 7 | B7 | 4 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 7 | A7 | 4 | D6 | 0 |
| H | 8 | B9 | 7 | A8 | 4 | D7 | 0 |
| H | 8 | B10 | 7 | A9 | 4 | D8 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 7 | B11 | 4 | A10 | 2 | D9 | 0 |
| O | 7 | B12 | 4 | A11 | 2 | D10 | 0 |
| H | 7 | B13 | 4 | A12 | 2 | D11 | 0 |
| H | 1 | B14 | 2 | A13 | 5 | D12 | 0 |
| H | 1 | B15 | 2 | A14 | 5 | D13 | 0 |
| H | 1 | B16 | 2 | A15 | 5 | D14 | 0 |
| O | 2 | B17 | 1 | A16 | 5 | D15 | 0 |
| C | 18 | B18 | 2 | A17 | 1 | D16 | 0 |
| H | 19 | B19 | 18 | A18 | 2 | D17 | 0 |
| C | 19 | B20 | 18 | A19 | 2 | D18 | 0 |
| H | 21 | B21 | 19 | A20 | 18 | D19 | 0 |
| H | 21 | B22 | 19 | A21 | 18 | D20 | 0 |
| H | 21 | B23 | 19 | A22 | 18 | D21 | 0 |
| O | 19 | B24 | 18 | A23 | 2 | D22 | 0 |
| O | 25 | B25 | 19 | A24 | 18 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 19 | D24 | 0 |

Variables:

| | |
|-----|--------------|
| B1 | 1.51037622 |
| B2 | 1.09404777 |
| B3 | 2.31748575 |
| B4 | 1.40675945 |
| B5 | 2.63746862 |
| B6 | 1.41258533 |
| B7 | 1.50987687 |
| B8 | 1.08545935 |
| B9 | 1.08764722 |
| B10 | 1.08801005 |
| B11 | 2.31320778 |
| B12 | 1.40611002 |
| B13 | 1.09238081 |
| B14 | 1.08756228 |
| B15 | 1.08761385 |
| B16 | 1.08698888 |
| B17 | 1.40970981 |
| B18 | 1.41915319 |
| B19 | 1.09429854 |
| B20 | 1.50808293 |
| B21 | 1.08697564 |
| B22 | 1.08736322 |
| B23 | 1.08750912 |
| B24 | 1.40191067 |
| B25 | 1.41617150 |
| B26 | 0.97244872 |
| A1 | 111.59152347 |

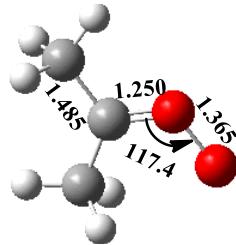
| | |
|-----|---------------|
| A2 | 85.22497751 |
| A3 | 113.76621574 |
| A4 | 66.95918870 |
| A5 | 128.77634772 |
| A6 | 114.44182151 |
| A7 | 112.00341507 |
| A8 | 108.38515873 |
| A9 | 109.20726483 |
| A10 | 98.96044606 |
| A11 | 110.67018242 |
| A12 | 103.37634136 |
| A13 | 108.98410509 |
| A14 | 109.99618754 |
| A15 | 110.22366049 |
| A16 | 108.42767768 |
| A17 | 115.73055313 |
| A18 | 108.15772300 |
| A19 | 107.85253448 |
| A20 | 110.48660912 |
| A21 | 109.69575004 |
| A22 | 109.04210883 |
| A23 | 112.43513230 |
| A24 | 111.08035088 |
| A25 | 103.13871838 |
| D1 | -135.24045782 |
| D2 | 21.31696023 |
| D3 | -104.90770045 |
| D4 | -143.68693540 |
| D5 | -61.48950710 |
| D6 | 61.57490877 |
| D7 | -177.01158260 |
| D8 | -57.86019380 |
| D9 | 35.53293368 |
| D10 | 69.65833247 |
| D11 | 177.13167157 |
| D12 | -167.66866202 |
| D13 | -47.37266197 |
| D14 | 72.75345507 |
| D15 | -126.05987199 |
| D16 | -147.58634571 |
| D17 | 39.65488219 |
| D18 | 160.49918005 |
| D19 | 53.77394492 |
| D20 | 173.57584731 |

D21 -66.12868612
D22 -72.39186670
D23 -86.08939000
D24 86.12215251

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-------------------------------|---------|---------|---------|-----------|-----------|-----------|---------|---------|--------|--------|
| 33.43 | 52.70 | 72.95 | 92.59 | 131.80 | 173.69 | 211.02 | 218.51 | 228.24 | 244.20 | 264.34 |
| 294.49 | 305.04 | 322.59 | 336.56 | 355.57 | 395.98 | 458.12 | 484.58 | 511.82 | 554.57 | |
| 600.67 | 639.88 | 667.66 | 697.40 | 731.32 | 845.88 | 863.05 | 887.74 | 926.86 | 939.92 | |
| 969.32 | 1000.09 | 1021.09 | 1026.52 | 1109.83 | 1128.37 | 1142.55 | 1151.31 | 1163.36 | | |
| 1173.68 | 1178.29 | 1192.92 | 1223.93 | 1354.97 | 1370.34 | 1386.25 | 1391.50 | 1404.48 | | |
| 1424.33 | 1429.04 | 1434.45 | 1448.60 | 1464.61 | 1483.43 | 1487.59 | 1489.01 | 1496.14 | | |
| 1499.48 | 1506.33 | 1510.84 | 3077.10 | 3077.27 | 3079.04 | 3083.18 | 3097.99 | 3117.81 | | |
| 3155.90 | 3159.72 | 3160.47 | 3165.92 | 3166.25 | 3181.06 | 3682.68 | 3708.78 | | | |
| Rotational constants (B/GHZ): | | | | 1.0039743 | 0.6955716 | 0.5293500 | | | | |

Figure S8. Optimized geometries, z-matrices and vibrational frequencies of all stationary points in the reaction of $(\text{CH}_3)_2\text{COO}$ with $\text{HO-C(CH}_3)_2\text{OO-H}$ at the M06-2X/6-311+G(2df,2p) level of theory



C

| | | | | | | | |
|---|---|-----|---|----|---|----|---|
| O | 1 | B1 | | | | | |
| O | 2 | B2 | 1 | A1 | | | |
| C | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| C | 1 | B4 | 2 | A3 | 3 | D2 | 0 |
| H | 4 | B5 | 1 | A4 | 2 | D3 | 0 |
| H | 4 | B6 | 1 | A5 | 2 | D4 | 0 |
| H | 4 | B7 | 1 | A6 | 2 | D5 | 0 |
| H | 5 | B8 | 1 | A7 | 2 | D6 | 0 |
| H | 5 | B9 | 1 | A8 | 2 | D7 | 0 |
| H | 5 | B10 | 1 | A9 | 2 | D8 | 0 |

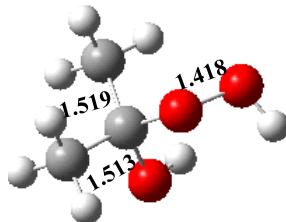
Variables:

| | |
|-----|--------------|
| B1 | 1.24973026 |
| B2 | 1.36521073 |
| B3 | 1.47294272 |
| B4 | 1.48491383 |
| B5 | 1.08561662 |
| B6 | 1.09251273 |
| B7 | 1.09251273 |
| B8 | 1.09132373 |
| B9 | 1.09132373 |
| B10 | 1.08604848 |
| A1 | 117.44317761 |
| A2 | 119.44468526 |
| A3 | 116.56507938 |
| A4 | 111.53606452 |
| A5 | 108.40498430 |
| A6 | 108.40498430 |
| A7 | 109.64754076 |
| A8 | 109.64754076 |
| A9 | 110.67329046 |
| D1 | 0.00000000 |
| D2 | 180.00000000 |
| D3 | 180.00000000 |
| D4 | -56.61851850 |

| | |
|----|---------------|
| D5 | 56.61851850 |
| D6 | 121.30347974 |
| D7 | -121.30347974 |
| D8 | 0.00000000 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|-------------------------------|---------|---------|---------|---------|-----------|-----------|-----------|---------|--------|
| 176.63 | 240.57 | 299.75 | 332.56 | 366.97 | 499.88 | 613.93 | 830.47 | 932.62 | 961.15 |
| 990.72 | 1089.85 | 1104.30 | 1320.14 | 1404.43 | 1413.61 | 1447.36 | 1470.97 | 1474.71 | |
| 1490.08 | 1654.29 | 3053.89 | 3060.79 | 3112.97 | 3114.84 | 3169.31 | 3176.48 | | |
| Rotational constants (B/GHZ): | | | | | 8.9366443 | 4.3782394 | 3.0471758 | | |



Pa₃(HO-C(CH₃)₂OO-H)

| | | | | | | |
|---|----|-----|---|-----|---|-------|
| C | | | | | | |
| O | 1 | B1 | | | | |
| O | 2 | B2 | 1 | A1 | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 0 |
| H | 3 | B4 | 2 | A3 | 1 | D2 0 |
| H | 4 | B5 | 1 | A4 | 2 | D3 0 |
| C | 1 | B6 | 4 | A5 | 2 | D4 0 |
| H | 7 | B7 | 1 | A6 | 4 | D5 0 |
| H | 7 | B8 | 1 | A7 | 4 | D6 0 |
| H | 7 | B9 | 1 | A8 | 4 | D7 0 |
| C | 1 | B10 | 4 | A9 | 2 | D8 0 |
| H | 11 | B11 | 1 | A10 | 4 | D9 0 |
| H | 11 | B12 | 1 | A11 | 4 | D10 0 |
| H | 11 | B13 | 1 | A12 | 4 | D11 0 |

Variables:

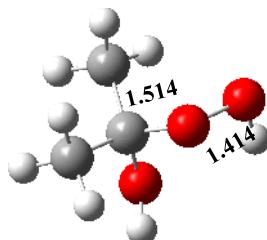
| | |
|-----|------------|
| B1 | 1.42803919 |
| B2 | 1.41800530 |
| B3 | 1.39759751 |
| B4 | 0.96418076 |
| B5 | 0.96115215 |
| B6 | 1.51302090 |
| B7 | 1.08771177 |
| B8 | 1.08772335 |
| B9 | 1.08778728 |
| B10 | 1.51907972 |
| B11 | 1.08858997 |
| B12 | 1.08832637 |
| B13 | 1.08934092 |

| | |
|-----|---------------|
| A1 | 108.25990832 |
| A2 | 110.17159819 |
| A3 | 101.12148048 |
| A4 | 108.38858916 |
| A5 | 107.86333905 |
| A6 | 110.19455398 |
| A7 | 109.21211180 |
| A8 | 109.40787479 |
| A9 | 111.49446172 |
| A10 | 109.55770894 |
| A11 | 110.04067083 |
| A12 | 110.35289730 |
| D1 | 60.09421131 |
| D2 | -107.24435152 |
| D3 | -78.39442433 |
| D4 | -112.40333608 |
| D5 | 174.17307356 |
| D6 | -65.61309310 |
| D7 | 53.78620215 |
| D8 | 122.64462128 |
| D9 | 59.21801019 |
| D10 | 179.39905446 |
| D11 | -61.01471649 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| 157.10 | 215.45 | 254.64 | 266.88 | 289.13 | 351.63 | 395.94 | 438.87 | 469.01 | 533.39 |
| 610.62 | 811.41 | 900.45 | 942.08 | 1009.93 | 1018.99 | 1052.21 | 1156.25 | 1222.47 | 1275.33 |
| 1379.33 | 1414.04 | 1419.69 | 1440.88 | 1488.01 | 1488.58 | 1504.38 | 1512.80 | 3065.61 | |
| 3073.57 | 3143.79 | 3154.79 | 3158.62 | 3161.33 | 3840.02 | 3882.61 | | | |

Rotational constants (B/GHZ): 4.8013572 2.9558337 2.8668841



Pb₃(HO-C(CH₃)₂OO-H)

| | | | | | | | |
|---|---|----|---|----|---|----|---|
| C | | | | | | | |
| O | 1 | B1 | | | | | |
| O | 2 | B2 | 1 | A1 | | | |
| O | 1 | B3 | 2 | A2 | 3 | D1 | 0 |
| H | 3 | B4 | 2 | A3 | 1 | D2 | 0 |
| H | 4 | B5 | 1 | A4 | 2 | D3 | 0 |
| C | 1 | B6 | 4 | A5 | 2 | D4 | 0 |
| H | 7 | B7 | 1 | A6 | 4 | D5 | 0 |

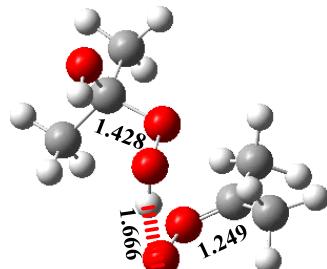
| | | | | | | | |
|---|----|-----|---|-----|---|-----|---|
| H | 7 | B8 | 1 | A7 | 4 | D6 | 0 |
| H | 7 | B9 | 1 | A8 | 4 | D7 | 0 |
| C | 1 | B10 | 4 | A9 | 2 | D8 | 0 |
| H | 11 | B11 | 1 | A10 | 4 | D9 | 0 |
| H | 11 | B12 | 1 | A11 | 4 | D10 | 0 |
| H | 11 | B13 | 1 | A12 | 4 | D11 | 0 |

Variables:

| | |
|-----|---------------|
| B1 | 1.42036903 |
| B2 | 1.41353351 |
| B3 | 1.40771550 |
| B4 | 0.96704094 |
| B5 | 0.96174753 |
| B6 | 1.51724115 |
| B7 | 1.08774105 |
| B8 | 1.08800934 |
| B9 | 1.09065644 |
| B10 | 1.51409413 |
| B11 | 1.08817133 |
| B12 | 1.08811607 |
| B13 | 1.08592678 |
| A1 | 109.52808369 |
| A2 | 109.02539061 |
| A3 | 102.33339650 |
| A4 | 108.69209589 |
| A5 | 111.87981629 |
| A6 | 110.32651224 |
| A7 | 109.29683717 |
| A8 | 110.15669170 |
| A9 | 107.22797735 |
| A10 | 109.38232930 |
| A11 | 109.51457284 |
| A12 | 110.32563548 |
| D1 | 63.69901589 |
| D2 | -70.42057341 |
| D3 | 71.96629503 |
| D4 | -113.82811305 |
| D5 | -179.46084328 |
| D6 | -59.25388260 |
| D7 | 60.90401865 |
| D8 | 121.63715387 |
| D9 | 67.14427196 |
| D10 | -172.83920079 |
| D11 | -52.78580086 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|-------------------------------|---------|---------|---------|---------|-----------|-----------|-----------|---------|---------|
| 140.02 | 192.88 | 235.58 | 278.54 | 333.98 | 360.45 | 406.19 | 425.30 | 447.14 | 535.06 |
| 617.12 | 812.26 | 901.87 | 945.22 | 1000.84 | 1020.04 | 1060.14 | 1161.65 | 1223.07 | 1270.83 |
| 1377.42 | 1418.11 | 1433.91 | 1443.52 | 1482.28 | 1487.67 | 1499.81 | 1510.99 | 3059.83 | |
| 3074.83 | 3138.10 | 3152.22 | 3157.57 | 3167.12 | 3791.52 | 3873.47 | | | |
| Rotational constants (B/GHZ): | | | | | 4.7743794 | 2.9637751 | 2.8780998 | | |



IM7a

C

| | | | | | | |
|---|----|-----|---|-----|---|-------|
| O | 1 | B1 | | | | |
| O | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| C | 3 | B4 | 2 | A3 | 1 | D2 0 |
| C | 5 | B5 | 3 | A4 | 2 | D3 0 |
| H | 6 | B6 | 5 | A5 | 3 | D4 0 |
| H | 6 | B7 | 5 | A6 | 3 | D5 0 |
| H | 6 | B8 | 5 | A7 | 3 | D6 0 |
| C | 5 | B9 | 3 | A8 | 2 | D7 0 |
| H | 10 | B10 | 5 | A9 | 3 | D8 0 |
| H | 10 | B11 | 5 | A10 | 3 | D9 0 |
| H | 10 | B12 | 5 | A11 | 3 | D10 0 |
| O | 5 | B13 | 3 | A12 | 2 | D11 0 |
| O | 5 | B14 | 3 | A13 | 2 | D12 0 |
| C | 1 | B15 | 3 | A14 | 2 | D13 0 |
| H | 16 | B16 | 1 | A15 | 3 | D14 0 |
| H | 16 | B17 | 1 | A16 | 3 | D15 0 |
| H | 16 | B18 | 1 | A17 | 3 | D16 0 |
| C | 1 | B19 | 3 | A18 | 2 | D17 0 |
| H | 20 | B20 | 1 | A19 | 3 | D18 0 |
| H | 20 | B21 | 1 | A20 | 3 | D19 0 |
| H | 20 | B22 | 1 | A21 | 3 | D20 0 |
| O | 1 | B23 | 3 | A22 | 2 | D21 0 |
| H | 24 | B24 | 1 | A23 | 3 | D22 0 |

Variables:

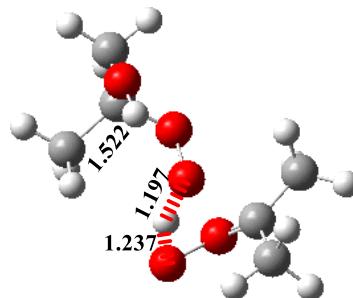
| | |
|----|------------|
| B1 | 2.30994866 |
| B2 | 1.42211604 |
| B3 | 0.99843776 |
| B4 | 2.79618710 |
| B5 | 1.48168363 |

| | |
|-----|---------------|
| B6 | 1.09006107 |
| B7 | 1.08587289 |
| B8 | 1.09265242 |
| B9 | 1.47232181 |
| B10 | 1.09380200 |
| B11 | 1.09000982 |
| B12 | 1.08579104 |
| B13 | 2.25260185 |
| B14 | 1.24854891 |
| B15 | 1.51350945 |
| B16 | 1.08788603 |
| B17 | 1.08822470 |
| B18 | 1.08903814 |
| B19 | 1.52108723 |
| B20 | 1.08823829 |
| B21 | 1.08855579 |
| B22 | 1.08915728 |
| B23 | 1.39546628 |
| B24 | 0.96344045 |
| A1 | 35.93192591 |
| A2 | 105.41595123 |
| A3 | 95.30499225 |
| A4 | 101.49527504 |
| A5 | 110.05142669 |
| A6 | 111.13924999 |
| A7 | 107.45889653 |
| A8 | 88.88193845 |
| A9 | 108.13676696 |
| A10 | 108.91371112 |
| A11 | 110.64801682 |
| A12 | 73.67567531 |
| A13 | 78.71323115 |
| A14 | 104.21642285 |
| A15 | 109.09102198 |
| A16 | 109.47103905 |
| A17 | 110.41026475 |
| A18 | 110.73296624 |
| A19 | 110.61062393 |
| A20 | 109.06225400 |
| A21 | 110.73356189 |
| A22 | 109.61652926 |
| A23 | 106.96024250 |
| D1 | -87.55734855 |
| D2 | -134.98283473 |

| | |
|-----|---------------|
| D3 | -176.02956737 |
| D4 | 151.37311366 |
| D5 | -85.78033606 |
| D6 | 34.42173545 |
| D7 | -52.88037573 |
| D8 | 4.09999543 |
| D9 | 119.46283527 |
| D10 | -116.61175937 |
| D11 | 35.76249037 |
| D12 | 69.61050685 |
| D13 | 175.48984732 |
| D14 | -175.99046789 |
| D15 | -56.81423625 |
| D16 | 64.31193115 |
| D17 | -62.89038753 |
| D18 | 64.96293393 |
| D19 | -175.61793030 |
| D20 | -55.04328821 |
| D21 | 60.43622906 |
| D22 | -56.21232413 |

Harmonic Vibrational Frequencies (cm^{-1}):

Rotational constants (B/GHZ): 1.6042967 0.7175580 0.6477149



TS7a

| | | | | | | | | |
|---|---|----|---|----|---|----|---|--|
| C | | | | | | | | |
| O | 1 | B1 | | | | | | |
| O | 2 | B2 | 1 | A1 | | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 | |
| C | 2 | B4 | 1 | A3 | 3 | D2 | 0 | |

| | | | | | | | |
|---|----|-----|---|-----|---|-----|---|
| C | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 6 | B6 | 5 | A5 | 2 | D4 | 0 |
| H | 6 | B7 | 5 | A6 | 2 | D5 | 0 |
| H | 6 | B8 | 5 | A7 | 2 | D6 | 0 |
| C | 5 | B9 | 2 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 5 | A9 | 2 | D8 | 0 |
| H | 10 | B11 | 5 | A10 | 2 | D9 | 0 |
| H | 10 | B12 | 5 | A11 | 2 | D10 | 0 |
| O | 5 | B13 | 2 | A12 | 1 | D11 | 0 |
| O | 5 | B14 | 2 | A13 | 1 | D12 | 0 |
| C | 1 | B15 | 3 | A14 | 2 | D13 | 0 |
| H | 16 | B16 | 1 | A15 | 3 | D14 | 0 |
| H | 16 | B17 | 1 | A16 | 3 | D15 | 0 |
| H | 16 | B18 | 1 | A17 | 3 | D16 | 0 |
| C | 1 | B19 | 3 | A18 | 2 | D17 | 0 |
| H | 20 | B20 | 1 | A19 | 3 | D18 | 0 |
| H | 20 | B21 | 1 | A20 | 3 | D19 | 0 |
| H | 20 | B22 | 1 | A21 | 3 | D20 | 0 |
| O | 1 | B23 | 3 | A22 | 2 | D21 | 0 |
| H | 24 | B24 | 1 | A23 | 3 | D22 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 2.30587951 |
| B2 | 1.42029801 |
| B3 | 1.19661251 |
| B4 | 2.12665176 |
| B5 | 1.48139931 |
| B6 | 1.08782503 |
| B7 | 1.08628347 |
| B8 | 1.09280403 |
| B9 | 1.48602114 |
| B10 | 1.08658587 |
| B11 | 1.08265787 |
| B12 | 1.09435380 |
| B13 | 2.21718167 |
| B14 | 1.27984906 |
| B15 | 1.51301310 |
| B16 | 1.08794896 |
| B17 | 1.08794379 |
| B18 | 1.08803628 |
| B19 | 1.52213984 |
| B20 | 1.08926000 |
| B21 | 1.08847705 |
| B22 | 1.08898851 |
| B23 | 1.39930155 |

| | |
|-----|---------------|
| B24 | 0.96315731 |
| A1 | 35.83803365 |
| A2 | 102.50876962 |
| A3 | 133.68778180 |
| A4 | 107.71111012 |
| A5 | 111.06572004 |
| A6 | 110.62536248 |
| A7 | 105.94723297 |
| A8 | 89.71485017 |
| A9 | 109.33822751 |
| A10 | 112.18720316 |
| A11 | 106.22855010 |
| A12 | 66.10533091 |
| A13 | 89.20506929 |
| A14 | 104.41883384 |
| A15 | 109.04959610 |
| A16 | 109.40569395 |
| A17 | 110.32367851 |
| A18 | 110.59789523 |
| A19 | 110.64868051 |
| A20 | 109.20452138 |
| A21 | 110.36947028 |
| A22 | 109.79157084 |
| A23 | 106.78025961 |
| D1 | -95.26408199 |
| D2 | -18.41756165 |
| D3 | 56.85862266 |
| D4 | 129.39295618 |
| D5 | -106.14255269 |
| D6 | 11.10801703 |
| D7 | 178.42483015 |
| D8 | -63.55549936 |
| D9 | 59.97693823 |
| D10 | 179.64737076 |
| D11 | -87.61971874 |
| D12 | -58.22783812 |
| D13 | 176.93526894 |
| D14 | -176.17895241 |
| D15 | -57.07171307 |
| D16 | 63.67123527 |
| D17 | -61.53339509 |
| D18 | 67.88568348 |
| D19 | -173.04361901 |
| D20 | -52.45989794 |

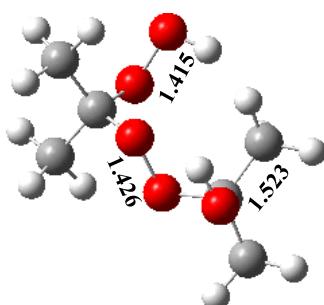
D21 61.62177637

D22 -55.63844055

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|------------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 1021.22 <i>i</i> | 34.14 | 42.48 | 60.79 | 87.49 | 173.09 | 183.06 | 202.05 | 206.32 | 211.63 | 267.60 |
| 304.61 | 332.58 | 356.59 | 373.77 | 383.44 | 402.53 | 438.17 | 453.30 | 522.45 | 553.22 | |
| 580.55 | 625.64 | 730.11 | 815.82 | 821.98 | 911.58 | 943.08 | 954.71 | 959.72 | 986.92 | |
| 1006.92 | 1014.11 | 1066.57 | 1084.06 | 1105.74 | 1147.82 | 1242.80 | 1267.39 | 1316.37 | | |
| 1378.22 | 1401.27 | 1412.22 | 1423.78 | 1433.06 | 1438.91 | 1457.13 | 1477.36 | 1485.91 | | |
| 1487.14 | 1493.24 | 1503.17 | 1510.24 | 1543.59 | 1588.20 | 1830.56 | 3052.57 | 3057.51 | | |
| 3062.11 | 3075.41 | 3132.35 | 3142.72 | 3146.46 | 3146.64 | 3160.17 | 3163.32 | 3172.81 | | |
| 3217.82 | 3863.02 | | | | | | | | | |

Rotational constants (B/GHZ): 1.8611556 0.6571852 0.6168925



P7a

C

| | | | | | | |
|---|----|-----|---|-----|---|-------|
| O | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| C | 2 | B4 | 1 | A3 | 3 | D2 0 |
| C | 5 | B5 | 2 | A4 | 1 | D3 0 |
| H | 6 | B6 | 5 | A5 | 2 | D4 0 |
| H | 6 | B7 | 5 | A6 | 2 | D5 0 |
| H | 6 | B8 | 5 | A7 | 2 | D6 0 |
| C | 5 | B9 | 2 | A8 | 1 | D7 0 |
| H | 10 | B10 | 5 | A9 | 2 | D8 0 |
| H | 10 | B11 | 5 | A10 | 2 | D9 0 |
| H | 10 | B12 | 5 | A11 | 2 | D10 0 |
| O | 5 | B13 | 2 | A12 | 1 | D11 0 |
| O | 5 | B14 | 2 | A13 | 1 | D12 0 |
| C | 1 | B15 | 3 | A14 | 2 | D13 0 |
| H | 16 | B16 | 1 | A15 | 3 | D14 0 |
| H | 16 | B17 | 1 | A16 | 3 | D15 0 |
| H | 16 | B18 | 1 | A17 | 3 | D16 0 |
| C | 1 | B19 | 3 | A18 | 2 | D17 0 |
| H | 20 | B20 | 1 | A19 | 3 | D18 0 |
| H | 20 | B21 | 1 | A20 | 3 | D19 0 |
| H | 20 | B22 | 1 | A21 | 3 | D20 0 |

| | | | | | | | |
|---|----|-----|---|-----|---|-----|---|
| O | 1 | B23 | 3 | A22 | 2 | D21 | 0 |
| H | 24 | B24 | 1 | A23 | 3 | D22 | 0 |

Variables:

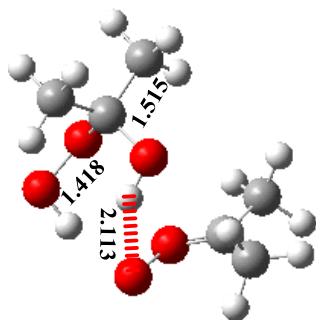
| | |
|-----|--------------|
| B1 | 2.29384480 |
| B2 | 1.41991671 |
| B3 | 2.77181151 |
| B4 | 1.41563488 |
| B5 | 1.51728812 |
| B6 | 1.08764905 |
| B7 | 1.08617650 |
| B8 | 1.08789207 |
| B9 | 1.51671525 |
| B10 | 1.08765668 |
| B11 | 1.08606173 |
| B12 | 1.08799280 |
| B13 | 2.31572911 |
| B14 | 1.41117263 |
| B15 | 1.51388283 |
| B16 | 1.08776132 |
| B17 | 1.08760462 |
| B18 | 1.08792566 |
| B19 | 1.52265333 |
| B20 | 1.09004253 |
| B21 | 1.08803858 |
| B22 | 1.09125397 |
| B23 | 1.39767133 |
| B24 | 0.96216003 |
| A1 | 36.38133949 |
| A2 | 85.52290916 |
| A3 | 135.40767946 |
| A4 | 112.37419632 |
| A5 | 109.19952253 |
| A6 | 110.58992543 |
| A7 | 109.03597300 |
| A8 | 104.14563950 |
| A9 | 109.33528602 |
| A10 | 110.80978867 |
| A11 | 108.75616587 |
| A12 | 95.80308420 |
| A13 | 110.62684998 |
| A14 | 103.81168838 |
| A15 | 108.90985249 |
| A16 | 109.29889992 |
| A17 | 110.41727385 |

| | |
|-----|---------------|
| A18 | 111.04645212 |
| A19 | 110.19355451 |
| A20 | 109.35028182 |
| A21 | 109.83046578 |
| A22 | 110.45008760 |
| A23 | 108.29381451 |
| D1 | -111.10611994 |
| D2 | -51.78079758 |
| D3 | 75.42219827 |
| D4 | 168.02421496 |
| D5 | -71.68699072 |
| D6 | 48.26708841 |
| D7 | -161.86460697 |
| D8 | -70.99514665 |
| D9 | 49.79038951 |
| D10 | 169.45649836 |
| D11 | -73.13700182 |
| D12 | -40.39593049 |
| D13 | 177.90328299 |
| D14 | -176.30675413 |
| D15 | -57.25506156 |
| D16 | 63.47108447 |
| D17 | -60.86698402 |
| D18 | 71.34161754 |
| D19 | -170.08907487 |
| D20 | -50.46411455 |
| D21 | 62.87615714 |
| D22 | -59.93356923 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 44.60 | 81.92 | 119.11 | 159.04 | 198.21 | 208.50 | 232.54 | 236.86 | 244.12 | 266.78 | 284.27 |
| 328.52 | 359.33 | 370.67 | 375.64 | 390.26 | 410.17 | 452.89 | 463.93 | 537.98 | 590.50 | |
| 607.60 | 619.05 | 812.34 | 846.62 | 907.81 | 927.49 | 946.56 | 960.44 | 974.63 | 1010.71 | |
| 1026.22 | 1030.27 | 1054.70 | 1066.04 | 1155.43 | 1207.34 | 1246.33 | 1255.52 | 1269.86 | | |
| 1313.94 | 1377.50 | 1405.31 | 1414.35 | 1423.90 | 1429.68 | 1439.70 | 1481.87 | 1487.21 | | |
| 1487.95 | 1492.98 | 1497.10 | 1504.98 | 1510.39 | 1529.69 | 3049.53 | 3072.82 | 3083.14 | | |
| 3085.96 | 3128.87 | 3143.74 | 3159.15 | 3160.93 | 3162.20 | 3167.27 | 3176.21 | 3181.38 | | |
| 3842.24 | 3877.61 | | | | | | | | | |

Rotational constants (B/GHZ): 1.7988145 0.7309428 0.6661869



IM7b

C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| C | 1 | B1 | | | | |
| H | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| H | 2 | B4 | 1 | A3 | 4 | D2 0 |
| C | 1 | B5 | 2 | A4 | 3 | D3 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 0 |
| H | 6 | B7 | 1 | A6 | 2 | D5 0 |
| H | 6 | B8 | 1 | A7 | 2 | D6 0 |
| O | 1 | B9 | 6 | A8 | 2 | D7 0 |
| H | 10 | B10 | 1 | A9 | 6 | D8 0 |
| O | 1 | B11 | 10 | A10 | 6 | D9 0 |
| C | 10 | B12 | 1 | A11 | 6 | D10 0 |
| C | 13 | B13 | 10 | A12 | 1 | D11 0 |
| H | 14 | B14 | 13 | A13 | 10 | D12 0 |
| H | 14 | B15 | 13 | A14 | 10 | D13 0 |
| H | 14 | B16 | 13 | A15 | 10 | D14 0 |
| C | 13 | B17 | 10 | A16 | 1 | D15 0 |
| H | 18 | B18 | 13 | A17 | 10 | D16 0 |
| H | 18 | B19 | 13 | A18 | 10 | D17 0 |
| H | 18 | B20 | 13 | A19 | 10 | D18 0 |
| O | 13 | B21 | 10 | A20 | 1 | D19 0 |
| O | 13 | B22 | 10 | A21 | 1 | D20 0 |
| O | 1 | B23 | 10 | A22 | 6 | D21 0 |
| H | 12 | B24 | 1 | A23 | 10 | D22 0 |

Variables:

| | |
|----|------------|
| B1 | 1.51912522 |
| B2 | 1.08666541 |
| B3 | 1.08870560 |
| B4 | 1.08886031 |
| B5 | 1.51467507 |
| B6 | 1.08909095 |
| B7 | 1.08754406 |
| B8 | 1.08813772 |
| B9 | 1.41146083 |

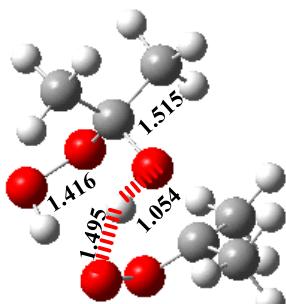
| | |
|-----|---------------|
| B10 | 0.96929819 |
| B11 | 2.31632335 |
| B12 | 2.96479402 |
| B13 | 1.48190801 |
| B14 | 1.09184188 |
| B15 | 1.09080734 |
| B16 | 1.08574494 |
| B17 | 1.47302927 |
| B18 | 1.09259673 |
| B19 | 1.08958266 |
| B20 | 1.08596796 |
| B21 | 2.24756788 |
| B22 | 1.24695040 |
| B23 | 1.41527190 |
| B24 | 0.98294912 |
| A1 | 110.46521688 |
| A2 | 109.13296872 |
| A3 | 110.03360884 |
| A4 | 112.70390304 |
| A5 | 109.43502513 |
| A6 | 110.37291320 |
| A7 | 109.23982934 |
| A8 | 107.11708914 |
| A9 | 107.95300410 |
| A10 | 96.35845866 |
| A11 | 117.42934070 |
| A12 | 112.80938637 |
| A13 | 108.04598173 |
| A14 | 109.75687501 |
| A15 | 110.95799654 |
| A16 | 82.71749073 |
| A17 | 107.76469556 |
| A18 | 109.07558139 |
| A19 | 110.68169179 |
| A20 | 64.97485761 |
| A21 | 74.90335490 |
| A22 | 110.13469824 |
| A23 | 101.79388520 |
| D1 | 119.88699709 |
| D2 | 120.11734103 |
| D3 | -176.44539623 |
| D4 | -175.09092970 |
| D5 | -55.02475699 |
| D6 | 65.42921691 |

| | |
|-----|---------------|
| D7 | -122.13652958 |
| D8 | -161.86038955 |
| D9 | 146.06370822 |
| D10 | -78.92314007 |
| D11 | 56.45916003 |
| D12 | 38.78233848 |
| D13 | 155.55831450 |
| D14 | -81.89096438 |
| D15 | 179.26521920 |
| D16 | -4.83226908 |
| D17 | 110.93706419 |
| D18 | -125.05719537 |
| D19 | -89.43149150 |
| D20 | -55.53915016 |
| D21 | 112.64700173 |
| D22 | -21.32732074 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 28.00 | 54.96 | 74.22 | 98.79 | 128.92 | 131.86 | 156.07 | 176.53 | 194.91 | 228.09 | 268.45 |
| 294.48 | 325.16 | 356.74 | 361.33 | 379.17 | 400.56 | 444.30 | 489.45 | 525.04 | 551.30 | |
| 606.64 | 616.86 | 738.89 | 810.41 | 830.64 | 907.80 | 910.64 | 943.81 | 965.27 | 993.66 | |
| 1000.92 | 1015.21 | 1062.93 | 1096.05 | 1105.62 | 1181.33 | 1239.99 | 1267.99 | 1320.10 | | |
| 1383.66 | 1386.15 | 1411.94 | 1413.79 | 1434.89 | 1458.44 | 1468.25 | 1477.20 | 1482.13 | | |
| 1484.45 | 1492.04 | 1498.52 | 1510.82 | 1575.54 | 1679.24 | 3052.60 | 3056.50 | 3061.10 | | |
| 3066.30 | 3117.84 | 3120.74 | 3139.80 | 3141.69 | 3151.01 | 3161.59 | 3168.61 | 3182.01 | | |
| 3455.59 | 3739.52 | | | | | | | | | |

Rotational constants (B/GHZ): 1.5806841 0.7163457 0.6334593



TS7b

| | | | | | | | |
|---|---|--|----|---|----|---|------|
| C | | | | | | | |
| C | 1 | | B1 | | | | |
| H | 2 | | B2 | 1 | A1 | | |
| H | 2 | | B3 | 1 | A2 | 3 | D1 0 |
| H | 2 | | B4 | 1 | A3 | 4 | D2 0 |
| C | 1 | | B5 | 2 | A4 | 3 | D3 0 |
| H | 6 | | B6 | 1 | A5 | 2 | D4 0 |
| H | 6 | | B7 | 1 | A6 | 2 | D5 0 |
| H | 6 | | B8 | 1 | A7 | 2 | D6 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 1 | B9 | 6 | A8 | 2 | D7 | 0 |
| H | 10 | B10 | 1 | A9 | 6 | D8 | 0 |
| O | 1 | B11 | 10 | A10 | 2 | D9 | 0 |
| C | 10 | B12 | 1 | A11 | 6 | D10 | 0 |
| C | 13 | B13 | 10 | A12 | 1 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 10 | D12 | 0 |
| H | 14 | B15 | 13 | A14 | 10 | D13 | 0 |
| H | 14 | B16 | 13 | A15 | 10 | D14 | 0 |
| C | 13 | B17 | 10 | A16 | 1 | D15 | 0 |
| H | 18 | B18 | 13 | A17 | 10 | D16 | 0 |
| H | 18 | B19 | 13 | A18 | 10 | D17 | 0 |
| H | 18 | B20 | 13 | A19 | 10 | D18 | 0 |
| O | 13 | B21 | 10 | A20 | 1 | D19 | 0 |
| O | 13 | B22 | 10 | A21 | 1 | D20 | 0 |
| O | 1 | B23 | 10 | A22 | 13 | D21 | 0 |
| H | 12 | B24 | 1 | A23 | 24 | D22 | 0 |

Variables:

| | |
|-----|--------------|
| B1 | 1.51793124 |
| B2 | 1.08683102 |
| B3 | 1.08826680 |
| B4 | 1.08839803 |
| B5 | 1.51542228 |
| B6 | 1.08740288 |
| B7 | 1.08756003 |
| B8 | 1.08804320 |
| B9 | 1.43103489 |
| B10 | 1.05380252 |
| B11 | 2.33143227 |
| B12 | 1.92870523 |
| B13 | 1.49058817 |
| B14 | 1.08707406 |
| B15 | 1.09194538 |
| B16 | 1.08631594 |
| B17 | 1.49488298 |
| B18 | 1.08563631 |
| B19 | 1.08380553 |
| B20 | 1.09312044 |
| B21 | 2.23457018 |
| B22 | 1.29274492 |
| B23 | 1.40750391 |
| B24 | 0.97904523 |
| A1 | 110.95657346 |
| A2 | 109.01826097 |
| A3 | 109.39474188 |

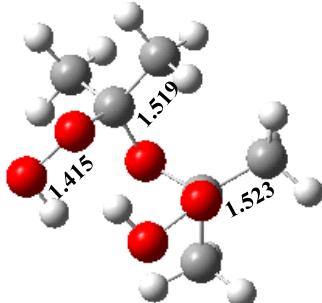
| | |
|-----|---------------|
| A4 | 112.43505581 |
| A5 | 110.69396512 |
| A6 | 109.59455493 |
| A7 | 109.25702145 |
| A8 | 108.40061155 |
| A9 | 108.69906868 |
| A10 | 100.85572238 |
| A11 | 122.96840554 |
| A12 | 109.67233791 |
| A13 | 110.13278609 |
| A14 | 107.50459589 |
| A15 | 110.37651183 |
| A16 | 93.01875964 |
| A17 | 110.37445754 |
| A18 | 111.33002613 |
| A19 | 106.15690301 |
| A20 | 71.24528107 |
| A21 | 95.84259798 |
| A22 | 110.21663850 |
| A23 | 94.28445951 |
| D1 | 120.39119833 |
| D2 | 119.98823918 |
| D3 | -172.50452175 |
| D4 | -171.92428843 |
| D5 | -52.25939734 |
| D6 | 67.60809322 |
| D7 | -119.32008888 |
| D8 | -173.75650334 |
| D9 | -89.19244136 |
| D10 | -84.16805698 |
| D11 | 46.03441556 |
| D12 | 56.57286927 |
| D13 | 174.27846511 |
| D14 | -66.54691392 |
| D15 | 167.75586601 |
| D16 | -61.89314937 |
| D17 | 61.70496038 |
| D18 | -179.76365708 |
| D19 | -99.13876586 |
| D20 | -71.07370870 |
| D21 | 30.07421026 |
| D22 | 108.47346682 |

Harmonic Vibrational Frequencies (cm⁻¹):

389.61*i* 62.31 120.67 145.61 162.48 195.53 208.44 225.07 235.09 245.37

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 283.81 | 313.88 | 326.24 | 354.59 | 376.05 | 386.10 | 407.72 | 476.36 | 502.10 | 572.97 |
| 577.71 | 622.55 | 632.69 | 784.62 | 829.32 | 900.93 | 927.61 | 939.42 | 951.07 | 982.87 |
| 998.80 | 1017.96 | 1069.03 | 1082.53 | 1094.94 | 1166.74 | 1230.07 | 1267.37 | 1278.89 | |
| 1316.91 | 1405.87 | 1411.25 | 1421.06 | 1422.99 | 1440.20 | 1456.90 | 1474.30 | 1481.15 | |
| 1486.03 | 1492.48 | 1500.78 | 1510.88 | 1517.24 | 1554.37 | 1587.30 | 2313.40 | 3057.11 | |
| 3066.29 | 3067.86 | 3071.07 | 3138.76 | 3147.69 | 3150.02 | 3153.52 | 3160.06 | 3162.67 | |
| 3182.94 | 3203.52 | 3568.40 | | | | | | | |

Rotational constants (B/GHZ): 1.5136497 0.9238782 0.7943765



P7b

C

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| C | 1 | B5 | 2 | A4 | 3 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| H | 6 | B7 | 1 | A6 | 2 | D5 | 0 |
| H | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| O | 1 | B9 | 2 | A8 | 6 | D7 | 0 |
| H | 10 | B10 | 1 | A9 | 2 | D8 | 0 |
| O | 1 | B11 | 10 | A10 | 2 | D9 | 0 |
| C | 10 | B12 | 1 | A11 | 2 | D10 | 0 |
| C | 13 | B13 | 10 | A12 | 1 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 10 | D12 | 0 |
| H | 14 | B15 | 13 | A14 | 10 | D13 | 0 |
| H | 14 | B16 | 13 | A15 | 10 | D14 | 0 |
| C | 13 | B17 | 10 | A16 | 1 | D15 | 0 |
| H | 18 | B18 | 13 | A17 | 10 | D16 | 0 |
| H | 18 | B19 | 13 | A18 | 10 | D17 | 0 |
| H | 18 | B20 | 13 | A19 | 10 | D18 | 0 |
| O | 13 | B21 | 10 | A20 | 1 | D19 | 0 |
| O | 22 | B22 | 13 | A21 | 10 | D20 | 0 |
| O | 1 | B23 | 10 | A22 | 13 | D21 | 0 |
| H | 12 | B24 | 1 | A23 | 24 | D22 | 0 |

Variables:

B1 1.51796960

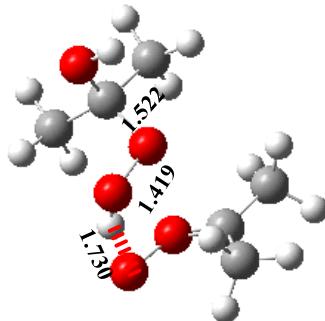
| | |
|-----|--------------|
| B2 | 1.08631684 |
| B3 | 1.08829144 |
| B4 | 1.08808809 |
| B5 | 1.52325025 |
| B6 | 1.08565516 |
| B7 | 1.08797718 |
| B8 | 1.08811447 |
| B9 | 1.42255353 |
| B10 | 2.29473798 |
| B11 | 2.32069363 |
| B12 | 1.40884321 |
| B13 | 1.51920615 |
| B14 | 1.08785477 |
| B15 | 1.08813714 |
| B16 | 1.08646695 |
| B17 | 1.51720452 |
| B18 | 1.08835907 |
| B19 | 1.08581886 |
| B20 | 1.08816468 |
| B21 | 2.32495472 |
| B22 | 1.41502654 |
| B23 | 1.40940663 |
| B24 | 0.96914405 |
| A1 | 110.50374449 |
| A2 | 109.28436959 |
| A3 | 109.46802991 |
| A4 | 111.11830414 |
| A5 | 111.89257328 |
| A6 | 109.40296879 |
| A7 | 108.72989545 |
| A8 | 104.83494213 |
| A9 | 106.24586544 |
| A10 | 95.67208426 |
| A11 | 124.32100140 |
| A12 | 116.73269760 |
| A13 | 109.55514170 |
| A14 | 108.33357807 |
| A15 | 111.39150013 |
| A16 | 105.45983152 |
| A17 | 109.19833860 |
| A18 | 110.35968385 |
| A19 | 109.54484776 |
| A20 | 89.02886257 |
| A21 | 35.38133353 |

| | |
|-----|---------------|
| A22 | 112.64923397 |
| A23 | 107.21663867 |
| D1 | 119.95094209 |
| D2 | 119.89265735 |
| D3 | -178.06251157 |
| D4 | -166.65239770 |
| D5 | -46.70314912 |
| D6 | 72.38135463 |
| D7 | 121.87549827 |
| D8 | 70.25016533 |
| D9 | -90.37857456 |
| D10 | 158.58911122 |
| D11 | 38.99692642 |
| D12 | 58.23453085 |
| D13 | 176.55327352 |
| D14 | -63.60747206 |
| D15 | 163.74389055 |
| D16 | -69.79780907 |
| D17 | 50.01722280 |
| D18 | 170.29621483 |
| D19 | -106.68644926 |
| D20 | 125.98673456 |
| D21 | 36.57631911 |
| D22 | 83.22823206 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 76.46 | 126.86 | 165.68 | 178.61 | 201.92 | 210.86 | 227.73 | 242.71 | 282.21 | 288.60 |
| 315.54 | 335.99 | 343.49 | 372.90 | 385.66 | 388.48 | 416.35 | 475.06 | 504.86 | 581.16 |
| 601.99 | 644.21 | 662.48 | 775.68 | 834.71 | 881.45 | 926.99 | 945.24 | 955.13 | 967.39 |
| 1019.15 | 1027.33 | 1050.62 | 1060.85 | 1072.79 | 1183.36 | 1225.82 | 1257.37 | 1262.65 | |
| 1270.56 | 1317.30 | 1407.04 | 1411.13 | 1418.23 | 1423.08 | 1457.86 | 1474.24 | 1480.94 | |
| 1481.96 | 1487.38 | 1490.70 | 1498.28 | 1501.81 | 1515.04 | 1525.70 | 3071.28 | 3074.41 | |
| 3077.03 | 3078.60 | 3146.09 | 3150.93 | 3153.64 | 3161.70 | 3162.75 | 3173.21 | 3174.57 | |
| 3178.02 | 3743.11 | 3757.11 | | | | | | | |

Rotational constants (B/GHZ): 1.4905567 0.9870946 0.8211376



IM7c

| | | | | | | | |
|---|----|-----|---|-----|---|-----|---|
| O | 1 | B1 | | A1 | | | |
| O | 2 | B2 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B3 | 1 | A3 | 1 | D2 | 0 |
| C | 3 | B4 | 2 | A4 | 2 | D3 | 0 |
| C | 5 | B5 | 3 | A5 | 3 | D4 | 0 |
| H | 6 | B6 | 5 | A6 | 3 | D5 | 0 |
| H | 6 | B7 | 5 | A7 | 3 | D6 | 0 |
| C | 5 | B8 | 3 | A8 | 2 | D7 | 0 |
| H | 10 | B9 | 3 | A9 | 3 | D8 | 0 |
| H | 10 | B10 | 5 | A10 | 3 | D9 | 0 |
| H | 10 | B11 | 5 | A11 | 3 | D10 | 0 |
| O | 5 | B12 | 5 | A12 | 2 | D11 | 0 |
| O | 5 | B13 | 3 | A13 | 2 | D12 | 0 |
| C | 1 | B14 | 3 | A14 | 2 | D13 | 0 |
| H | 16 | B15 | 3 | A15 | 3 | D14 | 0 |
| H | 16 | B16 | 1 | A16 | 3 | D15 | 0 |
| H | 16 | B17 | 1 | A17 | 3 | D16 | 0 |
| C | 1 | B18 | 1 | A18 | 2 | D17 | 0 |
| H | 20 | B19 | 3 | A19 | 3 | D18 | 0 |
| H | 20 | B20 | 1 | A20 | 3 | D19 | 0 |
| H | 20 | B21 | 1 | A21 | 3 | D20 | 0 |
| O | 1 | B22 | 3 | A22 | 2 | D21 | 0 |
| H | 24 | B23 | 1 | A23 | 3 | D22 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 2.33690441 |
| B2 | 1.41895120 |
| B3 | 0.99080142 |
| B4 | 2.81671118 |
| B5 | 1.48243491 |
| B6 | 1.08597064 |
| B7 | 1.09249738 |
| B8 | 1.09019034 |
| B9 | 1.47215910 |
| B10 | 1.09373609 |
| B11 | 1.09042399 |
| B12 | 1.08574587 |
| B13 | 2.25101099 |
| B14 | 1.24840694 |
| B15 | 1.52246351 |
| B16 | 1.08772020 |
| B17 | 1.09120934 |
| B18 | 1.08947578 |
| B19 | 1.51409828 |

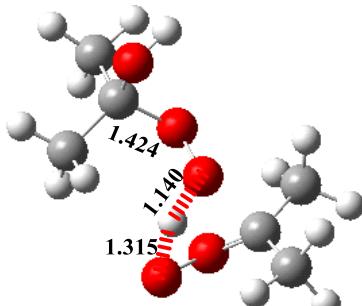
| | |
|-----|---------------|
| B20 | 1.08623343 |
| B21 | 1.08850967 |
| B22 | 1.08868638 |
| B23 | 1.39822778 |
| B24 | 0.96154362 |
| A1 | 34.75486579 |
| A2 | 102.83540669 |
| A3 | 97.00073580 |
| A4 | 103.49862069 |
| A5 | 111.15704869 |
| A6 | 107.83869880 |
| A7 | 109.86181039 |
| A8 | 88.19096701 |
| A9 | 108.22559825 |
| A10 | 108.76293200 |
| A11 | 110.74827249 |
| A12 | 72.79107041 |
| A13 | 77.91856722 |
| A14 | 102.79669386 |
| A15 | 109.01471973 |
| A16 | 110.11304635 |
| A17 | 110.61291504 |
| A18 | 112.40902089 |
| A19 | 109.70608626 |
| A20 | 109.18169219 |
| A21 | 110.14673269 |
| A22 | 110.23639208 |
| A23 | 108.38277272 |
| D1 | -89.60573413 |
| D2 | -132.60189661 |
| D3 | -174.00933323 |
| D4 | -86.31818671 |
| D5 | 34.09321727 |
| D6 | 151.10760556 |
| D7 | -50.73300214 |
| D8 | 4.45184323 |
| D9 | 119.57782651 |
| D10 | -116.63097843 |
| D11 | 37.98335264 |
| D12 | 71.89990250 |
| D13 | -172.75310203 |
| D14 | -172.96335224 |
| D15 | -53.62400233 |
| D16 | 67.08664701 |

| | |
|-----|---------------|
| D17 | -51.34205653 |
| D18 | 69.64992991 |
| D19 | -171.10239214 |
| D20 | -50.53017296 |
| D21 | 68.23188301 |
| D22 | 48.74910928 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 41.59 | 67.66 | 70.49 | 78.90 | 124.35 | 161.84 | 175.65 | 181.79 | 230.26 | 244.59 | 269.22 |
| 286.27 | 308.75 | 328.72 | 344.73 | 362.48 | 378.57 | 397.32 | 449.69 | 492.33 | 529.01 | |
| 602.47 | 606.05 | 810.14 | 823.73 | 858.72 | 903.13 | 909.69 | 941.13 | 951.60 | 988.00 | |
| 1004.73 | 1019.84 | 1061.68 | 1089.76 | 1106.84 | 1149.62 | 1228.14 | 1271.86 | 1316.06 | | |
| 1372.98 | 1392.38 | 1406.88 | 1409.22 | 1431.27 | 1450.43 | 1462.62 | 1474.73 | 1485.00 | | |
| 1488.48 | 1492.35 | 1502.89 | 1512.09 | 1602.24 | 1667.42 | 3044.98 | 3052.37 | 3058.02 | | |
| 3071.75 | 3112.40 | 3117.93 | 3134.70 | 3147.28 | 3153.52 | 3169.98 | 3175.81 | 3176.19 | | |
| 3279.23 | 3884.86 | | | | | | | | | |

Rotational constants (B/GHZ): 1.5915018 0.7252717 0.6538639



TS7c

C

| | | | | | | | |
|---|----|-----|---|-----|---|-----|---|
| O | 1 | B1 | | | | | |
| O | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| C | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| C | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 6 | B6 | 5 | A5 | 2 | D4 | 0 |
| H | 6 | B7 | 5 | A6 | 2 | D5 | 0 |
| H | 6 | B8 | 5 | A7 | 2 | D6 | 0 |
| C | 5 | B9 | 2 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 5 | A9 | 2 | D8 | 0 |
| H | 10 | B11 | 5 | A10 | 2 | D9 | 0 |
| H | 10 | B12 | 5 | A11 | 2 | D10 | 0 |
| O | 5 | B13 | 2 | A12 | 1 | D11 | 0 |
| O | 5 | B14 | 2 | A13 | 1 | D12 | 0 |
| C | 1 | B15 | 3 | A14 | 2 | D13 | 0 |
| H | 16 | B16 | 1 | A15 | 3 | D14 | 0 |
| H | 16 | B17 | 1 | A16 | 3 | D15 | 0 |
| H | 16 | B18 | 1 | A17 | 3 | D16 | 0 |

| | | | | | | | |
|---|----|-----|---|-----|---|-----|---|
| C | 1 | B19 | 3 | A18 | 2 | D17 | 0 |
| H | 20 | B20 | 1 | A19 | 3 | D18 | 0 |
| H | 20 | B21 | 1 | A20 | 3 | D19 | 0 |
| H | 20 | B22 | 1 | A21 | 3 | D20 | 0 |
| O | 1 | B23 | 3 | A22 | 2 | D21 | 0 |
| H | 24 | B24 | 1 | A23 | 3 | D22 | 0 |

Variables:

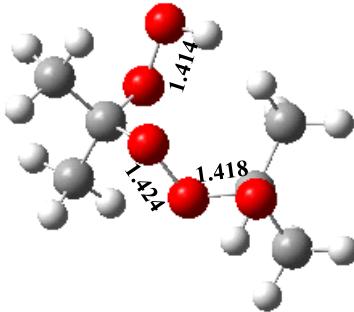
| | |
|-----|--------------|
| B1 | 2.33450667 |
| B2 | 1.41576394 |
| B3 | 1.14015447 |
| B4 | 2.06849195 |
| B5 | 1.48482479 |
| B6 | 1.08546220 |
| B7 | 1.09037854 |
| B8 | 1.08959154 |
| B9 | 1.48922545 |
| B10 | 1.08653314 |
| B11 | 1.08284678 |
| B12 | 1.09385049 |
| B13 | 2.21383823 |
| B14 | 1.28087117 |
| B15 | 1.52090371 |
| B16 | 1.08781970 |
| B17 | 1.09071678 |
| B18 | 1.08799670 |
| B19 | 1.51471941 |
| B20 | 1.08758826 |
| B21 | 1.08825803 |
| B22 | 1.08831732 |
| B23 | 1.39904341 |
| B24 | 0.96133824 |
| A1 | 34.80333571 |
| A2 | 97.22019966 |
| A3 | 132.60857670 |
| A4 | 107.53436679 |
| A5 | 110.66645403 |
| A6 | 107.19026734 |
| A7 | 110.17775288 |
| A8 | 90.76312854 |
| A9 | 109.55795648 |
| A10 | 111.95840167 |
| A11 | 106.40094650 |
| A12 | 67.59274225 |
| A13 | 90.80709895 |

| | |
|-----|---------------|
| A14 | 102.76272050 |
| A15 | 108.91387081 |
| A16 | 110.06024341 |
| A17 | 110.63019972 |
| A18 | 112.19422569 |
| A19 | 109.94006364 |
| A20 | 109.16623950 |
| A21 | 110.06984658 |
| A22 | 110.47471355 |
| A23 | 108.44263541 |
| D1 | -103.00535301 |
| D2 | -28.71512577 |
| D3 | 63.71487937 |
| D4 | -93.49447900 |
| D5 | 25.53261919 |
| D6 | 143.24692415 |
| D7 | -175.11668455 |
| D8 | -64.54974324 |
| D9 | 58.90201580 |
| D10 | 178.19473478 |
| D11 | -81.74818894 |
| D12 | -52.21231230 |
| D13 | -174.33223843 |
| D14 | -174.96287212 |
| D15 | -55.54732773 |
| D16 | 64.65649235 |
| D17 | -52.93181149 |
| D18 | 69.49225863 |
| D19 | -171.68861691 |
| D20 | -51.15363952 |
| D21 | 66.33937695 |
| D22 | 54.94104970 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|--------|
| 774.33 <i>i</i> | 41.79 | 65.22 | 81.55 | 87.04 | 149.22 | 167.63 | 185.53 | 209.06 | 221.04 | 261.54 |
| 292.66 | 325.39 | 334.83 | 363.06 | 380.16 | 409.93 | 445.34 | 448.93 | 522.13 | 548.36 | |
| 581.11 | 620.46 | 806.70 | 815.90 | 891.65 | 908.62 | 943.76 | 944.88 | 959.75 | 983.79 | |
| 1004.65 | 1020.09 | 1079.26 | 1082.67 | 1126.36 | 1153.56 | 1230.31 | 1274.47 | 1314.55 | | |
| 1373.05 | 1402.46 | 1412.76 | 1422.27 | 1432.99 | 1447.55 | 1457.23 | 1470.00 | 1482.02 | | |
| 1485.86 | 1493.06 | 1502.62 | 1512.27 | 1588.04 | 1604.33 | 1786.55 | 3055.04 | 3058.06 | | |
| 3065.87 | 3072.04 | 3136.25 | 3136.38 | 3144.18 | 3152.25 | 3157.44 | 3160.19 | 3176.32 | | |
| 3213.07 | 3875.44 | | | | | | | | | |

Rotational constants (B/GHZ): 1.8634429 0.6631601 0.6226989



P7c

C

| | | | | | | |
|---|----|-----|---|-----|---|-------|
| O | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| C | 2 | B4 | 1 | A3 | 3 | D2 0 |
| C | 5 | B5 | 2 | A4 | 1 | D3 0 |
| H | 6 | B6 | 5 | A5 | 2 | D4 0 |
| H | 6 | B7 | 5 | A6 | 2 | D5 0 |
| H | 6 | B8 | 5 | A7 | 2 | D6 0 |
| C | 5 | B9 | 2 | A8 | 1 | D7 0 |
| H | 10 | B10 | 5 | A9 | 2 | D8 0 |
| H | 10 | B11 | 5 | A10 | 2 | D9 0 |
| H | 10 | B12 | 5 | A11 | 2 | D10 0 |
| O | 5 | B13 | 2 | A12 | 1 | D11 0 |
| O | 5 | B14 | 2 | A13 | 1 | D12 0 |
| C | 1 | B15 | 3 | A14 | 2 | D13 0 |
| H | 16 | B16 | 1 | A15 | 3 | D14 0 |
| H | 16 | B17 | 1 | A16 | 3 | D15 0 |
| H | 16 | B18 | 1 | A17 | 3 | D16 0 |
| C | 1 | B19 | 3 | A18 | 2 | D17 0 |
| H | 20 | B20 | 1 | A19 | 3 | D18 0 |
| H | 20 | B21 | 1 | A20 | 3 | D19 0 |
| H | 20 | B22 | 1 | A21 | 3 | D20 0 |
| O | 1 | B23 | 3 | A22 | 2 | D21 0 |
| H | 24 | B24 | 1 | A23 | 3 | D22 0 |

Variables:

| | |
|----|------------|
| B1 | 2.32041754 |
| B2 | 1.41793950 |
| B3 | 2.69121487 |
| B4 | 1.41544267 |
| B5 | 1.51746648 |
| B6 | 1.08615272 |
| B7 | 1.08799285 |
| B8 | 1.08769628 |
| B9 | 1.51706057 |

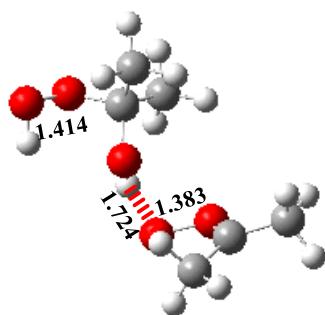
| | |
|-----|---------------|
| B10 | 1.08766149 |
| B11 | 1.08583801 |
| B12 | 1.08790715 |
| B13 | 2.31752023 |
| B14 | 1.41310791 |
| B15 | 1.52139292 |
| B16 | 1.08775033 |
| B17 | 1.09016254 |
| B18 | 1.08817114 |
| B19 | 1.51544068 |
| B20 | 1.08890228 |
| B21 | 1.08792015 |
| B22 | 1.09018726 |
| B23 | 1.39785127 |
| B24 | 0.96173873 |
| A1 | 35.35543874 |
| A2 | 85.43264168 |
| A3 | 132.03010964 |
| A4 | 112.76374466 |
| A5 | 110.66381344 |
| A6 | 109.10055389 |
| A7 | 109.14831159 |
| A8 | 104.01980557 |
| A9 | 109.20087335 |
| A10 | 110.86240715 |
| A11 | 108.84495993 |
| A12 | 96.36497666 |
| A13 | 110.46633638 |
| A14 | 102.65815351 |
| A15 | 108.86686466 |
| A16 | 109.93582699 |
| A17 | 110.76140721 |
| A18 | 112.52158495 |
| A19 | 109.18452195 |
| A20 | 109.52817862 |
| A21 | 109.55678851 |
| A22 | 110.64316925 |
| A23 | 108.58025354 |
| D1 | -118.95618914 |
| D2 | -56.93075538 |
| D3 | 75.10730044 |
| D4 | -72.54917223 |
| D5 | 47.53042304 |
| D6 | 167.20383946 |

| | |
|-----|---------------|
| D7 | -162.19588705 |
| D8 | -72.97587626 |
| D9 | 47.54122160 |
| D10 | 167.38697170 |
| D11 | -73.84091976 |
| D12 | -40.83006114 |
| D13 | -176.36573308 |
| D14 | -175.40650350 |
| D15 | -56.07286275 |
| D16 | 64.07024469 |
| D17 | -55.03507989 |
| D18 | 72.04070069 |
| D19 | -169.81285633 |
| D20 | -50.13815036 |
| D21 | 64.10535551 |
| D22 | 54.31641570 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 53.26 | 87.59 | 118.96 | 155.72 | 192.87 | 219.14 | 231.90 | 237.98 | 254.76 | 268.65 | 283.51 |
| 310.11 | 333.45 | 363.74 | 375.24 | 380.00 | 411.11 | 451.05 | 464.43 | 526.29 | 596.36 | |
| 607.78 | 620.39 | 812.44 | 842.52 | 903.23 | 925.88 | 947.45 | 958.60 | 971.97 | 1013.24 | |
| 1019.63 | 1028.44 | 1055.70 | 1065.50 | 1155.49 | 1209.22 | 1230.79 | 1251.87 | 1281.03 | | |
| 1313.58 | 1368.04 | 1412.27 | 1415.55 | 1421.09 | 1424.81 | 1430.95 | 1478.90 | 1487.05 | | |
| 1488.15 | 1493.82 | 1494.93 | 1503.04 | 1508.43 | 1529.29 | 3057.81 | 3063.48 | 3076.47 | | |
| 3081.50 | 3141.85 | 3144.26 | 3149.42 | 3156.88 | 3159.79 | 3161.92 | 3169.96 | 3175.16 | | |
| 3826.81 | 3883.11 | | | | | | | | | |

Rotational constants (B/GHZ): 1.7919387 0.7346323 0.6691134



IM7d

| | | | | | | | |
|---|---|----|---|----|---|----|---|
| C | | B1 | | | | | |
| C | 1 | | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| C | 1 | B5 | 2 | A4 | 5 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| H | 6 | B7 | 1 | A6 | 2 | D5 | 0 |
| H | 6 | B8 | 1 | A7 | 2 | D6 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 1 | B9 | 6 | A8 | 2 | D7 | 0 |
| H | 10 | B10 | 1 | A9 | 6 | D8 | 0 |
| O | 1 | B11 | 10 | A10 | 6 | D9 | 0 |
| C | 10 | B12 | 1 | A11 | 6 | D10 | 0 |
| C | 13 | B13 | 10 | A12 | 1 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 10 | D12 | 0 |
| H | 14 | B15 | 13 | A14 | 10 | D13 | 0 |
| H | 14 | B16 | 13 | A15 | 10 | D14 | 0 |
| C | 13 | B17 | 10 | A16 | 1 | D15 | 0 |
| H | 18 | B18 | 13 | A17 | 10 | D16 | 0 |
| H | 18 | B19 | 13 | A18 | 10 | D17 | 0 |
| H | 18 | B20 | 13 | A19 | 10 | D18 | 0 |
| O | 13 | B21 | 10 | A20 | 1 | D19 | 0 |
| O | 13 | B22 | 10 | A21 | 1 | D20 | 0 |
| O | 12 | B23 | 1 | A22 | 10 | D21 | 0 |
| H | 12 | B24 | 1 | A23 | 10 | D22 | 0 |

Variables:

| | |
|-----|--------------|
| B1 | 1.51935236 |
| B2 | 1.08948458 |
| B3 | 1.08953774 |
| B4 | 1.08819841 |
| B5 | 1.51610767 |
| B6 | 1.08903208 |
| B7 | 1.08833762 |
| B8 | 1.08664537 |
| B9 | 1.39928720 |
| B10 | 0.98674675 |
| B11 | 2.31266600 |
| B12 | 3.12791732 |
| B13 | 1.48324666 |
| B14 | 1.09190625 |
| B15 | 1.09071787 |
| B16 | 1.08579597 |
| B17 | 1.47257889 |
| B18 | 1.09404573 |
| B19 | 1.09034209 |
| B20 | 1.08570871 |
| B21 | 2.24848582 |
| B22 | 1.24936484 |
| B23 | 1.41397679 |
| B24 | 0.96680923 |
| A1 | 109.18980975 |
| A2 | 109.97340333 |
| A3 | 110.29604306 |

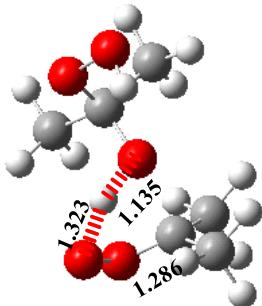
| | |
|-----|---------------|
| A4 | 113.08088007 |
| A5 | 109.46342504 |
| A6 | 109.88853742 |
| A7 | 110.06523363 |
| A8 | 107.94800798 |
| A9 | 109.81889551 |
| A10 | 89.78275673 |
| A11 | 122.73287256 |
| A12 | 123.67155223 |
| A13 | 108.53704990 |
| A14 | 109.51959725 |
| A15 | 111.11497556 |
| A16 | 77.35542522 |
| A17 | 107.84916989 |
| A18 | 108.77009665 |
| A19 | 110.86139864 |
| A20 | 56.74562939 |
| A21 | 70.49563163 |
| A22 | 35.58274494 |
| A23 | 87.23848434 |
| D1 | 119.47598533 |
| D2 | -119.78129867 |
| D3 | -62.04506226 |
| D4 | -60.20981946 |
| D5 | 59.80438117 |
| D6 | 179.93933073 |
| D7 | 124.37751295 |
| D8 | -164.50633581 |
| D9 | -91.20075804 |
| D10 | -100.38428653 |
| D11 | 48.09315491 |
| D12 | 37.28149027 |
| D13 | 154.06698654 |
| D14 | -83.84732302 |
| D15 | 169.54931514 |
| D16 | -12.19185258 |
| D17 | 102.84631150 |
| D18 | -133.11348862 |
| D19 | -94.52323292 |
| D20 | -60.60163843 |
| D21 | -125.37564924 |
| D22 | -10.58183698 |

Harmonic Vibrational Frequencies (cm⁻¹):

35.82 42.15 67.45 88.69 111.10 148.44 166.36 187.65 207.34 222.48 252.78

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 279.12 | 321.93 | 337.47 | 342.61 | 360.61 | 374.77 | 423.66 | 451.44 | 495.22 | 552.24 |
| 603.29 | 615.42 | 814.79 | 828.46 | 904.88 | 909.89 | 941.98 | 946.29 | 968.62 | 991.06 |
| 1010.35 | 1026.92 | 1061.35 | 1091.76 | 1106.05 | 1220.64 | 1227.40 | 1280.79 | 1318.62 | |
| 1388.69 | 1395.86 | 1412.85 | 1420.36 | 1445.63 | 1452.79 | 1457.81 | 1465.23 | 1475.42 | |
| 1483.43 | 1489.24 | 1495.72 | 1504.72 | 1514.50 | 1665.85 | 3046.74 | 3057.96 | 3062.56 | |
| 3068.07 | 3113.08 | 3121.45 | 3139.30 | 3145.77 | 3154.43 | 3158.94 | 3169.96 | 3173.02 | |
| 3313.22 | 3788.54 | | | | | | | | |

Rotational constants (B/GHZ): 1.7748628 0.5471228 0.5256580



TS7d

C

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| C | 1 | B5 | 2 | A4 | 5 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| H | 6 | B7 | 1 | A6 | 2 | D5 | 0 |
| H | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| O | 1 | B9 | 6 | A8 | 2 | D7 | 0 |
| H | 10 | B10 | 1 | A9 | 6 | D8 | 0 |
| O | 1 | B11 | 10 | A10 | 6 | D9 | 0 |
| C | 10 | B12 | 1 | A11 | 6 | D10 | 0 |
| C | 13 | B13 | 10 | A12 | 1 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 10 | D12 | 0 |
| H | 14 | B15 | 13 | A14 | 10 | D13 | 0 |
| H | 14 | B16 | 13 | A15 | 10 | D14 | 0 |
| C | 13 | B17 | 10 | A16 | 1 | D15 | 0 |
| H | 18 | B18 | 13 | A17 | 10 | D16 | 0 |
| H | 18 | B19 | 13 | A18 | 10 | D17 | 0 |
| H | 18 | B20 | 13 | A19 | 10 | D18 | 0 |
| O | 13 | B21 | 10 | A20 | 1 | D19 | 0 |
| O | 13 | B22 | 10 | A21 | 1 | D20 | 0 |
| O | 12 | B23 | 1 | A22 | 10 | D21 | 0 |
| H | 12 | B24 | 1 | A23 | 10 | D22 | 0 |

Variables:

B1 1.52017477

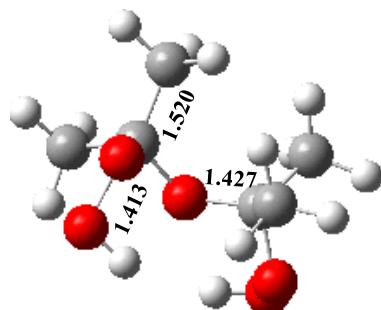
| | |
|-----|--------------|
| B2 | 1.08822179 |
| B3 | 1.08835353 |
| B4 | 1.08810005 |
| B5 | 1.51785486 |
| B6 | 1.08886157 |
| B7 | 1.08868961 |
| B8 | 1.08688076 |
| B9 | 1.40885578 |
| B10 | 1.13514638 |
| B11 | 2.31451369 |
| B12 | 2.00971629 |
| B13 | 1.48873615 |
| B14 | 1.08737058 |
| B15 | 1.09189561 |
| B16 | 1.08593925 |
| B17 | 1.49193143 |
| B18 | 1.08557186 |
| B19 | 1.08245384 |
| B20 | 1.09386159 |
| B21 | 2.21445415 |
| B22 | 1.28551325 |
| B23 | 1.41409901 |
| B24 | 0.96599734 |
| A1 | 109.99217325 |
| A2 | 110.28310897 |
| A3 | 109.49390842 |
| A4 | 112.89320513 |
| A5 | 110.05371781 |
| A6 | 109.57320180 |
| A7 | 110.26625911 |
| A8 | 109.42525331 |
| A9 | 110.72129389 |
| A10 | 89.53758679 |
| A11 | 125.88002182 |
| A12 | 110.56062128 |
| A13 | 109.53072092 |
| A14 | 108.09629381 |
| A15 | 111.23926397 |
| A16 | 91.16096194 |
| A17 | 110.00381547 |
| A18 | 111.58583342 |
| A19 | 106.09893433 |
| A20 | 68.38275298 |
| A21 | 92.83893192 |

| | |
|-----|---------------|
| A22 | 35.35211810 |
| A23 | 90.94224359 |
| D1 | 119.63256267 |
| D2 | -119.73964054 |
| D3 | -59.85221532 |
| D4 | -55.04929014 |
| D5 | 64.30026564 |
| D6 | -175.81090149 |
| D7 | 126.66682366 |
| D8 | -164.57720631 |
| D9 | -89.63307280 |
| D10 | -78.01548674 |
| D11 | 43.36468269 |
| D12 | 49.91400549 |
| D13 | 167.41648044 |
| D14 | -72.72368277 |
| D15 | 164.05271536 |
| D16 | -62.58583517 |
| D17 | 60.92866682 |
| D18 | 179.91845969 |
| D19 | -102.63007406 |
| D20 | -73.86177324 |
| D21 | -121.62153940 |
| D22 | -12.14042462 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 774.49 <i>i</i> | 49.74 | 114.29 | 118.06 | 144.31 | 163.33 | 179.41 | 202.61 | 213.46 | 233.49 |
| 257.60 | 295.97 | 317.57 | 338.66 | 360.16 | 364.54 | 394.90 | 423.08 | 443.47 | 529.89 |
| 567.61 | 583.78 | 637.49 | 755.33 | 833.85 | 895.62 | 912.85 | 926.12 | 942.53 | 953.25 |
| 994.27 | 1013.47 | 1032.20 | 1062.32 | 1082.00 | 1109.86 | 1228.52 | 1258.21 | 1270.52 | |
| 1314.27 | 1404.26 | 1408.08 | 1422.25 | 1425.07 | 1443.30 | 1444.98 | 1455.75 | 1473.92 | |
| 1476.73 | 1479.62 | 1495.70 | 1500.54 | 1501.58 | 1518.61 | 1576.11 | 1854.01 | 3055.10 | |
| 3064.84 | 3067.68 | 3075.00 | 3137.77 | 3149.18 | 3151.88 | 3152.46 | 3154.66 | 3166.87 | |
| 3186.36 | 3207.22 | 3809.33 | | | | | | | |

Rotational constants (B/GHZ): 1.5995969 0.7416070 0.7201273



P7d

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| C | 1 | B5 | 2 | A4 | 3 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |
| H | 6 | B7 | 1 | A6 | 2 | D5 | 0 |
| H | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| O | 1 | B9 | 2 | A8 | 6 | D7 | 0 |
| H | 10 | B10 | 1 | A9 | 2 | D8 | 0 |
| O | 1 | B11 | 10 | A10 | 6 | D9 | 0 |
| C | 10 | B12 | 1 | A11 | 2 | D10 | 0 |
| C | 13 | B13 | 10 | A12 | 1 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 10 | D12 | 0 |
| H | 14 | B15 | 13 | A14 | 10 | D13 | 0 |
| H | 14 | B16 | 13 | A15 | 10 | D14 | 0 |
| C | 13 | B17 | 10 | A16 | 1 | D15 | 0 |
| H | 18 | B18 | 13 | A17 | 10 | D16 | 0 |
| H | 18 | B19 | 13 | A18 | 10 | D17 | 0 |
| H | 18 | B20 | 13 | A19 | 10 | D18 | 0 |
| O | 13 | B21 | 10 | A20 | 1 | D19 | 0 |
| O | 22 | B22 | 13 | A21 | 10 | D20 | 0 |
| O | 1 | B23 | 10 | A22 | 13 | D21 | 0 |
| H | 12 | B24 | 1 | A23 | 24 | D22 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.51975844 |
| B2 | 1.08510851 |
| B3 | 1.08831892 |
| B4 | 1.08849776 |
| B5 | 1.52089814 |
| B6 | 1.08694474 |
| B7 | 1.08863574 |
| B8 | 1.08644301 |
| B9 | 1.42740681 |
| B10 | 2.35894884 |
| B11 | 2.31046110 |
| B12 | 1.40993266 |
| B13 | 1.52022979 |
| B14 | 1.08793957 |
| B15 | 1.08787123 |
| B16 | 1.08703109 |
| B17 | 1.51834295 |
| B18 | 1.08841555 |
| B19 | 1.08585966 |

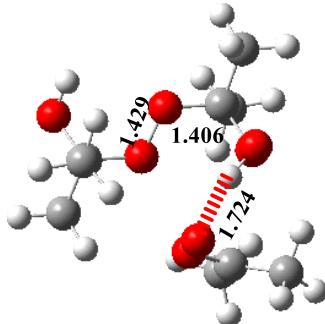
| | |
|-----|---------------|
| B20 | 1.08802660 |
| B21 | 2.31356060 |
| B22 | 1.41273241 |
| B23 | 1.41290913 |
| B24 | 0.96657963 |
| A1 | 111.52128219 |
| A2 | 110.85853846 |
| A3 | 108.04806701 |
| A4 | 112.84620699 |
| A5 | 110.97598616 |
| A6 | 108.65228146 |
| A7 | 110.32134206 |
| A8 | 114.98573393 |
| A9 | 101.16071446 |
| A10 | 86.36020338 |
| A11 | 124.86474696 |
| A12 | 115.28817617 |
| A13 | 109.43189990 |
| A14 | 108.70713214 |
| A15 | 112.04165269 |
| A16 | 105.19988632 |
| A17 | 109.33648987 |
| A18 | 110.39085652 |
| A19 | 109.42589555 |
| A20 | 90.99216125 |
| A21 | 35.23093048 |
| A22 | 103.28018597 |
| A23 | 91.26800033 |
| D1 | 121.01719067 |
| D2 | 118.88689337 |
| D3 | 63.61090912 |
| D4 | -51.37173866 |
| D5 | 67.96401097 |
| D6 | -172.83122748 |
| D7 | -129.40868284 |
| D8 | -36.67435283 |
| D9 | -87.84312708 |
| D10 | 46.27258105 |
| D11 | 47.98797546 |
| D12 | 53.50978221 |
| D13 | 172.48843577 |
| D14 | -68.04775717 |
| D15 | 170.92537626 |
| D16 | -68.71298204 |

| | |
|-----|--------------|
| D17 | 51.42836618 |
| D18 | 171.42415332 |
| D19 | -99.09829213 |
| D20 | 124.09315111 |
| D21 | 157.27375643 |
| D22 | 108.92634121 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 54.46 | 106.02 | 136.80 | 161.28 | 205.40 | 223.22 | 241.23 | 258.97 | 273.25 | 289.25 |
| 302.42 | 324.73 | 340.11 | 358.83 | 373.39 | 380.90 | 398.37 | 404.10 | 491.79 | 539.38 |
| 558.34 | 603.47 | 641.66 | 752.33 | 849.45 | 899.42 | 925.81 | 939.16 | 948.44 | 972.48 |
| 1017.99 | 1022.21 | 1052.37 | 1063.94 | 1074.19 | 1196.00 | 1231.87 | 1249.32 | 1261.80 | |
| 1280.31 | 1307.65 | 1410.77 | 1412.68 | 1419.87 | 1429.97 | 1441.85 | 1450.05 | 1474.40 | |
| 1483.25 | 1487.94 | 1494.65 | 1495.58 | 1504.63 | 1511.27 | 1520.74 | 3074.88 | 3075.59 | |
| 3078.01 | 3081.30 | 3149.27 | 3152.36 | 3154.64 | 3160.43 | 3166.98 | 3168.92 | 3172.26 | |
| 3193.58 | 3779.71 | 3809.13 | | | | | | | |

Rotational constants (B/GHZ): 1.5565329 0.8072245 0.7806714



IM8a

| | | | | | | | | | |
|---|----|--|-----|---|-----|---|-----|---|--|
| C | | | | | | | | | |
| O | 1 | | B1 | | | | | | |
| O | 1 | | B2 | 2 | A1 | | | | |
| H | 2 | | B3 | 1 | A2 | 3 | D1 | 0 | |
| C | 3 | | B4 | 1 | A3 | 2 | D2 | 0 | |
| O | 5 | | B5 | 3 | A4 | 1 | D3 | 0 | |
| O | 5 | | B6 | 3 | A5 | 1 | D4 | 0 | |
| C | 1 | | B7 | 3 | A6 | 2 | D5 | 0 | |
| H | 8 | | B8 | 1 | A7 | 3 | D6 | 0 | |
| H | 8 | | B9 | 1 | A8 | 3 | D7 | 0 | |
| H | 8 | | B10 | 1 | A9 | 3 | D8 | 0 | |
| O | 1 | | B11 | 3 | A10 | 2 | D9 | 0 | |
| C | 12 | | B12 | 1 | A11 | 3 | D10 | 0 | |
| C | 5 | | B13 | 3 | A12 | 1 | D11 | 0 | |
| H | 14 | | B14 | 5 | A13 | 3 | D12 | 0 | |
| H | 14 | | B15 | 5 | A14 | 3 | D13 | 0 | |
| H | 14 | | B16 | 5 | A15 | 3 | D14 | 0 | |
| C | 5 | | B17 | 3 | A16 | 1 | D15 | 0 | |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 18 | B18 | 5 | A17 | 3 | D16 | 0 |
| H | 18 | B19 | 5 | A18 | 3 | D17 | 0 |
| H | 18 | B20 | 5 | A19 | 3 | D18 | 0 |
| C | 1 | B21 | 12 | A20 | 13 | D19 | 0 |
| H | 22 | B22 | 1 | A21 | 12 | D20 | 0 |
| H | 22 | B23 | 1 | A22 | 12 | D21 | 0 |
| H | 22 | B24 | 1 | A23 | 12 | D22 | 0 |
| O | 13 | B25 | 12 | A24 | 1 | D23 | 0 |
| C | 13 | B26 | 12 | A25 | 1 | D24 | 0 |
| H | 27 | B27 | 13 | A26 | 12 | D25 | 0 |
| H | 27 | B28 | 13 | A27 | 12 | D26 | 0 |
| H | 27 | B29 | 13 | A28 | 12 | D27 | 0 |
| C | 13 | B30 | 12 | A29 | 1 | D28 | 0 |
| H | 31 | B31 | 13 | A30 | 12 | D29 | 0 |
| H | 31 | B32 | 13 | A31 | 12 | D30 | 0 |
| H | 31 | B33 | 13 | A32 | 12 | D31 | 0 |
| O | 13 | B34 | 12 | A33 | 1 | D32 | 0 |
| H | 35 | B35 | 13 | A34 | 12 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 2.31968155 |
| B2 | 1.41073015 |
| B3 | 0.99240356 |
| B4 | 2.79512694 |
| B5 | 2.24983357 |
| B6 | 1.24736331 |
| B7 | 1.51881329 |
| B8 | 1.08788767 |
| B9 | 1.08639059 |
| B10 | 1.08796568 |
| B11 | 1.40648711 |
| B12 | 2.28389634 |
| B13 | 1.48148482 |
| B14 | 1.08628662 |
| B15 | 1.09124945 |
| B16 | 1.09140505 |
| B17 | 1.47406083 |
| B18 | 1.09253058 |
| B19 | 1.09041646 |
| B20 | 1.08586134 |
| B21 | 1.51725893 |
| B22 | 1.08807250 |
| B23 | 1.08792238 |
| B24 | 1.08567861 |
| B25 | 1.42471061 |

| | |
|-----|--------------|
| B26 | 1.51448664 |
| B27 | 1.08904415 |
| B28 | 1.08790724 |
| B29 | 1.08766472 |
| B30 | 1.51937191 |
| B31 | 1.08940057 |
| B32 | 1.08861881 |
| B33 | 1.08884347 |
| B34 | 1.39982303 |
| B35 | 0.96141261 |
| A1 | 35.13324428 |
| A2 | 110.68768202 |
| A3 | 131.14698969 |
| A4 | 77.88597221 |
| A5 | 83.67622646 |
| A6 | 104.51901777 |
| A7 | 109.58868384 |
| A8 | 110.71945938 |
| A9 | 108.90630313 |
| A10 | 110.79722842 |
| A11 | 144.70602573 |
| A12 | 99.30508026 |
| A13 | 110.84414679 |
| A14 | 107.79940001 |
| A15 | 109.70512477 |
| A16 | 87.24006640 |
| A17 | 108.56045476 |
| A18 | 108.58629338 |
| A19 | 110.65881243 |
| A20 | 104.22536140 |
| A21 | 108.77728410 |
| A22 | 109.59125879 |
| A23 | 110.30649333 |
| A24 | 36.89425555 |
| A25 | 140.48903187 |
| A26 | 109.64216898 |
| A27 | 110.14081877 |
| A28 | 108.74286797 |
| A29 | 89.06939618 |
| A30 | 110.56054919 |
| A31 | 110.59465807 |
| A32 | 108.77329832 |
| A33 | 93.04697218 |
| A34 | 108.05585123 |

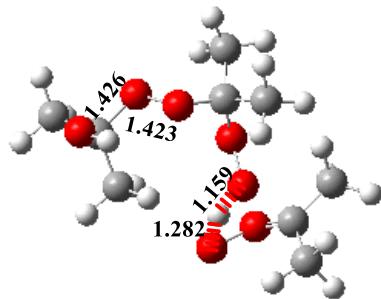
| | |
|-----|---------------|
| D1 | -81.80759302 |
| D2 | 116.88058604 |
| D3 | -97.18246834 |
| D4 | -63.89471874 |
| D5 | 171.61575420 |
| D6 | -67.81797423 |
| D7 | 53.26297116 |
| D8 | 172.43428268 |
| D9 | -67.20895478 |
| D10 | -60.43575250 |
| D11 | 51.32686259 |
| D12 | -81.30555133 |
| D13 | 39.10657522 |
| D14 | 155.92395966 |
| D15 | 174.36824032 |
| D16 | 11.83670620 |
| D17 | 127.11344084 |
| D18 | -109.36652676 |
| D19 | 178.50669780 |
| D20 | 171.24055265 |
| D21 | -69.17048010 |
| D22 | 51.76156921 |
| D23 | -5.39950991 |
| D24 | -2.99886798 |
| D25 | -57.09044284 |
| D26 | 64.40066710 |
| D27 | -175.88202491 |
| D28 | 123.10310053 |
| D29 | -81.55632291 |
| D30 | 38.39650041 |
| D31 | 157.70733099 |
| D32 | -125.09956499 |
| D33 | -34.73845411 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 35.22 | 56.04 | 73.25 | 84.73 | 88.63 | 95.84 | 114.42 | 132.82 | 139.72 | 164.50 | 175.98 |
| 191.50 | 200.12 | 204.42 | 222.69 | 246.40 | 265.90 | 274.30 | 287.79 | 323.20 | 335.04 | |
| 348.28 | 361.79 | 371.07 | 380.65 | 395.91 | 406.62 | 442.91 | 470.67 | 504.58 | 538.70 | |
| 581.33 | 596.45 | 603.73 | 615.02 | 771.50 | 815.11 | 831.90 | 855.56 | 912.31 | 918.86 | |
| 930.42 | 947.33 | 953.54 | 960.68 | 972.19 | 993.84 | 1012.12 | 1023.74 | 1033.52 | 1057.62 | |
| 1068.41 | 1094.07 | 1110.58 | 1156.18 | 1208.49 | 1237.22 | 1258.31 | 1271.93 | 1310.03 | | |
| 1319.19 | 1378.00 | 1397.67 | 1406.65 | 1410.78 | 1415.40 | 1432.60 | 1433.69 | 1457.07 | | |
| 1462.43 | 1474.87 | 1481.25 | 1486.14 | 1488.62 | 1490.98 | 1492.23 | 1496.63 | 1504.32 | | |
| 1509.73 | 1515.80 | 1625.41 | 1673.66 | 3057.05 | 3061.80 | 3062.33 | 3065.62 | 3071.79 | | |
| 3075.60 | 3125.16 | 3125.90 | 3143.01 | 3146.67 | 3150.56 | 3150.95 | 3155.90 | 3157.46 | | |

3163.76 3169.09 3170.74 3173.74 3231.19 3889.84

Rotational constants (B/GHZ): 0.5932267 0.4720037 0.3590494



TS8a

C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| O | 1 | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| C | 2 | B4 | 1 | A3 | 3 | D2 0 |
| O | 5 | B5 | 2 | A4 | 1 | D3 0 |
| O | 5 | B6 | 2 | A5 | 1 | D4 0 |
| C | 1 | B7 | 3 | A6 | 2 | D5 0 |
| H | 8 | B8 | 1 | A7 | 3 | D6 0 |
| H | 8 | B9 | 1 | A8 | 3 | D7 0 |
| H | 8 | B10 | 1 | A9 | 3 | D8 0 |
| O | 1 | B11 | 3 | A10 | 2 | D9 0 |
| C | 12 | B12 | 1 | A11 | 3 | D10 0 |
| C | 5 | B13 | 2 | A12 | 1 | D11 0 |
| H | 14 | B14 | 5 | A13 | 2 | D12 0 |
| H | 14 | B15 | 5 | A14 | 2 | D13 0 |
| H | 14 | B16 | 5 | A15 | 2 | D14 0 |
| C | 5 | B17 | 2 | A16 | 1 | D15 0 |
| H | 18 | B18 | 5 | A17 | 2 | D16 0 |
| H | 18 | B19 | 5 | A18 | 2 | D17 0 |
| H | 18 | B20 | 5 | A19 | 2 | D18 0 |
| C | 1 | B21 | 3 | A20 | 2 | D19 0 |
| H | 22 | B22 | 1 | A21 | 3 | D20 0 |
| H | 22 | B23 | 1 | A22 | 3 | D21 0 |
| H | 22 | B24 | 1 | A23 | 3 | D22 0 |
| O | 12 | B25 | 1 | A24 | 3 | D23 0 |
| C | 13 | B26 | 12 | A25 | 1 | D24 0 |
| H | 27 | B27 | 13 | A26 | 12 | D25 0 |
| H | 27 | B28 | 13 | A27 | 12 | D26 0 |
| H | 27 | B29 | 13 | A28 | 12 | D27 0 |
| C | 13 | B30 | 12 | A29 | 1 | D28 0 |
| H | 31 | B31 | 13 | A30 | 12 | D29 0 |
| H | 31 | B32 | 13 | A31 | 12 | D30 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 31 | B33 | 13 | A32 | 12 | D31 | 0 |
| O | 13 | B34 | 12 | A33 | 1 | D32 | 0 |
| H | 35 | B35 | 13 | A34 | 12 | D33 | 0 |

Variables:

| | |
|-----|--------------|
| B1 | 2.31326192 |
| B2 | 1.41023439 |
| B3 | 1.15901384 |
| B4 | 2.11704371 |
| B5 | 2.21839799 |
| B6 | 1.27982971 |
| B7 | 1.51882049 |
| B8 | 1.08852137 |
| B9 | 1.08605009 |
| B10 | 1.08787818 |
| B11 | 1.41042674 |
| B12 | 2.30071068 |
| B13 | 1.48269256 |
| B14 | 1.08736657 |
| B15 | 1.09326133 |
| B16 | 1.08671050 |
| B17 | 1.48638690 |
| B18 | 1.08262707 |
| B19 | 1.09466325 |
| B20 | 1.08668649 |
| B21 | 1.51872724 |
| B22 | 1.08896338 |
| B23 | 1.08772513 |
| B24 | 1.08617550 |
| B25 | 1.42279617 |
| B26 | 1.51391167 |
| B27 | 1.08782097 |
| B28 | 1.08772480 |
| B29 | 1.08775376 |
| B30 | 1.51791713 |
| B31 | 1.08899958 |
| B32 | 1.08937375 |
| B33 | 1.08859079 |
| B34 | 1.39890900 |
| B35 | 0.96176878 |
| A1 | 35.18218477 |
| A2 | 126.40637646 |
| A3 | 130.14059860 |
| A4 | 66.32413606 |
| A5 | 89.67816031 |

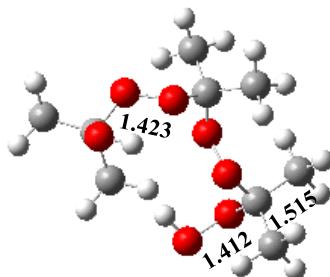
| | |
|-----|---------------|
| A6 | 104.15087633 |
| A7 | 109.47740940 |
| A8 | 110.40664496 |
| A9 | 109.04414490 |
| A10 | 111.45723426 |
| A11 | 131.68103828 |
| A12 | 107.66684882 |
| A13 | 110.24538513 |
| A14 | 105.94350667 |
| A15 | 111.70297372 |
| A16 | 89.63924695 |
| A17 | 112.07625955 |
| A18 | 106.15884191 |
| A19 | 109.55093716 |
| A20 | 112.69868640 |
| A21 | 109.28294600 |
| A22 | 109.33904463 |
| A23 | 110.54349600 |
| A24 | 108.90195231 |
| A25 | 139.49127567 |
| A26 | 109.43671501 |
| A27 | 110.33105670 |
| A28 | 108.81284181 |
| A29 | 91.89463276 |
| A30 | 110.55581070 |
| A31 | 110.46353133 |
| A32 | 109.07902793 |
| A33 | 90.91882098 |
| A34 | 107.99806822 |
| D1 | -53.81015742 |
| D2 | 44.75654729 |
| D3 | -121.86649866 |
| D4 | -92.68738650 |
| D5 | 166.99014646 |
| D6 | -72.38574704 |
| D7 | 48.09181886 |
| D8 | 167.86151006 |
| D9 | -71.89787126 |
| D10 | -37.02595165 |
| D11 | 22.12174168 |
| D12 | -117.40348400 |
| D13 | -1.07156017 |
| D14 | 118.19682126 |
| D15 | 144.16861735 |

| | |
|-----|---------------|
| D16 | 58.98332448 |
| D17 | 178.45551645 |
| D18 | -64.72677988 |
| D19 | 44.30949488 |
| D20 | 48.96155429 |
| D21 | 168.40310633 |
| D22 | -71.02860377 |
| D23 | -70.18177856 |
| D24 | -66.30914134 |
| D25 | -54.63541830 |
| D26 | 66.21813816 |
| D27 | -173.78449002 |
| D28 | 63.41139262 |
| D29 | -84.38205004 |
| D30 | 35.71117815 |
| D31 | 155.25180405 |
| D32 | 175.02972869 |
| D33 | -34.38888159 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 849.05 <i>i</i> | 36.98 | 48.81 | 57.82 | 74.62 | 88.09 | 102.11 | 111.37 | 143.87 | 173.72 | 192.69 |
| 199.09 | 210.69 | 232.61 | 243.82 | 252.89 | 277.75 | 297.54 | 300.61 | 322.79 | 335.34 | |
| 361.33 | 379.39 | 383.78 | 392.83 | 405.32 | 428.34 | 452.71 | 456.94 | 535.57 | 538.60 | |
| 563.11 | 598.25 | 616.66 | 634.01 | 798.40 | 814.68 | 842.77 | 847.49 | 908.85 | 915.67 | |
| 948.51 | 950.73 | 956.70 | 959.60 | 973.13 | 987.09 | 1013.03 | 1023.44 | 1027.39 | 1061.32 | |
| 1076.09 | 1082.69 | 1109.47 | 1155.87 | 1209.91 | 1239.37 | 1252.44 | 1273.74 | 1307.28 | | |
| 1314.83 | 1379.95 | 1400.06 | 1405.63 | 1416.56 | 1417.70 | 1421.00 | 1435.34 | 1439.56 | | |
| 1463.36 | 1476.57 | 1481.12 | 1485.00 | 1487.43 | 1489.26 | 1491.38 | 1492.23 | 1503.14 | | |
| 1507.68 | 1523.23 | 1582.18 | 1591.39 | 1792.90 | 3045.87 | 3061.95 | 3064.82 | 3070.26 | | |
| 3070.73 | 3081.58 | 3139.06 | 3139.70 | 3147.53 | 3148.20 | 3149.57 | 3155.04 | 3160.49 | | |
| 3162.22 | 3166.43 | 3172.53 | 3175.08 | 3205.63 | 3884.61 | | | | | |

Rotational constants (B/GHZ): 0.7952050 0.3330921 0.2780785



P8a

| | | | | | | | |
|---|---|----|---|----|---|----|---|
| C | | | | | | | |
| O | 1 | B1 | | | | | |
| O | 1 | B2 | 2 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| C | 2 | B4 | 1 | A3 | 3 | D2 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| O | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| C | 1 | B7 | 3 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 1 | A7 | 3 | D6 | 0 |
| H | 8 | B9 | 1 | A8 | 3 | D7 | 0 |
| H | 8 | B10 | 1 | A9 | 3 | D8 | 0 |
| O | 1 | B11 | 3 | A10 | 2 | D9 | 0 |
| C | 12 | B12 | 1 | A11 | 3 | D10 | 0 |
| C | 5 | B13 | 2 | A12 | 1 | D11 | 0 |
| H | 14 | B14 | 5 | A13 | 2 | D12 | 0 |
| H | 14 | B15 | 5 | A14 | 2 | D13 | 0 |
| H | 14 | B16 | 5 | A15 | 2 | D14 | 0 |
| C | 5 | B17 | 2 | A16 | 1 | D15 | 0 |
| H | 18 | B18 | 5 | A17 | 2 | D16 | 0 |
| H | 18 | B19 | 5 | A18 | 2 | D17 | 0 |
| H | 18 | B20 | 5 | A19 | 2 | D18 | 0 |
| C | 1 | B21 | 12 | A20 | 13 | D19 | 0 |
| H | 22 | B22 | 1 | A21 | 12 | D20 | 0 |
| H | 22 | B23 | 1 | A22 | 12 | D21 | 0 |
| H | 22 | B24 | 1 | A23 | 12 | D22 | 0 |
| O | 12 | B25 | 1 | A24 | 3 | D23 | 0 |
| C | 13 | B26 | 12 | A25 | 1 | D24 | 0 |
| H | 27 | B27 | 13 | A26 | 12 | D25 | 0 |
| H | 27 | B28 | 13 | A27 | 12 | D26 | 0 |
| H | 27 | B29 | 13 | A28 | 12 | D27 | 0 |
| C | 13 | B30 | 12 | A29 | 1 | D28 | 0 |
| H | 31 | B31 | 13 | A30 | 12 | D29 | 0 |
| H | 31 | B32 | 13 | A31 | 12 | D30 | 0 |
| H | 31 | B33 | 13 | A32 | 12 | D31 | 0 |
| O | 13 | B34 | 12 | A33 | 1 | D32 | 0 |
| H | 35 | B35 | 13 | A34 | 12 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 2.30908939 |
| B2 | 1.41514003 |
| B3 | 2.46130847 |
| B4 | 1.41824510 |
| B5 | 2.30541365 |
| B6 | 1.40889451 |
| B7 | 1.51769783 |
| B8 | 1.08795609 |
| B9 | 1.08589278 |
| B10 | 1.08777834 |
| B11 | 1.41055401 |
| B12 | 2.30709555 |

| | |
|-----|--------------|
| B13 | 1.51541517 |
| B14 | 1.08780055 |
| B15 | 1.08718928 |
| B16 | 1.08843281 |
| B17 | 1.51636819 |
| B18 | 1.08629214 |
| B19 | 1.08816886 |
| B20 | 1.08822181 |
| B21 | 1.51800790 |
| B22 | 1.08803484 |
| B23 | 1.08755312 |
| B24 | 1.08648794 |
| B25 | 1.42255904 |
| B26 | 1.51393200 |
| B27 | 1.08743287 |
| B28 | 1.08814905 |
| B29 | 1.08787236 |
| B30 | 1.51968437 |
| B31 | 1.09118388 |
| B32 | 1.08914846 |
| B33 | 1.08840247 |
| B34 | 1.39460138 |
| B35 | 0.96219433 |
| A1 | 35.74007698 |
| A2 | 109.11323312 |
| A3 | 133.66469209 |
| A4 | 88.92188066 |
| A5 | 109.81257454 |
| A6 | 103.85823732 |
| A7 | 109.19834436 |
| A8 | 110.62851480 |
| A9 | 108.97011961 |
| A10 | 110.96440846 |
| A11 | 130.87661854 |
| A12 | 113.02854803 |
| A13 | 109.41028452 |
| A14 | 110.21454072 |
| A15 | 109.22858423 |
| A16 | 103.78420199 |
| A17 | 110.27246445 |
| A18 | 108.63423337 |
| A19 | 110.01285835 |
| A20 | 103.95217064 |
| A21 | 109.20321262 |

| | |
|-----|---------------|
| A22 | 108.97111217 |
| A23 | 110.94289935 |
| A24 | 109.94430385 |
| A25 | 138.74273832 |
| A26 | 109.32663130 |
| A27 | 110.44390640 |
| A28 | 108.89757599 |
| A29 | 94.93898393 |
| A30 | 109.11499059 |
| A31 | 110.75169860 |
| A32 | 109.25016912 |
| A33 | 88.20478830 |
| A34 | 108.10074895 |
| D1 | -37.44451449 |
| D2 | 54.53773797 |
| D3 | -114.96791900 |
| D4 | -86.00771262 |
| D5 | 171.22973549 |
| D6 | -72.27191213 |
| D7 | 48.26471804 |
| D8 | 168.02416362 |
| D9 | -67.33607946 |
| D10 | -41.42945877 |
| D11 | 29.96220233 |
| D12 | -179.11136690 |
| D13 | -59.21070008 |
| D14 | 61.57625895 |
| D15 | 153.34524441 |
| D16 | 58.21697803 |
| D17 | 177.78062874 |
| D18 | -62.67782159 |
| D19 | -163.03765445 |
| D20 | 172.41195369 |
| D21 | -68.38335850 |
| D22 | 51.83685414 |
| D23 | -76.05280088 |
| D24 | -79.47633929 |
| D25 | -51.62608081 |
| D26 | 69.09725425 |
| D27 | -170.85021729 |
| D28 | 54.04164616 |
| D29 | -91.65146504 |
| D30 | 28.77598499 |
| D31 | 149.10903180 |

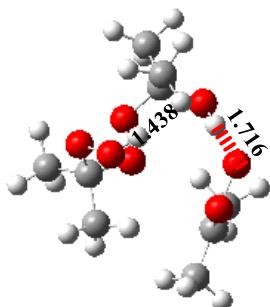
D32 165.53981495

D33 -34.21983325

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 35.19 | 52.52 | 67.69 | 82.09 | 106.38 | 120.22 | 141.20 | 174.84 | 187.80 | 217.51 | 223.81 |
| 232.67 | 250.58 | 262.79 | 270.39 | 287.64 | 297.40 | 305.39 | 327.61 | 350.23 | 358.14 | |
| 373.32 | 380.66 | 389.51 | 407.48 | 424.38 | 439.91 | 460.67 | 479.14 | 534.41 | 574.94 | |
| 591.73 | 602.52 | 614.80 | 631.03 | 812.69 | 831.22 | 866.23 | 904.55 | 912.93 | 917.10 | |
| 944.54 | 951.53 | 955.12 | 962.19 | 982.34 | 1017.03 | 1023.89 | 1028.26 | 1034.90 | 1049.24 | |
| 1062.07 | 1068.97 | 1154.05 | 1193.73 | 1225.50 | 1238.57 | 1250.82 | 1256.09 | 1277.48 | | |
| 1297.91 | 1323.02 | 1381.99 | 1407.67 | 1411.79 | 1413.28 | 1415.20 | 1420.52 | 1437.30 | | |
| 1448.62 | 1478.20 | 1483.22 | 1486.00 | 1486.67 | 1488.83 | 1495.03 | 1496.84 | 1499.46 | | |
| 1507.70 | 1510.76 | 1513.43 | 1525.90 | 3057.21 | 3074.19 | 3076.02 | 3077.42 | 3078.92 | | |
| 3081.03 | 3137.17 | 3153.42 | 3156.08 | 3158.14 | 3159.73 | 3161.30 | 3162.75 | 3167.21 | | |
| 3168.14 | 3169.99 | 3170.10 | 3170.91 | 3799.00 | 3878.96 | | | | | |

Rotational constants (B/GHZ): 0.7749678 0.3589879 0.2955461



IM8b

| C | | B1 | | | | |
|---|----|-----|----|-----|----|-------|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 0 |
| C | 1 | B5 | 2 | A4 | 3 | D3 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 0 |
| H | 6 | B7 | 1 | A6 | 2 | D5 0 |
| H | 6 | B8 | 1 | A7 | 2 | D6 0 |
| O | 1 | B9 | 2 | A8 | 6 | D7 0 |
| H | 10 | B10 | 1 | A9 | 2 | D8 0 |
| C | 10 | B11 | 1 | A10 | 2 | D9 0 |
| C | 12 | B12 | 10 | A11 | 1 | D10 0 |
| H | 13 | B13 | 12 | A12 | 10 | D11 0 |
| H | 13 | B14 | 12 | A13 | 10 | D12 0 |
| H | 13 | B15 | 12 | A14 | 10 | D13 0 |
| C | 12 | B16 | 10 | A15 | 1 | D14 0 |
| H | 17 | B17 | 12 | A16 | 10 | D15 0 |
| H | 17 | B18 | 12 | A17 | 10 | D16 0 |
| H | 17 | B19 | 12 | A18 | 10 | D17 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 12 | B20 | 10 | A19 | 1 | D18 | 0 |
| O | 12 | B21 | 10 | A20 | 1 | D19 | 0 |
| O | 1 | B22 | 10 | A21 | 2 | D20 | 0 |
| O | 23 | B23 | 1 | A22 | 10 | D21 | 0 |
| C | 24 | B24 | 23 | A23 | 1 | D22 | 0 |
| C | 25 | B25 | 24 | A24 | 23 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 24 | D24 | 0 |
| H | 26 | B27 | 25 | A26 | 24 | D25 | 0 |
| H | 26 | B28 | 25 | A27 | 24 | D26 | 0 |
| C | 25 | B29 | 24 | A28 | 23 | D27 | 0 |
| H | 30 | B30 | 25 | A29 | 24 | D28 | 0 |
| H | 30 | B31 | 25 | A30 | 24 | D29 | 0 |
| H | 30 | B32 | 25 | A31 | 24 | D30 | 0 |
| O | 25 | B33 | 24 | A32 | 23 | D31 | 0 |
| O | 34 | B34 | 25 | A33 | 24 | D32 | 0 |
| H | 35 | B35 | 34 | A34 | 25 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.51730555 |
| B2 | 1.08753630 |
| B3 | 1.08821852 |
| B4 | 1.08825952 |
| B5 | 1.52213938 |
| B6 | 1.08865668 |
| B7 | 1.08914895 |
| B8 | 1.09109496 |
| B9 | 1.38278939 |
| B10 | 0.98397369 |
| B11 | 3.69130209 |
| B12 | 1.48428764 |
| B13 | 1.08552829 |
| B14 | 1.09041186 |
| B15 | 1.09187943 |
| B16 | 1.47094734 |
| B17 | 1.09510810 |
| B18 | 1.09051260 |
| B19 | 1.08595366 |
| B20 | 2.25855798 |
| B21 | 1.24905942 |
| B22 | 1.43778211 |
| B23 | 1.42421409 |
| B24 | 1.41913110 |
| B25 | 1.51768533 |
| B26 | 1.08655121 |
| B27 | 1.08799923 |

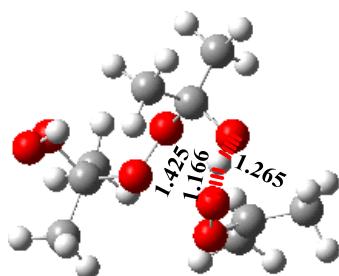
| | |
|-----|---------------|
| B28 | 1.08841320 |
| B29 | 1.51729775 |
| B30 | 1.08565126 |
| B31 | 1.08804648 |
| B32 | 1.08786489 |
| B33 | 1.40961621 |
| B34 | 1.41339449 |
| B35 | 0.96683142 |
| A1 | 108.55230834 |
| A2 | 109.51274678 |
| A3 | 110.74233419 |
| A4 | 112.64674933 |
| A5 | 108.84609217 |
| A6 | 110.95741928 |
| A7 | 109.34473611 |
| A8 | 108.60548826 |
| A9 | 108.84205278 |
| A10 | 110.46461269 |
| A11 | 153.28763450 |
| A12 | 111.47098701 |
| A13 | 109.09653828 |
| A14 | 108.60103925 |
| A15 | 54.91445558 |
| A16 | 108.38977903 |
| A17 | 109.36970677 |
| A18 | 110.67011323 |
| A19 | 46.68262382 |
| A20 | 74.01286267 |
| A21 | 110.57504946 |
| A22 | 109.92105939 |
| A23 | 108.51280392 |
| A24 | 104.52721952 |
| A25 | 110.66731027 |
| A26 | 108.83549142 |
| A27 | 109.32502593 |
| A28 | 112.80752640 |
| A29 | 110.54120271 |
| A30 | 109.32300830 |
| A31 | 109.05347636 |
| A32 | 110.46673031 |
| A33 | 109.93582435 |
| A34 | 102.51828441 |
| D1 | 118.81408731 |
| D2 | -120.27556037 |

| | |
|-----|---------------|
| D3 | 64.01965328 |
| D4 | -49.13747622 |
| D5 | 71.13314538 |
| D6 | -165.72416520 |
| D7 | -123.56162073 |
| D8 | 168.41992115 |
| D9 | -151.64813968 |
| D10 | 42.01211735 |
| D11 | -102.13017764 |
| D12 | 19.93586893 |
| D13 | 136.53039638 |
| D14 | 135.11863361 |
| D15 | -38.56074792 |
| D16 | 76.51097647 |
| D17 | -159.53642966 |
| D18 | -94.65697155 |
| D19 | -74.11807770 |
| D20 | 111.11953106 |
| D21 | 65.26394781 |
| D22 | 132.82810384 |
| D23 | 164.24013634 |
| D24 | 47.83190920 |
| D25 | 167.12361888 |
| D26 | -73.63810326 |
| D27 | 41.45546951 |
| D28 | -72.96493746 |
| D29 | 46.95950645 |
| D30 | 166.79861019 |
| D31 | -74.87410950 |
| D32 | -70.85260150 |
| D33 | 82.57674467 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 19.72 | 45.50 | 63.58 | 77.53 | 101.46 | 119.94 | 120.62 | 135.30 | 153.59 | 161.32 | 177.59 |
| 215.19 | 217.19 | 230.42 | 245.52 | 268.74 | 279.63 | 305.94 | 316.87 | 321.59 | 343.91 | |
| 351.83 | 368.93 | 378.22 | 383.61 | 390.14 | 420.81 | 459.00 | 469.70 | 493.40 | 544.28 | |
| 598.34 | 604.42 | 613.40 | 626.45 | 811.61 | 826.61 | 843.75 | 898.24 | 900.81 | 912.08 | |
| 920.97 | 950.32 | 952.99 | 962.96 | 970.92 | 992.61 | 1018.34 | 1026.79 | 1036.42 | 1055.70 | |
| 1067.65 | 1096.57 | 1104.16 | 1191.38 | 1210.39 | 1240.68 | 1252.47 | 1287.65 | 1311.21 | | |
| 1321.87 | 1386.91 | 1399.20 | 1407.79 | 1411.27 | 1413.10 | 1416.04 | 1428.06 | 1456.32 | | |
| 1466.07 | 1470.94 | 1473.39 | 1480.88 | 1490.19 | 1491.80 | 1496.44 | 1498.67 | 1499.64 | | |
| 1514.55 | 1525.87 | 1546.27 | 1665.24 | 3044.69 | 3051.35 | 3056.55 | 3073.32 | 3073.89 | | |
| 3077.57 | 3109.36 | 3123.00 | 3129.90 | 3149.12 | 3153.44 | 3159.14 | 3159.29 | 3160.07 | | |
| 3167.22 | 3170.50 | 3175.33 | 3176.69 | 3345.74 | 3803.56 | | | | | |

Rotational constants (B/GHZ): 0.5626837 0.4730170 0.3462310



TS8b

| C | | B1 | | | | |
|---|----|-----|----|-----|----|-------|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| H | 2 | B4 | 1 | A3 | 3 | D2 0 |
| C | 1 | B5 | 2 | A4 | 3 | D3 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 0 |
| H | 6 | B7 | 1 | A6 | 2 | D5 0 |
| H | 6 | B8 | 1 | A7 | 2 | D6 0 |
| O | 1 | B9 | 2 | A8 | 6 | D7 0 |
| H | 10 | B10 | 1 | A9 | 2 | D8 0 |
| C | 10 | B11 | 1 | A10 | 2 | D9 0 |
| C | 12 | B12 | 10 | A11 | 1 | D10 0 |
| H | 13 | B13 | 12 | A12 | 10 | D11 0 |
| H | 13 | B14 | 12 | A13 | 10 | D12 0 |
| H | 13 | B15 | 12 | A14 | 10 | D13 0 |
| C | 12 | B16 | 10 | A15 | 1 | D14 0 |
| H | 17 | B17 | 12 | A16 | 10 | D15 0 |
| H | 17 | B18 | 12 | A17 | 10 | D16 0 |
| H | 17 | B19 | 12 | A18 | 10 | D17 0 |
| O | 12 | B20 | 10 | A19 | 1 | D18 0 |
| O | 12 | B21 | 10 | A20 | 1 | D19 0 |
| O | 1 | B22 | 10 | A21 | 12 | D20 0 |
| O | 23 | B23 | 1 | A22 | 10 | D21 0 |
| C | 24 | B24 | 23 | A23 | 1 | D22 0 |
| C | 25 | B25 | 24 | A24 | 23 | D23 0 |
| H | 26 | B26 | 25 | A25 | 24 | D24 0 |
| H | 26 | B27 | 25 | A26 | 24 | D25 0 |
| H | 26 | B28 | 25 | A27 | 24 | D26 0 |
| C | 25 | B29 | 24 | A28 | 23 | D27 0 |
| H | 30 | B30 | 25 | A29 | 24 | D28 0 |
| H | 30 | B31 | 25 | A30 | 24 | D29 0 |
| H | 30 | B32 | 25 | A31 | 24 | D30 0 |
| O | 25 | B33 | 24 | A32 | 23 | D31 0 |
| O | 34 | B34 | 25 | A33 | 24 | D32 0 |
| H | 35 | B35 | 34 | A34 | 25 | D33 0 |

Variables:

| | |
|-----|--------------|
| B1 | 1.52311122 |
| B2 | 1.08792015 |
| B3 | 1.08890482 |
| B4 | 1.08871281 |
| B5 | 1.52443625 |
| B6 | 1.08894247 |
| B7 | 1.09114024 |
| B8 | 1.09071869 |
| B9 | 1.37844482 |
| B10 | 1.26474017 |
| B11 | 2.11126607 |
| B12 | 1.48392616 |
| B13 | 1.08537033 |
| B14 | 1.09152395 |
| B15 | 1.08883726 |
| B16 | 1.48726939 |
| B17 | 1.08569335 |
| B18 | 1.08140113 |
| B19 | 1.09494215 |
| B20 | 2.21735200 |
| B21 | 1.28387695 |
| B22 | 1.43599161 |
| B23 | 1.42466020 |
| B24 | 1.41440086 |
| B25 | 1.51811281 |
| B26 | 1.08631163 |
| B27 | 1.08790780 |
| B28 | 1.08852627 |
| B29 | 1.51768793 |
| B30 | 1.08607332 |
| B31 | 1.08871949 |
| B32 | 1.08780449 |
| B33 | 1.41106207 |
| B34 | 1.41386529 |
| B35 | 0.96576667 |
| A1 | 108.53875156 |
| A2 | 109.31928944 |
| A3 | 111.20129083 |
| A4 | 111.83431201 |
| A5 | 109.10407124 |
| A6 | 110.26755974 |
| A7 | 109.78585561 |
| A8 | 109.55982742 |

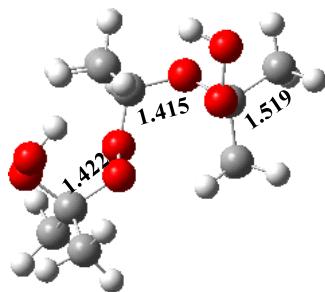
| | |
|-----|---------------|
| A9 | 116.07977239 |
| A10 | 129.18316204 |
| A11 | 112.46972470 |
| A12 | 110.68715916 |
| A13 | 106.66476645 |
| A14 | 110.05931375 |
| A15 | 87.24502451 |
| A16 | 109.36259769 |
| A17 | 112.55838544 |
| A18 | 105.57705711 |
| A19 | 66.22840656 |
| A20 | 91.29908197 |
| A21 | 111.54922700 |
| A22 | 108.86819868 |
| A23 | 108.83353981 |
| A24 | 103.94587119 |
| A25 | 110.76087281 |
| A26 | 109.00605355 |
| A27 | 109.37558585 |
| A28 | 112.63837078 |
| A29 | 110.56796248 |
| A30 | 109.13748839 |
| A31 | 109.26178416 |
| A32 | 110.57757803 |
| A33 | 109.95669524 |
| A34 | 102.21718438 |
| D1 | 118.44720802 |
| D2 | -120.60821959 |
| D3 | 65.31075318 |
| D4 | -55.38804774 |
| D5 | 64.07812490 |
| D6 | -173.33939667 |
| D7 | -123.91355848 |
| D8 | 146.59506370 |
| D9 | -126.44651589 |
| D10 | 36.45982770 |
| D11 | -104.56072470 |
| D12 | 13.33428715 |
| D13 | 131.44620027 |
| D14 | 156.78344929 |
| D15 | -67.42059270 |
| D16 | 55.89507138 |
| D17 | 175.68219676 |
| D18 | -107.97262289 |

| | |
|-----|--------------|
| D19 | -80.45505311 |
| D20 | -14.54368603 |
| D21 | 68.08310616 |
| D22 | 140.38632200 |
| D23 | 166.73471982 |
| D24 | 45.57129973 |
| D25 | 165.50378954 |
| D26 | -74.97922056 |
| D27 | 44.02507780 |
| D28 | -71.99029807 |
| D29 | 47.99484361 |
| D30 | 167.56961025 |
| D31 | -71.99363305 |
| D32 | -70.40935930 |
| D33 | 86.32197881 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 858.84 <i>i</i> | 29.25 | 37.32 | 59.11 | 98.11 | 119.17 | 134.06 | 156.53 | 180.63 | 196.45 | 213.34 |
| 220.55 | 231.58 | 234.18 | 248.37 | 252.54 | 274.41 | 279.20 | 283.47 | 316.74 | 336.06 | |
| 352.19 | 365.32 | 372.55 | 391.36 | 394.97 | 418.61 | 460.51 | 491.85 | 503.18 | 544.83 | |
| 598.84 | 607.42 | 619.36 | 622.04 | 703.15 | 810.33 | 817.75 | 853.51 | 903.22 | 911.62 | |
| 938.90 | 957.46 | 957.72 | 966.40 | 971.01 | 995.53 | 1017.02 | 1024.19 | 1030.71 | 1053.53 | |
| 1067.01 | 1087.27 | 1098.67 | 1197.64 | 1219.09 | 1250.44 | 1252.88 | 1283.26 | 1310.38 | | |
| 1323.85 | 1385.57 | 1393.79 | 1406.50 | 1410.25 | 1414.13 | 1419.80 | 1424.14 | 1430.79 | | |
| 1452.03 | 1465.63 | 1473.08 | 1481.03 | 1485.60 | 1485.92 | 1491.15 | 1494.27 | 1495.36 | | |
| 1500.31 | 1506.12 | 1534.21 | 1575.03 | 1921.67 | 3037.62 | 3054.54 | 3063.18 | 3068.37 | | |
| 3070.25 | 3073.02 | 3120.20 | 3130.06 | 3134.82 | 3147.51 | 3149.51 | 3153.36 | 3156.27 | | |
| 3162.19 | 3165.80 | 3166.68 | 3176.02 | 3214.90 | 3817.74 | | | | | |

Rotational constants (B/GHZ): 0.7279719 0.3936212 0.3535498



P8b

| | | | | | | | |
|---|---|----|---|----|---|----|---|
| C | | | | | | | |
| C | 1 | B1 | | | | | |
| H | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | B4 | 1 | A3 | 4 | D2 | 0 |
| C | 1 | B5 | 2 | A4 | 3 | D3 | 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 6 | B7 | 1 | A6 | 2 | D5 | 0 |
| H | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| O | 1 | B9 | 6 | A8 | 2 | D7 | 0 |
| H | 6 | B10 | 1 | A9 | 10 | D8 | 0 |
| C | 10 | B11 | 1 | A10 | 6 | D9 | 0 |
| C | 12 | B12 | 10 | A11 | 1 | D10 | 0 |
| H | 13 | B13 | 12 | A12 | 10 | D11 | 0 |
| H | 13 | B14 | 12 | A13 | 10 | D12 | 0 |
| H | 13 | B15 | 12 | A14 | 10 | D13 | 0 |
| C | 12 | B16 | 10 | A15 | 1 | D14 | 0 |
| H | 17 | B17 | 12 | A16 | 10 | D15 | 0 |
| H | 17 | B18 | 12 | A17 | 10 | D16 | 0 |
| H | 17 | B19 | 12 | A18 | 10 | D17 | 0 |
| O | 12 | B20 | 10 | A19 | 1 | D18 | 0 |
| O | 21 | B21 | 12 | A20 | 10 | D19 | 0 |
| O | 1 | B22 | 10 | A21 | 12 | D20 | 0 |
| O | 23 | B23 | 1 | A22 | 10 | D21 | 0 |
| C | 24 | B24 | 23 | A23 | 1 | D22 | 0 |
| C | 25 | B25 | 24 | A24 | 23 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 24 | D24 | 0 |
| H | 26 | B27 | 25 | A26 | 24 | D25 | 0 |
| H | 26 | B28 | 25 | A27 | 24 | D26 | 0 |
| C | 25 | B29 | 24 | A28 | 23 | D27 | 0 |
| H | 30 | B30 | 25 | A29 | 24 | D28 | 0 |
| H | 30 | B31 | 25 | A30 | 24 | D29 | 0 |
| H | 30 | B32 | 25 | A31 | 24 | D30 | 0 |
| O | 25 | B33 | 24 | A32 | 23 | D31 | 0 |
| O | 34 | B34 | 25 | A33 | 24 | D32 | 0 |
| H | 35 | B35 | 34 | A34 | 25 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.52108106 |
| B2 | 1.08769472 |
| B3 | 1.08813701 |
| B4 | 1.08798034 |
| B5 | 1.52070302 |
| B6 | 1.09025078 |
| B7 | 1.09003681 |
| B8 | 1.08843790 |
| B9 | 1.41492568 |
| B10 | 2.47023965 |
| B11 | 1.41666094 |
| B12 | 1.52198207 |
| B13 | 1.08377634 |
| B14 | 1.08796481 |

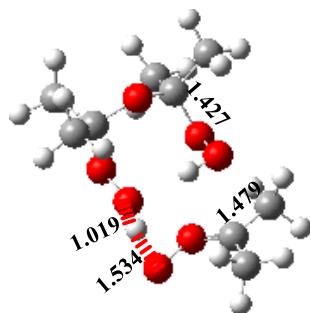
| | |
|-----|--------------|
| B15 | 1.08839260 |
| B16 | 1.51904027 |
| B17 | 1.08834640 |
| B18 | 1.08534959 |
| B19 | 1.08818908 |
| B20 | 2.32315013 |
| B21 | 1.41470646 |
| B22 | 1.41689474 |
| B23 | 1.42250691 |
| B24 | 1.42151250 |
| B25 | 1.51730254 |
| B26 | 1.08618309 |
| B27 | 1.08777258 |
| B28 | 1.08781546 |
| B29 | 1.51625901 |
| B30 | 1.08603262 |
| B31 | 1.08785495 |
| B32 | 1.08765782 |
| B33 | 1.41235739 |
| B34 | 1.41366128 |
| B35 | 0.96600246 |
| A1 | 109.31070787 |
| A2 | 109.19329888 |
| A3 | 110.04835237 |
| A4 | 111.20121293 |
| A5 | 108.29445314 |
| A6 | 109.15584829 |
| A7 | 111.06388448 |
| A8 | 112.00627143 |
| A9 | 96.23289555 |
| A10 | 125.46241953 |
| A11 | 114.35410162 |
| A12 | 111.80073692 |
| A13 | 108.73427053 |
| A14 | 108.65061308 |
| A15 | 104.48113588 |
| A16 | 108.86442221 |
| A17 | 110.89032831 |
| A18 | 109.34041552 |
| A19 | 96.31671829 |
| A20 | 34.91082502 |
| A21 | 113.15908449 |
| A22 | 113.02560960 |
| A23 | 108.92241075 |

| | |
|-----|---------------|
| A24 | 103.84240866 |
| A25 | 111.12419147 |
| A26 | 108.93954855 |
| A27 | 108.99134610 |
| A28 | 113.06219167 |
| A29 | 110.81806484 |
| A30 | 109.32332160 |
| A31 | 108.76555322 |
| A32 | 109.95160318 |
| A33 | 110.12981216 |
| A34 | 102.74891137 |
| D1 | 118.91213093 |
| D2 | 120.28062245 |
| D3 | 66.06279510 |
| D4 | -58.83208850 |
| D5 | 58.33177204 |
| D6 | -179.61039020 |
| D7 | 116.19334067 |
| D8 | -5.85427545 |
| D9 | 78.00356633 |
| D10 | 63.04843105 |
| D11 | -76.47332812 |
| D12 | 44.37250652 |
| D13 | 163.16909214 |
| D14 | -175.59711866 |
| D15 | -70.65266744 |
| D16 | 49.31558708 |
| D17 | 169.88432471 |
| D18 | -87.18300858 |
| D19 | 118.25440408 |
| D20 | -50.39515208 |
| D21 | 92.89896189 |
| D22 | 129.05692073 |
| D23 | 161.17321314 |
| D24 | 45.65789719 |
| D25 | 165.62952361 |
| D26 | -74.72846648 |
| D27 | 38.41166245 |
| D28 | -73.44328505 |
| D29 | 46.80938158 |
| D30 | 166.39464136 |
| D31 | -77.73656278 |
| D32 | -72.42633099 |
| D33 | 81.07444508 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 28.23 | 42.40 | 74.24 | 115.10 | 140.50 | 148.25 | 159.71 | 189.20 | 214.41 | 217.94 | 232.82 |
| 239.34 | 241.76 | 250.21 | 266.53 | 270.41 | 286.45 | 314.55 | 321.62 | 333.60 | 339.83 | |
| 360.88 | 379.77 | 388.33 | 403.39 | 415.15 | 438.58 | 447.17 | 495.32 | 527.27 | 548.18 | |
| 604.55 | 615.94 | 621.38 | 643.82 | 779.34 | 821.04 | 838.52 | 890.58 | 894.69 | 933.57 | |
| 950.91 | 961.47 | 966.26 | 970.35 | 975.73 | 1024.39 | 1027.03 | 1032.71 | 1053.26 | 1056.32 | |
| 1065.31 | 1079.79 | 1175.96 | 1210.05 | 1233.84 | 1248.24 | 1254.56 | 1258.29 | 1275.70 | | |
| 1304.74 | 1320.40 | 1394.68 | 1412.88 | 1415.77 | 1417.04 | 1424.67 | 1425.16 | 1426.73 | | |
| 1436.89 | 1481.32 | 1481.82 | 1486.27 | 1488.95 | 1491.14 | 1494.47 | 1496.78 | 1502.57 | | |
| 1508.79 | 1511.91 | 1521.02 | 1559.45 | 3057.83 | 3070.33 | 3077.56 | 3079.14 | 3081.37 | | |
| 3081.81 | 3132.45 | 3152.83 | 3152.93 | 3157.78 | 3158.19 | 3158.86 | 3162.39 | 3165.99 | | |
| 3172.71 | 3179.18 | 3179.39 | 3202.62 | 3807.51 | 3810.42 | | | | | |

Rotational constants (B/GHZ): 0.8346450 0.3441726 0.3375178



IM8c

| C | | | | | | | |
|---|----|--|-----|----|-----|----|-------|
| O | 1 | | B1 | | | | |
| O | 2 | | B2 | 1 | A1 | | |
| H | 2 | | B3 | 1 | A2 | 3 | D1 0 |
| C | 2 | | B4 | 1 | A3 | 3 | D2 0 |
| O | 5 | | B5 | 2 | A4 | 1 | D3 0 |
| O | 5 | | B6 | 2 | A5 | 1 | D4 0 |
| C | 1 | | B7 | 3 | A6 | 2 | D5 0 |
| H | 8 | | B8 | 1 | A7 | 3 | D6 0 |
| H | 8 | | B9 | 1 | A8 | 3 | D7 0 |
| H | 8 | | B10 | 1 | A9 | 3 | D8 0 |
| O | 1 | | B11 | 3 | A10 | 2 | D9 0 |
| C | 12 | | B12 | 1 | A11 | 3 | D10 0 |
| C | 13 | | B13 | 12 | A12 | 1 | D11 0 |
| H | 14 | | B14 | 13 | A13 | 12 | D12 0 |
| H | 14 | | B15 | 13 | A14 | 12 | D13 0 |
| H | 14 | | B16 | 13 | A15 | 12 | D14 0 |
| O | 13 | | B17 | 12 | A16 | 1 | D15 0 |
| O | 18 | | B18 | 13 | A17 | 12 | D16 0 |
| H | 19 | | B19 | 18 | A18 | 13 | D17 0 |
| C | 5 | | B20 | 2 | A19 | 1 | D18 0 |
| H | 21 | | B21 | 5 | A20 | 2 | D19 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 21 | B22 | 5 | A21 | 2 | D20 | 0 |
| H | 21 | B23 | 5 | A22 | 2 | D21 | 0 |
| C | 5 | B24 | 2 | A23 | 1 | D22 | 0 |
| H | 25 | B25 | 5 | A24 | 2 | D23 | 0 |
| H | 25 | B26 | 5 | A25 | 2 | D24 | 0 |
| H | 25 | B27 | 5 | A26 | 2 | D25 | 0 |
| C | 1 | B28 | 12 | A27 | 13 | D26 | 0 |
| H | 29 | B29 | 1 | A28 | 12 | D27 | 0 |
| H | 29 | B30 | 1 | A29 | 12 | D28 | 0 |
| H | 29 | B31 | 1 | A30 | 12 | D29 | 0 |
| C | 13 | B32 | 12 | A31 | 1 | D30 | 0 |
| H | 33 | B33 | 13 | A32 | 12 | D31 | 0 |
| H | 33 | B34 | 13 | A33 | 12 | D32 | 0 |
| H | 33 | B35 | 13 | A34 | 12 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 2.32959602 |
| B2 | 1.41521699 |
| B3 | 0.97918966 |
| B4 | 2.83161492 |
| B5 | 2.24648820 |
| B6 | 1.24849208 |
| B7 | 1.52074551 |
| B8 | 1.08852128 |
| B9 | 1.08700022 |
| B10 | 1.08790118 |
| B11 | 1.40210153 |
| B12 | 1.42408078 |
| B13 | 1.52050410 |
| B14 | 1.08855169 |
| B15 | 1.08821171 |
| B16 | 1.08541224 |
| B17 | 1.39871734 |
| B18 | 1.42701766 |
| B19 | 1.01878173 |
| B20 | 1.47934639 |
| B21 | 1.08509235 |
| B22 | 1.09033112 |
| B23 | 1.09160887 |
| B24 | 1.47542341 |
| B25 | 1.08914942 |
| B26 | 1.09236565 |
| B27 | 1.08508648 |
| B28 | 1.51835671 |
| B29 | 1.08858772 |

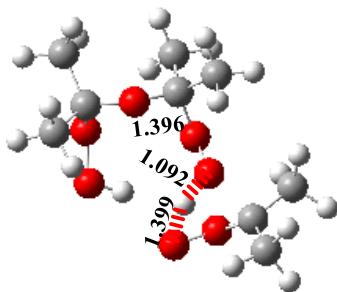
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|-----|---------------|
| B30 | 1.08847610 |
| B31 | 1.08673219 |
| B32 | 1.52541985 |
| B33 | 1.08845739 |
| B34 | 1.08522394 |
| B35 | 1.08804755 |
| A1 | 35.12038183 |
| A2 | 92.64429255 |
| A3 | 114.33643778 |
| A4 | 96.75800277 |
| A5 | 98.39289513 |
| A6 | 102.12785376 |
| A7 | 108.73581122 |
| A8 | 110.64113542 |
| A9 | 109.94217777 |
| A10 | 111.12502653 |
| A11 | 124.75520708 |
| A12 | 104.14800820 |
| A13 | 109.16600840 |
| A14 | 109.31121697 |
| A15 | 110.44313103 |
| A16 | 112.25533008 |
| A17 | 108.75730292 |
| A18 | 100.64023145 |
| A19 | 86.97922862 |
| A20 | 110.89962272 |
| A21 | 107.75270351 |
| A22 | 108.96305891 |
| A23 | 87.01408433 |
| A24 | 109.15975057 |
| A25 | 108.15046917 |
| A26 | 110.75813024 |
| A27 | 104.74542722 |
| A28 | 109.77801424 |
| A29 | 109.59962925 |
| A30 | 109.54931457 |
| A31 | 113.36892692 |
| A32 | 108.98562674 |
| A33 | 112.14718280 |
| A34 | 109.00138550 |
| D1 | -102.57867790 |
| D2 | -12.06866456 |
| D3 | -76.77576482 |
| D4 | -42.83744379 |

| | |
|-----|---------------|
| D5 | -178.48203379 |
| D6 | -66.68401384 |
| D7 | 52.53795174 |
| D8 | 174.37025970 |
| D9 | -53.79149656 |
| D10 | -70.46274827 |
| D11 | 165.08507380 |
| D12 | 67.96901279 |
| D13 | -172.19531797 |
| D14 | -51.96852848 |
| D15 | 43.18470503 |
| D16 | 69.05323071 |
| D17 | -171.01351873 |
| D18 | 73.36305119 |
| D19 | -96.01937674 |
| D20 | 24.36911091 |
| D21 | 141.70988394 |
| D22 | -163.37316201 |
| D23 | 42.89642844 |
| D24 | 157.73219746 |
| D25 | -79.73404355 |
| D26 | 170.23807743 |
| D27 | 174.15987847 |
| D28 | -65.65525212 |
| D29 | 53.92295213 |
| D30 | -74.73515991 |
| D31 | -41.25640360 |
| D32 | 80.21041861 |
| D33 | -160.05861183 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 32.34 | 42.10 | 60.68 | 93.21 | 103.23 | 127.24 | 147.04 | 175.73 | 184.94 | 197.03 | 215.97 |
| 230.55 | 239.86 | 246.66 | 266.32 | 271.71 | 282.08 | 302.77 | 311.46 | 331.79 | 341.77 | |
| 350.69 | 364.49 | 379.98 | 386.96 | 410.98 | 428.08 | 471.94 | 491.51 | 507.00 | 585.94 | |
| 603.30 | 609.06 | 649.25 | 736.61 | 779.44 | 826.97 | 837.17 | 887.92 | 919.13 | 923.16 | |
| 942.15 | 948.28 | 960.14 | 964.61 | 994.64 | 1015.64 | 1025.04 | 1056.21 | 1065.03 | 1072.16 | |
| 1087.69 | 1104.81 | 1116.46 | 1181.62 | 1226.69 | 1259.13 | 1263.17 | 1265.48 | 1312.39 | | |
| 1320.58 | 1396.06 | 1403.19 | 1409.26 | 1414.50 | 1415.25 | 1419.91 | 1452.01 | 1468.82 | | |
| 1471.57 | 1474.87 | 1479.82 | 1485.79 | 1489.35 | 1492.12 | 1495.00 | 1501.13 | 1511.39 | | |
| 1527.01 | 1532.55 | 1584.09 | 1671.59 | 2771.51 | 3058.53 | 3063.41 | 3068.00 | 3071.74 | | |
| 3072.94 | 3079.92 | 3134.59 | 3136.55 | 3143.21 | 3148.85 | 3149.89 | 3155.07 | 3161.78 | | |
| 3170.22 | 3174.60 | 3181.46 | 3182.48 | 3182.84 | 3555.21 | | | | | |

Rotational constants (B/GHZ): 0.7505620 0.3992725 0.3239009



TS8c

C

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 1 | B1 | | | | | |
| O | 2 | B2 | 1 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| C | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| O | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| O | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| C | 1 | B7 | 3 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 1 | A7 | 3 | D6 | 0 |
| H | 8 | B9 | 1 | A8 | 3 | D7 | 0 |
| H | 8 | B10 | 1 | A9 | 3 | D8 | 0 |
| O | 1 | B11 | 3 | A10 | 2 | D9 | 0 |
| C | 12 | B12 | 1 | A11 | 3 | D10 | 0 |
| C | 13 | B13 | 12 | A12 | 1 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 12 | D12 | 0 |
| H | 14 | B15 | 13 | A14 | 12 | D13 | 0 |
| H | 14 | B16 | 13 | A15 | 12 | D14 | 0 |
| O | 13 | B17 | 12 | A16 | 1 | D15 | 0 |
| O | 18 | B18 | 13 | A17 | 12 | D16 | 0 |
| H | 19 | B19 | 18 | A18 | 13 | D17 | 0 |
| C | 5 | B20 | 2 | A19 | 1 | D18 | 0 |
| H | 21 | B21 | 5 | A20 | 2 | D19 | 0 |
| H | 21 | B22 | 5 | A21 | 2 | D20 | 0 |
| H | 21 | B23 | 5 | A22 | 2 | D21 | 0 |
| C | 5 | B24 | 2 | A23 | 1 | D22 | 0 |
| H | 25 | B25 | 5 | A24 | 2 | D23 | 0 |
| H | 25 | B26 | 5 | A25 | 2 | D24 | 0 |
| H | 25 | B27 | 5 | A26 | 2 | D25 | 0 |
| C | 1 | B28 | 12 | A27 | 13 | D26 | 0 |
| H | 29 | B29 | 1 | A28 | 12 | D27 | 0 |
| H | 29 | B30 | 1 | A29 | 12 | D28 | 0 |
| H | 29 | B31 | 1 | A30 | 12 | D29 | 0 |
| C | 13 | B32 | 12 | A31 | 1 | D30 | 0 |
| H | 33 | B33 | 13 | A32 | 12 | D31 | 0 |
| H | 33 | B34 | 13 | A33 | 12 | D32 | 0 |

| | | | | | | | |
|------------|----|--------------|----|-----|----|-----|---|
| H | 33 | B35 | 13 | A34 | 12 | D33 | 0 |
| Variables: | | | | | | | |
| B1 | | 2.32648613 | | | | | |
| B2 | | 1.41738595 | | | | | |
| B3 | | 1.09149944 | | | | | |
| B4 | | 2.00224386 | | | | | |
| B5 | | 2.21670860 | | | | | |
| B6 | | 1.28481768 | | | | | |
| B7 | | 1.52291801 | | | | | |
| B8 | | 1.08833646 | | | | | |
| B9 | | 1.08675781 | | | | | |
| B10 | | 1.08754282 | | | | | |
| B11 | | 1.39571195 | | | | | |
| B12 | | 1.42590677 | | | | | |
| B13 | | 1.51801877 | | | | | |
| B14 | | 1.08874625 | | | | | |
| B15 | | 1.08819965 | | | | | |
| B16 | | 1.08490281 | | | | | |
| B17 | | 1.40611799 | | | | | |
| B18 | | 1.41439036 | | | | | |
| B19 | | 0.97237818 | | | | | |
| B20 | | 1.48635909 | | | | | |
| B21 | | 1.08542015 | | | | | |
| B22 | | 1.09008289 | | | | | |
| B23 | | 1.08988697 | | | | | |
| B24 | | 1.49164444 | | | | | |
| B25 | | 1.08348617 | | | | | |
| B26 | | 1.09339191 | | | | | |
| B27 | | 1.08677495 | | | | | |
| B28 | | 1.51921203 | | | | | |
| B29 | | 1.08933378 | | | | | |
| B30 | | 1.08837463 | | | | | |
| B31 | | 1.08601933 | | | | | |
| B32 | | 1.52626289 | | | | | |
| B33 | | 1.08853531 | | | | | |
| B34 | | 1.08550090 | | | | | |
| B35 | | 1.08818416 | | | | | |
| A1 | | 35.40824852 | | | | | |
| A2 | | 116.23681098 | | | | | |
| A3 | | 134.42374622 | | | | | |
| A4 | | 68.98207957 | | | | | |
| A5 | | 92.14321540 | | | | | |
| A6 | | 102.00527841 | | | | | |
| A7 | | 108.55949301 | | | | | |

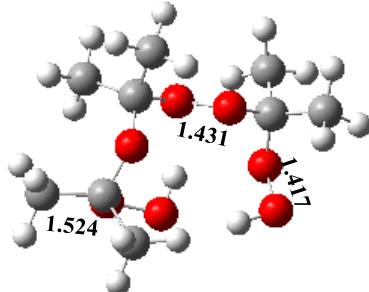
| | |
|-----|---------------|
| A8 | 111.06909875 |
| A9 | 109.61160946 |
| A10 | 110.60903860 |
| A11 | 123.99810037 |
| A12 | 104.31702037 |
| A13 | 108.91997757 |
| A14 | 109.46316248 |
| A15 | 110.24283053 |
| A16 | 112.81261124 |
| A17 | 110.49838473 |
| A18 | 104.44915380 |
| A19 | 106.79011332 |
| A20 | 110.59972278 |
| A21 | 107.62521746 |
| A22 | 109.89545465 |
| A23 | 92.33306011 |
| A24 | 111.96457236 |
| A25 | 106.34782307 |
| A26 | 109.78760126 |
| A27 | 105.43061293 |
| A28 | 110.03687375 |
| A29 | 109.08892875 |
| A30 | 109.98932895 |
| A31 | 112.54676471 |
| A32 | 109.24082564 |
| A33 | 112.08555237 |
| A34 | 108.93152600 |
| D1 | -69.86389231 |
| D2 | 27.31618746 |
| D3 | -107.29352319 |
| D4 | -77.64410753 |
| D5 | 170.37493596 |
| D6 | -63.75450038 |
| D7 | 56.00408926 |
| D8 | 177.72018241 |
| D9 | -64.71343679 |
| D10 | -78.89181326 |
| D11 | 162.55443712 |
| D12 | 67.61432415 |
| D13 | -172.65661426 |
| D14 | -52.39603285 |
| D15 | 39.99070599 |
| D16 | 77.51162135 |
| D17 | -109.19827224 |

| | |
|-----|---------------|
| D18 | 38.48480249 |
| D19 | -90.82503641 |
| D20 | 28.70778614 |
| D21 | 146.41503014 |
| D22 | 159.96138145 |
| D23 | 57.73554553 |
| D24 | 176.61333723 |
| D25 | -66.03211678 |
| D26 | 161.47634526 |
| D27 | 171.49817215 |
| D28 | -68.83103721 |
| D29 | 50.59971499 |
| D30 | -77.45406524 |
| D31 | -40.28043677 |
| D32 | 81.37142968 |
| D33 | -159.29221066 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 478.38 <i>i</i> | 35.08 | 50.29 | 69.75 | 100.91 | 106.67 | 132.65 | 155.98 | 171.92 | 192.13 | 193.49 |
| 212.36 | 222.87 | 236.58 | 246.70 | 264.24 | 301.98 | 322.38 | 326.03 | 338.89 | 345.40 | |
| 352.20 | 380.14 | 390.67 | 402.76 | 415.80 | 439.83 | 477.31 | 495.17 | 548.93 | 572.35 | |
| 582.39 | 610.01 | 633.00 | 652.94 | 776.21 | 819.62 | 836.71 | 890.10 | 926.59 | 943.66 | |
| 951.07 | 959.39 | 962.19 | 968.01 | 989.04 | 1021.84 | 1027.29 | 1039.86 | 1067.49 | 1078.19 | |
| 1082.69 | 1088.41 | 1170.35 | 1218.55 | 1246.65 | 1254.81 | 1268.76 | 1272.09 | 1314.22 | | |
| 1317.46 | 1401.36 | 1405.22 | 1410.99 | 1414.02 | 1418.08 | 1422.57 | 1427.37 | 1453.42 | | |
| 1462.05 | 1471.43 | 1478.06 | 1480.59 | 1488.41 | 1492.88 | 1496.46 | 1499.31 | 1502.87 | | |
| 1516.46 | 1531.51 | 1583.27 | 1632.26 | 2013.29 | 3063.81 | 3066.39 | 3070.11 | 3071.67 | | |
| 3079.88 | 3082.92 | 3142.02 | 3142.08 | 3145.65 | 3155.26 | 3156.75 | 3159.64 | 3171.13 | | |
| 3176.75 | 3179.48 | 3182.41 | 3182.53 | 3213.22 | 3687.43 | | | | | |

Rotational constants (B/GHZ): 0.8590051 0.3646711 0.3079698



P8c

| | | | | | | | |
|---|---|--|----|---|----|---|----|
| C | | | | | | | |
| O | 1 | | B1 | | | | |
| O | 1 | | B2 | 2 | A1 | | |
| H | 2 | | B3 | 1 | A2 | 3 | D1 |
| C | 2 | | B4 | 1 | A3 | 3 | D2 |
| O | 5 | | B5 | 2 | A4 | 1 | D3 |
| | | | | | | | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 5 | B6 | 2 | A5 | 1 | D4 | 0 |
| C | 1 | B7 | 3 | A6 | 2 | D5 | 0 |
| H | 8 | B8 | 1 | A7 | 3 | D6 | 0 |
| H | 8 | B9 | 1 | A8 | 3 | D7 | 0 |
| H | 8 | B10 | 1 | A9 | 3 | D8 | 0 |
| O | 1 | B11 | 3 | A10 | 2 | D9 | 0 |
| C | 12 | B12 | 1 | A11 | 3 | D10 | 0 |
| C | 13 | B13 | 12 | A12 | 1 | D11 | 0 |
| H | 14 | B14 | 13 | A13 | 12 | D12 | 0 |
| H | 14 | B15 | 13 | A14 | 12 | D13 | 0 |
| H | 14 | B16 | 13 | A15 | 12 | D14 | 0 |
| O | 13 | B17 | 12 | A16 | 1 | D15 | 0 |
| O | 18 | B18 | 13 | A17 | 12 | D16 | 0 |
| H | 19 | B19 | 18 | A18 | 13 | D17 | 0 |
| C | 5 | B20 | 2 | A19 | 1 | D18 | 0 |
| H | 21 | B21 | 5 | A20 | 2 | D19 | 0 |
| H | 21 | B22 | 5 | A21 | 2 | D20 | 0 |
| H | 21 | B23 | 5 | A22 | 2 | D21 | 0 |
| C | 5 | B24 | 2 | A23 | 1 | D22 | 0 |
| H | 25 | B25 | 5 | A24 | 2 | D23 | 0 |
| H | 25 | B26 | 5 | A25 | 2 | D24 | 0 |
| H | 25 | B27 | 5 | A26 | 2 | D25 | 0 |
| C | 1 | B28 | 12 | A27 | 13 | D26 | 0 |
| H | 29 | B29 | 1 | A28 | 12 | D27 | 0 |
| H | 29 | B30 | 1 | A29 | 12 | D28 | 0 |
| H | 29 | B31 | 1 | A30 | 12 | D29 | 0 |
| C | 13 | B32 | 12 | A31 | 1 | D30 | 0 |
| H | 33 | B33 | 13 | A32 | 12 | D31 | 0 |
| H | 33 | B34 | 13 | A33 | 12 | D32 | 0 |
| H | 33 | B35 | 13 | A34 | 12 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 2.30319829 |
| B2 | 1.43016996 |
| B3 | 2.81279029 |
| B4 | 1.40996294 |
| B5 | 2.31568951 |
| B6 | 1.41384865 |
| B7 | 1.52335628 |
| B8 | 1.08808936 |
| B9 | 1.08620588 |
| B10 | 1.08793409 |
| B11 | 1.39900735 |
| B12 | 1.42082666 |
| B13 | 1.51731637 |

| | |
|-----|--------------|
| B14 | 1.08830565 |
| B15 | 1.08819527 |
| B16 | 1.08628516 |
| B17 | 1.41012666 |
| B18 | 1.41206010 |
| B19 | 0.97203683 |
| B20 | 1.51757769 |
| B21 | 1.08658657 |
| B22 | 1.08813251 |
| B23 | 1.08750954 |
| B24 | 1.51682159 |
| B25 | 1.08590770 |
| B26 | 1.08807909 |
| B27 | 1.08773403 |
| B28 | 1.51970178 |
| B29 | 1.08865867 |
| B30 | 1.08825301 |
| B31 | 1.08538101 |
| B32 | 1.52362465 |
| B33 | 1.08797254 |
| B34 | 1.08638996 |
| B35 | 1.08815429 |
| A1 | 36.41996293 |
| A2 | 102.95257338 |
| A3 | 144.84159203 |
| A4 | 94.44126889 |
| A5 | 110.32711463 |
| A6 | 103.02870718 |
| A7 | 108.56713690 |
| A8 | 111.76633513 |
| A9 | 109.03065010 |
| A10 | 110.28797298 |
| A11 | 124.60580302 |
| A12 | 104.97669550 |
| A13 | 109.13674842 |
| A14 | 109.73420725 |
| A15 | 110.36514113 |
| A16 | 113.32577684 |
| A17 | 111.67793699 |
| A18 | 101.82424692 |
| A19 | 112.99879674 |
| A20 | 110.98836055 |
| A21 | 108.94098911 |
| A22 | 109.22400990 |

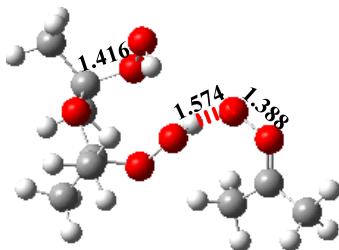
| | |
|-----|---------------|
| A23 | 103.91629696 |
| A24 | 110.50348967 |
| A25 | 108.69729456 |
| A26 | 109.52359046 |
| A27 | 105.40598437 |
| A28 | 109.76714375 |
| A29 | 108.90521843 |
| A30 | 110.23752723 |
| A31 | 111.77228323 |
| A32 | 108.73407221 |
| A33 | 111.45978398 |
| A34 | 109.58031539 |
| D1 | -80.78165207 |
| D2 | -2.28290853 |
| D3 | -99.03902231 |
| D4 | -66.80732091 |
| D5 | 170.02450629 |
| D6 | -63.94056787 |
| D7 | 56.55198250 |
| D8 | 177.97645021 |
| D9 | -64.94226943 |
| D10 | -76.97954870 |
| D11 | 153.66954162 |
| D12 | 66.95481769 |
| D13 | -173.11094312 |
| D14 | -52.02354573 |
| D15 | 30.77408800 |
| D16 | 69.54687540 |
| D17 | -96.47154429 |
| D18 | 49.39978250 |
| D19 | -70.97400319 |
| D20 | 49.13337442 |
| D21 | 168.67447484 |
| D22 | 172.42559678 |
| D23 | 48.27617800 |
| D24 | 167.84055732 |
| D25 | -72.51992023 |
| D26 | 163.60416377 |
| D27 | 168.43148043 |
| D28 | -71.85417564 |
| D29 | 47.75073479 |
| D30 | -85.41415721 |
| D31 | -46.41190321 |
| D32 | 74.26939422 |

D33 -165.80946040

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 38.59 | 54.32 | 101.03 | 130.44 | 139.83 | 169.26 | 179.48 | 198.40 | 210.10 | 213.68 | 219.31 |
| 227.22 | 239.93 | 256.20 | 277.59 | 285.90 | 293.36 | 321.93 | 326.99 | 347.61 | 358.65 | |
| 373.31 | 378.54 | 399.50 | 405.87 | 428.18 | 436.63 | 490.90 | 507.15 | 567.19 | 589.36 | |
| 600.77 | 608.55 | 641.87 | 666.48 | 779.32 | 827.24 | 854.30 | 895.73 | 918.71 | 928.70 | |
| 944.83 | 955.49 | 961.04 | 967.43 | 978.94 | 1020.25 | 1025.60 | 1034.67 | 1050.19 | 1065.25 | |
| 1073.20 | 1079.78 | 1175.81 | 1219.47 | 1225.48 | 1251.45 | 1254.66 | 1266.45 | 1271.21 | | |
| 1304.14 | 1325.58 | 1408.07 | 1410.39 | 1415.26 | 1419.84 | 1421.79 | 1424.76 | 1463.65 | | |
| 1479.93 | 1481.54 | 1481.77 | 1485.45 | 1489.67 | 1493.99 | 1497.67 | 1501.30 | 1501.64 | | |
| 1511.45 | 1515.27 | 1522.05 | 1526.85 | 3072.98 | 3074.53 | 3077.98 | 3078.42 | 3080.28 | | |
| 3086.32 | 3148.32 | 3152.54 | 3154.58 | 3157.90 | 3159.15 | 3164.37 | 3170.69 | 3170.75 | | |
| 3170.91 | 3175.64 | 3181.59 | 3188.68 | 3710.21 | 3742.96 | | | | | |

Rotational constants (B/GHZ): 0.8088231 0.4164583 0.3411174



IM8d

| C | | B1 | | | | |
|---|----|-----|----|-----|----|-------|
| C | 1 | | | | | |
| O | 2 | B2 | 1 | A1 | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 0 |
| H | 3 | B4 | 2 | A3 | 1 | D2 0 |
| C | 3 | B5 | 2 | A4 | 1 | D3 0 |
| C | 6 | B6 | 3 | A5 | 2 | D4 0 |
| H | 7 | B7 | 6 | A6 | 3 | D5 0 |
| H | 7 | B8 | 6 | A7 | 3 | D6 0 |
| H | 7 | B9 | 6 | A8 | 3 | D7 0 |
| O | 6 | B10 | 3 | A9 | 2 | D8 0 |
| O | 6 | B11 | 3 | A10 | 2 | D9 0 |
| H | 1 | B12 | 2 | A11 | 4 | D10 0 |
| H | 1 | B13 | 2 | A12 | 4 | D11 0 |
| H | 1 | B14 | 2 | A13 | 4 | D12 0 |
| O | 2 | B15 | 1 | A14 | 4 | D13 0 |
| C | 16 | B16 | 2 | A15 | 1 | D14 0 |
| C | 17 | B17 | 16 | A16 | 2 | D15 0 |
| H | 18 | B18 | 17 | A17 | 16 | D16 0 |
| H | 18 | B19 | 17 | A18 | 16 | D17 0 |
| H | 18 | B20 | 17 | A19 | 16 | D18 0 |
| O | 17 | B21 | 16 | A20 | 2 | D19 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 22 | B22 | 17 | A21 | 16 | D20 | 0 |
| H | 23 | B23 | 22 | A22 | 17 | D21 | 0 |
| C | 6 | B24 | 3 | A23 | 2 | D22 | 0 |
| H | 25 | B25 | 6 | A24 | 3 | D23 | 0 |
| H | 25 | B26 | 6 | A25 | 3 | D24 | 0 |
| H | 25 | B27 | 6 | A26 | 3 | D25 | 0 |
| C | 2 | B28 | 1 | A27 | 16 | D26 | 0 |
| H | 29 | B29 | 2 | A28 | 1 | D27 | 0 |
| H | 29 | B30 | 2 | A29 | 1 | D28 | 0 |
| H | 29 | B31 | 2 | A30 | 1 | D29 | 0 |
| C | 17 | B32 | 16 | A31 | 2 | D30 | 0 |
| H | 33 | B33 | 17 | A32 | 16 | D31 | 0 |
| H | 33 | B34 | 17 | A33 | 16 | D32 | 0 |
| H | 33 | B35 | 17 | A34 | 16 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.51984898 |
| B2 | 2.32251789 |
| B3 | 1.40885104 |
| B4 | 1.01291570 |
| B5 | 3.30687211 |
| B6 | 1.47169044 |
| B7 | 1.09491584 |
| B8 | 1.09120846 |
| B9 | 1.08568259 |
| B10 | 2.24680336 |
| B11 | 1.24878598 |
| B12 | 1.08849419 |
| B13 | 1.08852340 |
| B14 | 1.08584610 |
| B15 | 1.41190883 |
| B16 | 1.41186982 |
| B17 | 1.51833228 |
| B18 | 1.08619233 |
| B19 | 1.08830398 |
| B20 | 1.08866098 |
| B21 | 1.41657481 |
| B22 | 1.41201179 |
| B23 | 0.97004727 |
| B24 | 1.48313122 |
| B25 | 1.08557117 |
| B26 | 1.09118164 |
| B27 | 1.09101968 |
| B28 | 1.52605369 |
| B29 | 1.08842258 |

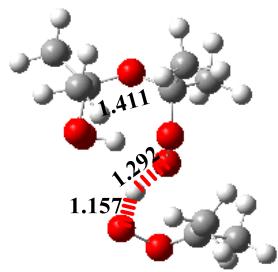
| | |
|-----|---------------|
| B30 | 1.08829181 |
| B31 | 1.08597430 |
| B32 | 1.52066603 |
| B33 | 1.08722113 |
| B34 | 1.08824112 |
| B35 | 1.08817121 |
| A1 | 87.90666797 |
| A2 | 111.63128225 |
| A3 | 122.76156981 |
| A4 | 129.62392146 |
| A5 | 81.55254121 |
| A6 | 108.60735459 |
| A7 | 108.43911686 |
| A8 | 110.94104942 |
| A9 | 50.76741577 |
| A10 | 63.25357400 |
| A11 | 109.18757296 |
| A12 | 109.76137003 |
| A13 | 110.08198036 |
| A14 | 104.74261964 |
| A15 | 124.56977020 |
| A16 | 104.65042700 |
| A17 | 109.66251693 |
| A18 | 109.53930892 |
| A19 | 109.60472886 |
| A20 | 110.61033599 |
| A21 | 109.55052958 |
| A22 | 100.54290519 |
| A23 | 126.63403186 |
| A24 | 111.05580507 |
| A25 | 108.73504170 |
| A26 | 109.27656864 |
| A27 | 110.87977700 |
| A28 | 109.63755822 |
| A29 | 108.65144535 |
| A30 | 111.80642836 |
| A31 | 115.89066989 |
| A32 | 110.74533153 |
| A33 | 109.91572777 |
| A34 | 108.46749000 |
| D1 | 26.42195236 |
| D2 | -168.65283426 |
| D3 | 126.91787508 |
| D4 | 13.97752610 |

| | |
|-----|---------------|
| D5 | -14.78421350 |
| D6 | 99.50616049 |
| D7 | -136.72366914 |
| D8 | 107.54944821 |
| D9 | 144.95650423 |
| D10 | -172.65092240 |
| D11 | -52.67438920 |
| D12 | 67.77541991 |
| D13 | -122.87495284 |
| D14 | 158.79632276 |
| D15 | 167.39626377 |
| D16 | 53.61873783 |
| D17 | 173.53388299 |
| D18 | -66.25353307 |
| D19 | -72.84152723 |
| D20 | -57.29042661 |
| D21 | 86.63242941 |
| D22 | -111.38402857 |
| D23 | -73.77387395 |
| D24 | 47.54824886 |
| D25 | 164.34880135 |
| D26 | -121.88457859 |
| D27 | -46.74695441 |
| D28 | 72.28374133 |
| D29 | -167.18240153 |
| D30 | 43.72757243 |
| D31 | -66.47698646 |
| D32 | 55.55772208 |
| D33 | 174.51004891 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 22.20 | 35.66 | 47.02 | 58.15 | 91.07 | 105.46 | 131.96 | 141.53 | 172.94 | 182.26 | 190.41 |
| 205.43 | 218.26 | 234.77 | 244.19 | 258.06 | 290.70 | 297.74 | 317.10 | 336.12 | 338.69 | |
| 345.91 | 372.46 | 380.02 | 385.73 | 394.05 | 415.54 | 459.88 | 490.90 | 503.29 | 524.01 | |
| 586.53 | 603.57 | 610.93 | 652.31 | 779.90 | 828.38 | 840.67 | 896.22 | 913.98 | 928.07 | |
| 945.16 | 946.28 | 947.68 | 964.55 | 991.52 | 1020.52 | 1028.25 | 1042.11 | 1061.11 | 1073.53 | |
| 1082.89 | 1093.44 | 1109.30 | 1189.91 | 1237.96 | 1258.43 | 1259.13 | 1267.58 | 1311.73 | | |
| 1318.50 | 1394.76 | 1404.07 | 1407.98 | 1411.27 | 1416.30 | 1418.64 | 1448.82 | 1466.67 | | |
| 1477.68 | 1478.75 | 1480.85 | 1485.08 | 1486.43 | 1490.19 | 1492.26 | 1500.78 | 1502.69 | | |
| 1514.16 | 1526.18 | 1588.02 | 1668.23 | 2895.84 | 3045.29 | 3058.81 | 3066.24 | 3068.28 | | |
| 3073.35 | 3080.84 | 3111.66 | 3123.18 | 3142.34 | 3145.84 | 3151.82 | 3159.72 | 3168.34 | | |
| 3169.22 | 3170.04 | 3170.82 | 3170.95 | 3174.11 | 3739.95 | | | | | |

Rotational constants (B/GHZ): 0.7879742 0.3169244 0.2789207



TS8d

| C | | B1 | | | | |
|---|----|-----|----|-----|----|-------|
| C | 1 | | | | | |
| O | 2 | B2 | 1 | A1 | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 0 |
| H | 3 | B4 | 2 | A3 | 1 | D2 0 |
| C | 3 | B5 | 2 | A4 | 1 | D3 0 |
| C | 6 | B6 | 3 | A5 | 2 | D4 0 |
| H | 7 | B7 | 6 | A6 | 3 | D5 0 |
| H | 7 | B8 | 6 | A7 | 3 | D6 0 |
| H | 7 | B9 | 6 | A8 | 3 | D7 0 |
| O | 6 | B10 | 3 | A9 | 2 | D8 0 |
| O | 6 | B11 | 3 | A10 | 2 | D9 0 |
| H | 1 | B12 | 2 | A11 | 4 | D10 0 |
| H | 1 | B13 | 2 | A12 | 4 | D11 0 |
| H | 1 | B14 | 2 | A13 | 4 | D12 0 |
| O | 2 | B15 | 1 | A14 | 4 | D13 0 |
| C | 16 | B16 | 2 | A15 | 1 | D14 0 |
| C | 17 | B17 | 16 | A16 | 2 | D15 0 |
| H | 18 | B18 | 17 | A17 | 16 | D16 0 |
| H | 18 | B19 | 17 | A18 | 16 | D17 0 |
| H | 18 | B20 | 17 | A19 | 16 | D18 0 |
| O | 17 | B21 | 16 | A20 | 2 | D19 0 |
| O | 22 | B22 | 17 | A21 | 16 | D20 0 |
| H | 23 | B23 | 22 | A22 | 17 | D21 0 |
| C | 6 | B24 | 3 | A23 | 2 | D22 0 |
| H | 25 | B25 | 6 | A24 | 3 | D23 0 |
| H | 25 | B26 | 6 | A25 | 3 | D24 0 |
| H | 25 | B27 | 6 | A26 | 3 | D25 0 |
| C | 2 | B28 | 1 | A27 | 16 | D26 0 |
| H | 29 | B29 | 2 | A28 | 1 | D27 0 |
| H | 29 | B30 | 2 | A29 | 1 | D28 0 |
| H | 29 | B31 | 2 | A30 | 1 | D29 0 |
| C | 17 | B32 | 16 | A31 | 2 | D30 0 |
| H | 33 | B33 | 17 | A32 | 16 | D31 0 |
| H | 33 | B34 | 17 | A33 | 16 | D32 0 |
| H | 33 | B35 | 17 | A34 | 16 | D33 0 |

Variables:

| | |
|-----|--------------|
| B1 | 1.52078622 |
| B2 | 2.31936148 |
| B3 | 1.40443606 |
| B4 | 1.29168429 |
| B5 | 2.27435536 |
| B6 | 1.47731291 |
| B7 | 1.08797363 |
| B8 | 1.08173973 |
| B9 | 1.09460900 |
| B10 | 2.23010100 |
| B11 | 1.27202304 |
| B12 | 1.08859755 |
| B13 | 1.08953608 |
| B14 | 1.08567855 |
| B15 | 1.41585983 |
| B16 | 1.41079385 |
| B17 | 1.51846886 |
| B18 | 1.08616790 |
| B19 | 1.08837525 |
| B20 | 1.08872053 |
| B21 | 1.41847576 |
| B22 | 1.41213963 |
| B23 | 0.97170844 |
| B24 | 1.48150343 |
| B25 | 1.08613104 |
| B26 | 1.09295231 |
| B27 | 1.08782472 |
| B28 | 1.52610070 |
| B29 | 1.08882788 |
| B30 | 1.08837309 |
| B31 | 1.08554390 |
| B32 | 1.52093295 |
| B33 | 1.08702565 |
| B34 | 1.08818605 |
| B35 | 1.08818700 |
| A1 | 88.09868936 |
| A2 | 111.98500603 |
| A3 | 124.22005603 |
| A4 | 140.22993995 |
| A5 | 90.06403067 |
| A6 | 109.24759674 |
| A7 | 112.21480461 |
| A8 | 106.03005575 |

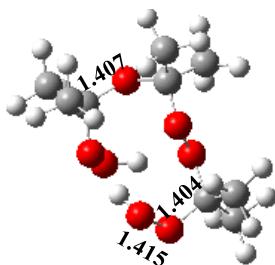
| | |
|-----|---------------|
| A9 | 63.76095663 |
| A10 | 83.53954898 |
| A11 | 109.29403032 |
| A12 | 109.57359001 |
| A13 | 110.11073676 |
| A14 | 104.55321826 |
| A15 | 124.10686459 |
| A16 | 104.64573302 |
| A17 | 109.66719888 |
| A18 | 109.55255794 |
| A19 | 109.59166181 |
| A20 | 110.86145766 |
| A21 | 109.50553961 |
| A22 | 99.88667073 |
| A23 | 108.42886967 |
| A24 | 111.12146511 |
| A25 | 105.63256434 |
| A26 | 111.03402951 |
| A27 | 110.65350871 |
| A28 | 109.52789102 |
| A29 | 108.83354855 |
| A30 | 111.82612337 |
| A31 | 115.89569781 |
| A32 | 110.69272391 |
| A33 | 109.93125881 |
| A34 | 108.50638261 |
| D1 | 26.29324589 |
| D2 | -169.85278926 |
| D3 | 90.84906031 |
| D4 | 30.12556954 |
| D5 | -58.85048819 |
| D6 | 63.39215248 |
| D7 | -175.55409678 |
| D8 | 123.14952010 |
| D9 | 154.69185946 |
| D10 | -171.99566928 |
| D11 | -52.36195718 |
| D12 | 68.20036771 |
| D13 | -122.41576785 |
| D14 | 159.73081017 |
| D15 | 168.55656568 |
| D16 | 53.82355269 |
| D17 | 173.74227414 |
| D18 | -66.05222708 |

| | |
|-----|---------------|
| D19 | -71.76747612 |
| D20 | -56.70506992 |
| D21 | 85.57853900 |
| D22 | -92.01698470 |
| D23 | -100.64755351 |
| D24 | 17.38547278 |
| D25 | 134.70927735 |
| D26 | -121.54777660 |
| D27 | -46.33577180 |
| D28 | 72.66262616 |
| D29 | -166.55442744 |
| D30 | 44.88261137 |
| D31 | -67.04801970 |
| D32 | 54.89559204 |
| D33 | 173.84973867 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 784.25 <i>i</i> | 25.65 | 45.64 | 65.61 | 91.36 | 112.83 | 123.21 | 140.72 | 173.84 | 176.51 | 197.78 |
| 202.32 | 212.27 | 229.60 | 255.33 | 259.72 | 288.10 | 293.24 | 316.03 | 326.90 | 340.98 | |
| 349.06 | 371.36 | 385.36 | 388.22 | 407.10 | 444.80 | 471.67 | 489.05 | 495.82 | 564.74 | |
| 594.57 | 603.96 | 613.53 | 655.27 | 756.30 | 785.57 | 818.37 | 843.02 | 895.76 | 928.70 | |
| 932.19 | 942.52 | 946.09 | 955.95 | 965.78 | 987.41 | 1017.46 | 1027.46 | 1058.96 | 1069.51 | |
| 1076.61 | 1090.08 | 1103.72 | 1190.63 | 1234.90 | 1253.86 | 1260.39 | 1265.73 | 1309.24 | | |
| 1319.52 | 1362.72 | 1397.26 | 1402.29 | 1407.39 | 1415.81 | 1418.57 | 1424.65 | 1441.58 | | |
| 1457.23 | 1470.55 | 1476.65 | 1480.20 | 1487.73 | 1490.10 | 1490.70 | 1495.26 | 1496.71 | | |
| 1502.60 | 1516.10 | 1526.99 | 1610.80 | 1927.26 | 3053.70 | 3059.94 | 3061.13 | 3070.93 | | |
| 3073.89 | 3077.02 | 3131.95 | 3135.51 | 3136.58 | 3148.43 | 3148.97 | 3156.38 | 3160.58 | | |
| 3160.97 | 3172.53 | 3174.27 | 3183.67 | 3209.90 | 3687.40 | | | | | |

Rotational constants (B/GHZ): 0.7989229 0.3705004 0.3140995



P8d

C

| | | | | | | | |
|---|---|----|---|----|---|----|---|
| C | 1 | B1 | | | | | |
| O | 2 | B2 | 1 | A1 | | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 4 | B4 | 2 | A3 | 1 | D2 | 0 |
| C | 3 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 6 | B6 | 3 | A5 | 2 | D4 | 0 |
| H | 7 | B7 | 6 | A6 | 3 | D5 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 7 | B8 | 6 | A7 | 3 | D6 | 0 |
| H | 7 | B9 | 6 | A8 | 3 | D7 | 0 |
| O | 6 | B10 | 3 | A9 | 2 | D8 | 0 |
| O | 6 | B11 | 3 | A10 | 2 | D9 | 0 |
| H | 1 | B12 | 2 | A11 | 4 | D10 | 0 |
| H | 1 | B13 | 2 | A12 | 4 | D11 | 0 |
| H | 1 | B14 | 2 | A13 | 4 | D12 | 0 |
| O | 2 | B15 | 1 | A14 | 4 | D13 | 0 |
| C | 16 | B16 | 2 | A15 | 1 | D14 | 0 |
| C | 17 | B17 | 16 | A16 | 2 | D15 | 0 |
| H | 18 | B18 | 17 | A17 | 16 | D16 | 0 |
| H | 18 | B19 | 17 | A18 | 16 | D17 | 0 |
| H | 18 | B20 | 17 | A19 | 16 | D18 | 0 |
| O | 17 | B21 | 16 | A20 | 2 | D19 | 0 |
| O | 22 | B22 | 17 | A21 | 16 | D20 | 0 |
| H | 23 | B23 | 22 | A22 | 17 | D21 | 0 |
| C | 6 | B24 | 3 | A23 | 2 | D22 | 0 |
| H | 25 | B25 | 6 | A24 | 3 | D23 | 0 |
| H | 25 | B26 | 6 | A25 | 3 | D24 | 0 |
| H | 25 | B27 | 6 | A26 | 3 | D25 | 0 |
| C | 2 | B28 | 1 | A27 | 16 | D26 | 0 |
| H | 29 | B29 | 2 | A28 | 1 | D27 | 0 |
| H | 29 | B30 | 2 | A29 | 1 | D28 | 0 |
| H | 29 | B31 | 2 | A30 | 1 | D29 | 0 |
| C | 17 | B32 | 16 | A31 | 2 | D30 | 0 |
| H | 33 | B33 | 17 | A32 | 16 | D31 | 0 |
| H | 33 | B34 | 17 | A33 | 16 | D32 | 0 |
| H | 33 | B35 | 17 | A34 | 16 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.52016370 |
| B2 | 2.29963054 |
| B3 | 1.41059122 |
| B4 | 2.60713139 |
| B5 | 1.42779127 |
| B6 | 1.51436369 |
| B7 | 1.08851039 |
| B8 | 1.08416930 |
| B9 | 1.08823600 |
| B10 | 2.31570622 |
| B11 | 1.40392251 |
| B12 | 1.08842625 |
| B13 | 1.08853775 |
| B14 | 1.08543077 |
| B15 | 1.41355338 |

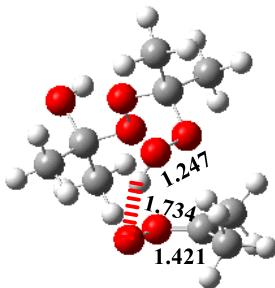
| | |
|-----|--------------|
| B16 | 1.40664548 |
| B17 | 1.51648534 |
| B18 | 1.08614036 |
| B19 | 1.08806768 |
| B20 | 1.08844939 |
| B21 | 1.42641054 |
| B22 | 1.40993238 |
| B23 | 0.97037467 |
| B24 | 1.51826934 |
| B25 | 1.08894773 |
| B26 | 1.08730640 |
| B27 | 1.08719607 |
| B28 | 1.52705524 |
| B29 | 1.08808127 |
| B30 | 1.08840824 |
| B31 | 1.08525381 |
| B32 | 1.52060750 |
| B33 | 1.08793761 |
| B34 | 1.08782299 |
| B35 | 1.08800943 |
| A1 | 86.30175837 |
| A2 | 112.45194201 |
| A3 | 125.20821276 |
| A4 | 145.10265987 |
| A5 | 112.29094243 |
| A6 | 109.70717096 |
| A7 | 110.94874871 |
| A8 | 108.24636255 |
| A9 | 95.99401266 |
| A10 | 110.15522544 |
| A11 | 108.84546011 |
| A12 | 109.53161303 |
| A13 | 110.69538535 |
| A14 | 104.76041354 |
| A15 | 124.44280307 |
| A16 | 104.92839659 |
| A17 | 109.70431919 |
| A18 | 109.62465302 |
| A19 | 109.39579987 |
| A20 | 110.78209748 |
| A21 | 110.50891683 |
| A22 | 100.42519573 |
| A23 | 103.63558559 |
| A24 | 110.02610851 |

| | |
|-----|---------------|
| A25 | 109.68937408 |
| A26 | 109.15050415 |
| A27 | 110.48069552 |
| A28 | 109.11899556 |
| A29 | 108.70110812 |
| A30 | 112.28987592 |
| A31 | 116.17739162 |
| A32 | 111.13520361 |
| A33 | 109.85504328 |
| A34 | 108.64687064 |
| D1 | 25.68184359 |
| D2 | -134.09282706 |
| D3 | 126.78519519 |
| D4 | -32.65265239 |
| D5 | -50.52424036 |
| D6 | 70.50681839 |
| D7 | -169.78745661 |
| D8 | 61.09225082 |
| D9 | 94.00240574 |
| D10 | -168.26508807 |
| D11 | -48.78722418 |
| D12 | 72.15535667 |
| D13 | -121.91487072 |
| D14 | 163.83047261 |
| D15 | 168.67748988 |
| D16 | 52.99597908 |
| D17 | 173.12540667 |
| D18 | -66.72026001 |
| D19 | -72.11545705 |
| D20 | -57.15472125 |
| D21 | 90.29220756 |
| D22 | -155.38582894 |
| D23 | -54.70033639 |
| D24 | 65.84416352 |
| D25 | -173.94062946 |
| D26 | -122.91923998 |
| D27 | -42.18896324 |
| D28 | 76.53316302 |
| D29 | -162.25697674 |
| D30 | 44.24395768 |
| D31 | -67.77125422 |
| D32 | 53.91318818 |
| D33 | 172.80687010 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 54.28 | 61.11 | 77.38 | 121.11 | 131.16 | 161.20 | 172.57 | 186.99 | 198.51 | 206.38 | 218.46 |
| 245.86 | 250.75 | 259.61 | 279.06 | 290.81 | 297.27 | 301.70 | 330.20 | 340.28 | 356.85 | |
| 366.08 | 375.70 | 397.08 | 431.66 | 440.72 | 456.40 | 499.92 | 503.36 | 533.60 | 541.69 | |
| 586.01 | 610.49 | 619.43 | 651.50 | 783.00 | 825.76 | 856.75 | 895.66 | 906.80 | 936.68 | |
| 947.02 | 960.20 | 961.00 | 970.22 | 974.11 | 1021.12 | 1022.04 | 1031.36 | 1057.68 | 1067.81 | |
| 1074.46 | 1077.78 | 1178.13 | 1213.64 | 1231.79 | 1252.32 | 1256.13 | 1262.96 | 1269.28 | | |
| 1307.54 | 1327.34 | 1407.53 | 1412.05 | 1415.28 | 1417.81 | 1421.31 | 1423.62 | 1477.38 | | |
| 1478.24 | 1482.37 | 1484.04 | 1487.33 | 1488.40 | 1492.53 | 1495.14 | 1502.85 | 1505.01 | | |
| 1511.46 | 1514.08 | 1526.53 | 1539.46 | 3067.81 | 3067.85 | 3076.91 | 3078.08 | 3080.04 | | |
| 3082.49 | 3145.08 | 3148.93 | 3150.95 | 3152.90 | 3158.01 | 3162.18 | 3165.02 | 3167.29 | | |
| 3170.15 | 3178.99 | 3185.48 | 3188.83 | 3695.05 | 3736.56 | | | | | |

Rotational constants (B/GHZ): 0.7550587 0.4454084 0.3758664



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| C | | | | | | | |
|---|----|--|-----|---|-----|---|-------|
| O | 1 | | B1 | | | | |
| O | 1 | | B2 | 2 | A1 | | |
| H | 2 | | B3 | 1 | A2 | 3 | D1 0 |
| C | 3 | | B4 | 1 | A3 | 2 | D2 0 |
| C | 5 | | B5 | 3 | A4 | 1 | D3 0 |
| H | 6 | | B6 | 5 | A5 | 3 | D4 0 |
| H | 6 | | B7 | 5 | A6 | 3 | D5 0 |
| H | 6 | | B8 | 5 | A7 | 3 | D6 0 |
| C | 5 | | B9 | 3 | A8 | 1 | D7 0 |
| H | 10 | | B10 | 5 | A9 | 3 | D8 0 |
| H | 10 | | B11 | 5 | A10 | 3 | D9 0 |
| H | 10 | | B12 | 5 | A11 | 3 | D10 0 |
| O | 5 | | B13 | 3 | A12 | 1 | D11 0 |
| O | 5 | | B14 | 3 | A13 | 1 | D12 0 |
| C | 1 | | B15 | 3 | A14 | 2 | D13 0 |
| H | 16 | | B16 | 1 | A15 | 3 | D14 0 |
| H | 16 | | B17 | 1 | A16 | 3 | D15 0 |
| H | 16 | | B18 | 1 | A17 | 3 | D16 0 |
| C | 1 | | B19 | 3 | A18 | 2 | D17 0 |
| H | 20 | | B20 | 1 | A19 | 3 | D18 0 |
| H | 20 | | B21 | 1 | A20 | 3 | D19 0 |
| H | 20 | | B22 | 1 | A21 | 3 | D20 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 1 | B23 | 3 | A22 | 2 | D21 | 0 |
| O | 24 | B24 | 1 | A23 | 3 | D22 | 0 |
| C | 25 | B25 | 24 | A24 | 1 | D23 | 0 |
| C | 26 | B26 | 25 | A25 | 24 | D24 | 0 |
| H | 27 | B27 | 26 | A26 | 25 | D25 | 0 |
| H | 27 | B28 | 26 | A27 | 25 | D26 | 0 |
| H | 27 | B29 | 26 | A28 | 25 | D27 | 0 |
| C | 26 | B30 | 25 | A29 | 24 | D28 | 0 |
| H | 31 | B31 | 26 | A30 | 25 | D29 | 0 |
| H | 31 | B32 | 26 | A31 | 25 | D30 | 0 |
| H | 31 | B33 | 26 | A32 | 25 | D31 | 0 |
| O | 26 | B34 | 25 | A33 | 24 | D32 | 0 |
| H | 35 | B35 | 26 | A34 | 25 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 2.32125941 |
| B2 | 1.41278768 |
| B3 | 0.99102410 |
| B4 | 2.76613958 |
| B5 | 1.48149396 |
| B6 | 1.09143067 |
| B7 | 1.08643016 |
| B8 | 1.09115544 |
| B9 | 1.47373363 |
| B10 | 1.08585998 |
| B11 | 1.09268948 |
| B12 | 1.09045898 |
| B13 | 2.24978577 |
| B14 | 1.24745543 |
| B15 | 1.51963346 |
| B16 | 1.08793249 |
| B17 | 1.08667844 |
| B18 | 1.08804845 |
| B19 | 1.51757303 |
| B20 | 1.08817704 |
| B21 | 1.08767342 |
| B22 | 1.08556727 |
| B23 | 1.40346740 |
| B24 | 1.42810111 |
| B25 | 1.42325418 |
| B26 | 1.51333629 |
| B27 | 1.08613898 |
| B28 | 1.08879280 |
| B29 | 1.08912202 |
| B30 | 1.52175184 |

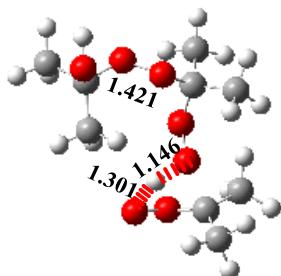
| | |
|-----|--------------|
| B31 | 1.08785587 |
| B32 | 1.09172365 |
| B33 | 1.08786117 |
| B34 | 1.40070056 |
| B35 | 0.96141230 |
| A1 | 35.10558118 |
| A2 | 111.36495150 |
| A3 | 132.88766006 |
| A4 | 98.56362877 |
| A5 | 109.69652263 |
| A6 | 110.80798023 |
| A7 | 107.85141376 |
| A8 | 88.13734041 |
| A9 | 110.71478426 |
| A10 | 108.43276856 |
| A11 | 108.62970227 |
| A12 | 78.33986778 |
| A13 | 83.46516013 |
| A14 | 104.27601160 |
| A15 | 109.59276944 |
| A16 | 110.76550406 |
| A17 | 108.88224707 |
| A18 | 112.24738176 |
| A19 | 108.81852872 |
| A20 | 109.53723895 |
| A21 | 110.24310944 |
| A22 | 111.29614017 |
| A23 | 108.12443459 |
| A24 | 107.58918944 |
| A25 | 112.48718503 |
| A26 | 109.87403342 |
| A27 | 108.78508156 |
| A28 | 110.15309207 |
| A29 | 102.80620634 |
| A30 | 108.56964614 |
| A31 | 110.27187085 |
| A32 | 110.57358090 |
| A33 | 110.04422314 |
| A34 | 108.53299505 |
| D1 | -80.79251249 |
| D2 | 118.97687172 |
| D3 | 50.61375542 |
| D4 | 156.75507809 |
| D5 | -80.59815266 |

| | |
|-----|---------------|
| D6 | 39.86634069 |
| D7 | 173.76168173 |
| D8 | -108.75834289 |
| D9 | 12.46005882 |
| D10 | 127.66046195 |
| D11 | -98.03279599 |
| D12 | -64.63707003 |
| D13 | 170.83099596 |
| D14 | -67.03364479 |
| D15 | 53.97122567 |
| D16 | 173.39151375 |
| D17 | 48.51878497 |
| D18 | 50.74390249 |
| D19 | 170.52852765 |
| D20 | -68.83770429 |
| D21 | -67.63507712 |
| D22 | -64.70193429 |
| D23 | 171.71351352 |
| D24 | -52.26454282 |
| D25 | 69.51571159 |
| D26 | -171.46346268 |
| D27 | -51.17582162 |
| D28 | -173.76234999 |
| D29 | -173.10868338 |
| D30 | -54.05789206 |
| D31 | 67.05078839 |
| D32 | 67.45134010 |
| D33 | 55.45084733 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 29.06 | 57.59 | 67.98 | 85.27 | 91.32 | 97.27 | 110.24 | 134.84 | 139.11 | 163.24 | 170.45 |
| 176.01 | 189.71 | 215.96 | 223.66 | 247.46 | 260.46 | 273.41 | 288.10 | 305.04 | 325.84 | |
| 337.81 | 350.98 | 368.15 | 372.56 | 380.40 | 404.25 | 443.23 | 468.62 | 503.26 | 524.62 | |
| 583.52 | 597.13 | 603.51 | 611.60 | 757.50 | 814.09 | 830.69 | 852.48 | 910.95 | 918.21 | |
| 928.48 | 948.39 | 951.24 | 959.95 | 972.98 | 993.61 | 1010.90 | 1018.29 | 1029.72 | 1056.18 | |
| 1067.98 | 1092.61 | 1111.35 | 1156.13 | 1212.25 | 1230.41 | 1256.08 | 1271.87 | 1309.30 | | |
| 1319.19 | 1380.02 | 1399.14 | 1403.36 | 1407.73 | 1411.18 | 1413.98 | 1442.32 | 1456.09 | | |
| 1464.31 | 1475.07 | 1479.76 | 1483.06 | 1488.95 | 1490.22 | 1494.35 | 1496.08 | 1505.47 | | |
| 1509.72 | 1516.83 | 1612.56 | 1672.13 | 3048.70 | 3054.48 | 3059.38 | 3069.37 | 3071.13 | | |
| 3072.67 | 3121.97 | 3122.37 | 3128.42 | 3147.57 | 3149.55 | 3152.82 | 3153.34 | 3162.55 | | |
| 3168.42 | 3171.05 | 3173.63 | 3174.76 | 3258.75 | 3882.03 | | | | | |

Rotational constants (B/GHZ): 0.5942399 0.4682707 0.3576222



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| C | | B1 | | | | |
|---|----|-----|----|-----|----|-------|
| O | 1 | | | | | |
| O | 1 | B2 | 2 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| C | 2 | B4 | 1 | A3 | 3 | D2 0 |
| C | 5 | B5 | 2 | A4 | 1 | D3 0 |
| H | 6 | B6 | 5 | A5 | 2 | D4 0 |
| H | 6 | B7 | 5 | A6 | 2 | D5 0 |
| H | 6 | B8 | 5 | A7 | 2 | D6 0 |
| C | 5 | B9 | 2 | A8 | 1 | D7 0 |
| H | 10 | B10 | 5 | A9 | 2 | D8 0 |
| H | 10 | B11 | 5 | A10 | 2 | D9 0 |
| H | 10 | B12 | 5 | A11 | 2 | D10 0 |
| O | 5 | B13 | 2 | A12 | 1 | D11 0 |
| O | 5 | B14 | 2 | A13 | 1 | D12 0 |
| C | 1 | B15 | 3 | A14 | 2 | D13 0 |
| H | 16 | B16 | 1 | A15 | 3 | D14 0 |
| H | 16 | B17 | 1 | A16 | 3 | D15 0 |
| H | 16 | B18 | 1 | A17 | 3 | D16 0 |
| C | 1 | B19 | 3 | A18 | 2 | D17 0 |
| H | 20 | B20 | 1 | A19 | 3 | D18 0 |
| H | 20 | B21 | 1 | A20 | 3 | D19 0 |
| H | 20 | B22 | 1 | A21 | 3 | D20 0 |
| O | 1 | B23 | 3 | A22 | 2 | D21 0 |
| O | 24 | B24 | 1 | A23 | 3 | D22 0 |
| C | 25 | B25 | 24 | A24 | 1 | D23 0 |
| C | 26 | B26 | 25 | A25 | 24 | D24 0 |
| H | 27 | B27 | 26 | A26 | 25 | D25 0 |
| H | 27 | B28 | 26 | A27 | 25 | D26 0 |
| H | 27 | B29 | 26 | A28 | 25 | D27 0 |
| C | 26 | B30 | 25 | A29 | 24 | D28 0 |
| H | 31 | B31 | 26 | A30 | 25 | D29 0 |
| H | 31 | B32 | 26 | A31 | 25 | D30 0 |
| H | 31 | B33 | 26 | A32 | 25 | D31 0 |
| O | 26 | B34 | 25 | A33 | 24 | D32 0 |
| H | 35 | B35 | 26 | A34 | 25 | D33 0 |

Variables:

| | |
|-----|--------------|
| B1 | 2.31261739 |
| B2 | 1.41239530 |
| B3 | 1.14627856 |
| B4 | 2.10128450 |
| B5 | 1.48348300 |
| B6 | 1.08670903 |
| B7 | 1.08743630 |
| B8 | 1.09300807 |
| B9 | 1.48703633 |
| B10 | 1.08671245 |
| B11 | 1.08272823 |
| B12 | 1.09456675 |
| B13 | 2.21820822 |
| B14 | 1.28042305 |
| B15 | 1.51925059 |
| B16 | 1.08854047 |
| B17 | 1.08613196 |
| B18 | 1.08795361 |
| B19 | 1.51892401 |
| B20 | 1.08901812 |
| B21 | 1.08775927 |
| B22 | 1.08609250 |
| B23 | 1.40833975 |
| B24 | 1.42145937 |
| B25 | 1.42382229 |
| B26 | 1.51157285 |
| B27 | 1.08706850 |
| B28 | 1.08843679 |
| B29 | 1.08848431 |
| B30 | 1.52149428 |
| B31 | 1.08781507 |
| B32 | 1.09045389 |
| B33 | 1.08803864 |
| B34 | 1.39958354 |
| B35 | 0.96153530 |
| A1 | 35.20320370 |
| A2 | 126.39216061 |
| A3 | 130.57471912 |
| A4 | 107.60014686 |
| A5 | 111.68623732 |
| A6 | 110.16732152 |
| A7 | 106.10860528 |
| A8 | 89.85405611 |

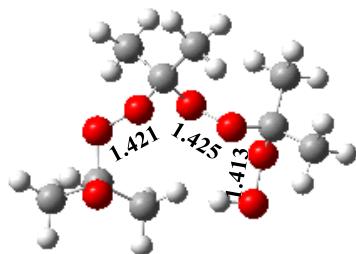
| | |
|-----|---------------|
| A9 | 109.58112011 |
| A10 | 112.02397141 |
| A11 | 106.18552042 |
| A12 | 66.67191498 |
| A13 | 90.07226943 |
| A14 | 103.95806638 |
| A15 | 109.50141564 |
| A16 | 110.46441840 |
| A17 | 109.03664898 |
| A18 | 112.61653682 |
| A19 | 109.34666829 |
| A20 | 109.33623065 |
| A21 | 110.42043416 |
| A22 | 111.51826315 |
| A23 | 108.62699959 |
| A24 | 109.35930118 |
| A25 | 112.61668619 |
| A26 | 109.71808281 |
| A27 | 109.06229601 |
| A28 | 110.13119288 |
| A29 | 102.42635171 |
| A30 | 108.75147312 |
| A31 | 110.12875299 |
| A32 | 110.67796095 |
| A33 | 110.06898385 |
| A34 | 108.34921473 |
| D1 | -54.37354883 |
| D2 | 45.48953420 |
| D3 | 21.80047562 |
| D4 | 117.57122642 |
| D5 | -118.19307601 |
| D6 | -1.80462590 |
| D7 | 143.85730464 |
| D8 | -64.59630932 |
| D9 | 59.06955695 |
| D10 | 178.51904205 |
| D11 | -122.28741270 |
| D12 | -93.11195286 |
| D13 | 166.87696431 |
| D14 | -72.32920171 |
| D15 | 48.14654239 |
| D16 | 168.00540633 |
| D17 | 44.36543703 |
| D18 | 48.25912482 |

| | |
|-----|---------------|
| D19 | 167.73889652 |
| D20 | -71.89020133 |
| D21 | -71.62536422 |
| D22 | -70.18025977 |
| D23 | 134.46054441 |
| D24 | -56.34684711 |
| D25 | 64.91669016 |
| D26 | -175.76178873 |
| D27 | -55.75160361 |
| D28 | -177.80312064 |
| D29 | -176.41915158 |
| D30 | -57.00459470 |
| D31 | 63.40013112 |
| D32 | 63.34338790 |
| D33 | 54.11233444 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 784.16 <i>i</i> | 17.28 | 43.40 | 51.83 | 62.74 | 86.03 | 97.32 | 104.53 | 145.39 | 172.77 | 201.87 |
| 209.95 | 213.33 | 232.56 | 239.40 | 253.46 | 275.97 | 293.49 | 300.92 | 326.01 | 335.03 | |
| 346.20 | 377.25 | 385.12 | 394.56 | 403.95 | 426.01 | 447.77 | 455.91 | 524.73 | 539.72 | |
| 564.09 | 601.42 | 615.18 | 635.51 | 805.89 | 814.79 | 842.46 | 880.89 | 907.91 | 915.52 | |
| 943.05 | 949.15 | 956.42 | 959.80 | 972.84 | 987.29 | 1003.10 | 1018.60 | 1027.55 | 1062.31 | |
| 1076.67 | 1081.82 | 1115.97 | 1156.26 | 1214.94 | 1229.90 | 1249.74 | 1275.33 | 1307.08 | | |
| 1314.27 | 1374.20 | 1400.67 | 1405.13 | 1409.47 | 1416.07 | 1420.45 | 1430.51 | 1440.01 | | |
| 1464.25 | 1476.42 | 1481.96 | 1483.65 | 1487.76 | 1490.99 | 1492.51 | 1494.25 | 1499.00 | | |
| 1507.45 | 1516.20 | 1582.51 | 1597.24 | 1788.59 | 3046.38 | 3054.29 | 3064.34 | 3067.10 | | |
| 3070.44 | 3079.62 | 3133.06 | 3139.19 | 3145.42 | 3146.47 | 3148.51 | 3151.14 | 3158.68 | | |
| 3162.18 | 3168.04 | 3171.67 | 3172.26 | 3205.37 | 3881.20 | | | | | |

Rotational constants (B/GHZ): 0.7900059 0.3350680 0.2791479



P8e

| | | | | | | | |
|---|---|----|----|----|---|----|---|
| C | | | | | | | |
| O | 1 | | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| C | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| C | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 6 | B6 | 5 | A5 | 2 | D4 | 0 |
| H | 6 | B7 | 5 | A6 | 2 | D5 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 6 | B8 | 5 | A7 | 2 | D6 | 0 |
| C | 5 | B9 | 2 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 5 | A9 | 2 | D8 | 0 |
| H | 10 | B11 | 5 | A10 | 2 | D9 | 0 |
| H | 10 | B12 | 5 | A11 | 2 | D10 | 0 |
| O | 5 | B13 | 2 | A12 | 1 | D11 | 0 |
| O | 5 | B14 | 2 | A13 | 1 | D12 | 0 |
| C | 1 | B15 | 3 | A14 | 2 | D13 | 0 |
| H | 16 | B16 | 1 | A15 | 3 | D14 | 0 |
| H | 16 | B17 | 1 | A16 | 3 | D15 | 0 |
| H | 16 | B18 | 1 | A17 | 3 | D16 | 0 |
| C | 1 | B19 | 3 | A18 | 2 | D17 | 0 |
| H | 20 | B20 | 1 | A19 | 3 | D18 | 0 |
| H | 20 | B21 | 1 | A20 | 3 | D19 | 0 |
| H | 20 | B22 | 1 | A21 | 3 | D20 | 0 |
| O | 1 | B23 | 3 | A22 | 2 | D21 | 0 |
| O | 24 | B24 | 1 | A23 | 3 | D22 | 0 |
| C | 25 | B25 | 24 | A24 | 1 | D23 | 0 |
| C | 26 | B26 | 25 | A25 | 24 | D24 | 0 |
| H | 27 | B27 | 26 | A26 | 25 | D25 | 0 |
| H | 27 | B28 | 26 | A27 | 25 | D26 | 0 |
| H | 27 | B29 | 26 | A28 | 25 | D27 | 0 |
| C | 26 | B30 | 25 | A29 | 24 | D28 | 0 |
| H | 31 | B31 | 26 | A30 | 25 | D29 | 0 |
| H | 31 | B32 | 26 | A31 | 25 | D30 | 0 |
| H | 31 | B33 | 26 | A32 | 25 | D31 | 0 |
| O | 26 | B34 | 25 | A33 | 24 | D32 | 0 |
| H | 35 | B35 | 26 | A34 | 25 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 2.30934914 |
| B2 | 1.41540656 |
| B3 | 2.43161017 |
| B4 | 1.41731621 |
| B5 | 1.51562526 |
| B6 | 1.08829273 |
| B7 | 1.08786162 |
| B8 | 1.08651151 |
| B9 | 1.51724277 |
| B10 | 1.08801841 |
| B11 | 1.08585494 |
| B12 | 1.08812818 |
| B13 | 2.30626682 |
| B14 | 1.40937688 |
| B15 | 1.51851585 |

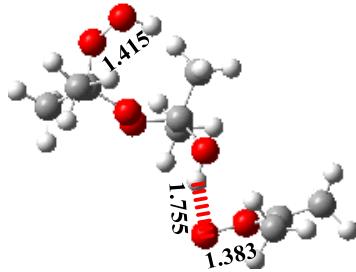
| | |
|-----|--------------|
| B16 | 1.08806195 |
| B17 | 1.08604131 |
| B18 | 1.08788564 |
| B19 | 1.51796499 |
| B20 | 1.08809936 |
| B21 | 1.08766784 |
| B22 | 1.08622324 |
| B23 | 1.41051625 |
| B24 | 1.42114561 |
| B25 | 1.42368513 |
| B26 | 1.51364179 |
| B27 | 1.08772811 |
| B28 | 1.08835318 |
| B29 | 1.09064688 |
| B30 | 1.52155608 |
| B31 | 1.08790418 |
| B32 | 1.09000140 |
| B33 | 1.08819587 |
| B34 | 1.39588862 |
| B35 | 0.96175774 |
| A1 | 35.75412821 |
| A2 | 115.99279212 |
| A3 | 134.53395820 |
| A4 | 113.38178498 |
| A5 | 109.26758619 |
| A6 | 109.13621944 |
| A7 | 110.62355187 |
| A8 | 103.82660210 |
| A9 | 109.84193324 |
| A10 | 110.52720649 |
| A11 | 108.58937793 |
| A12 | 90.52380610 |
| A13 | 109.58571940 |
| A14 | 103.71758915 |
| A15 | 109.17575202 |
| A16 | 110.69172156 |
| A17 | 109.04082000 |
| A18 | 112.97823819 |
| A19 | 109.18229857 |
| A20 | 108.96082593 |
| A21 | 110.83939664 |
| A22 | 110.98664960 |
| A23 | 109.41043541 |
| A24 | 109.93392349 |

| | |
|-----|---------------|
| A25 | 112.27080332 |
| A26 | 109.71755219 |
| A27 | 109.30964009 |
| A28 | 108.61323328 |
| A29 | 102.41575972 |
| A30 | 108.81837651 |
| A31 | 110.04165875 |
| A32 | 110.81845327 |
| A33 | 110.53146750 |
| A34 | 108.54058945 |
| D1 | -45.66705532 |
| D2 | 52.89145003 |
| D3 | 24.92354447 |
| D4 | 59.58759073 |
| D5 | 178.56365993 |
| D6 | -61.38704589 |
| D7 | 148.16768839 |
| D8 | -67.77572351 |
| D9 | 53.09217098 |
| D10 | 172.62097083 |
| D11 | -121.44939058 |
| D12 | -91.16742125 |
| D13 | 168.36500341 |
| D14 | -72.90227587 |
| D15 | 47.56780143 |
| D16 | 167.44293091 |
| D17 | 46.09789913 |
| D18 | 50.51746432 |
| D19 | 169.70326869 |
| D20 | -70.13864507 |
| D21 | -70.01166209 |
| D22 | -75.52853355 |
| D23 | 129.41980306 |
| D24 | -60.95661745 |
| D25 | 62.53351228 |
| D26 | -177.41314489 |
| D27 | -57.79746737 |
| D28 | 177.90228910 |
| D29 | -178.01619978 |
| D30 | -58.60279062 |
| D31 | 61.68309483 |
| D32 | 58.58696010 |
| D33 | 53.74109330 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 27.07 | 52.93 | 71.04 | 83.15 | 99.17 | 119.75 | 137.52 | 173.41 | 187.93 | 204.85 | 226.47 |
| 230.47 | 242.85 | 260.29 | 268.22 | 285.17 | 292.78 | 300.12 | 309.85 | 331.23 | 345.76 | |
| 359.12 | 373.24 | 388.45 | 390.01 | 423.85 | 439.96 | 461.64 | 477.33 | 528.51 | 582.91 | |
| 588.88 | 601.87 | 619.99 | 633.03 | 812.78 | 830.88 | 861.96 | 902.33 | 912.58 | 916.75 | |
| 948.29 | 949.89 | 956.48 | 963.63 | 981.13 | 1021.97 | 1026.39 | 1028.42 | 1033.48 | 1049.32 | |
| 1060.90 | 1068.54 | 1152.01 | 1197.25 | 1225.35 | 1230.35 | 1247.58 | 1258.05 | 1286.50 | | |
| 1299.87 | 1324.42 | 1375.93 | 1407.50 | 1409.40 | 1412.44 | 1415.78 | 1420.25 | 1429.53 | | |
| 1448.94 | 1476.59 | 1483.98 | 1485.30 | 1487.48 | 1487.63 | 1492.04 | 1495.31 | 1499.41 | | |
| 1503.50 | 1509.15 | 1512.96 | 1532.73 | 3054.41 | 3059.09 | 3073.24 | 3074.07 | 3077.82 | | |
| 3080.46 | 3137.50 | 3138.12 | 3152.45 | 3152.55 | 3153.35 | 3159.69 | 3161.44 | 3163.30 | | |
| 3164.02 | 3168.24 | 3170.37 | 3171.75 | 3804.46 | 3881.05 | | | | | |

Rotational constants (B/GHZ): 0.7660137 0.3617709 0.2938404



IM8f

C

| | | | | | | | | | | |
|---|----|-----|----|-----|----|-----|---|--|--|--|
| C | 1 | B1 | | | | | | | | |
| H | 2 | B2 | 1 | A1 | | | | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 | | | |
| H | 2 | B4 | 1 | A3 | 3 | D2 | 0 | | | |
| C | 1 | B5 | 2 | A4 | 5 | D3 | 0 | | | |
| H | 6 | B6 | 1 | A5 | 2 | D4 | 0 | | | |
| H | 6 | B7 | 1 | A6 | 2 | D5 | 0 | | | |
| H | 6 | B8 | 1 | A7 | 2 | D6 | 0 | | | |
| O | 1 | B9 | 6 | A8 | 2 | D7 | 0 | | | |
| H | 10 | B10 | 1 | A9 | 6 | D8 | 0 | | | |
| C | 10 | B11 | 1 | A10 | 6 | D9 | 0 | | | |
| C | 12 | B12 | 10 | A11 | 1 | D10 | 0 | | | |
| H | 13 | B13 | 12 | A12 | 10 | D11 | 0 | | | |
| H | 13 | B14 | 12 | A13 | 10 | D12 | 0 | | | |
| H | 13 | B15 | 12 | A14 | 10 | D13 | 0 | | | |
| C | 12 | B16 | 10 | A15 | 1 | D14 | 0 | | | |
| H | 17 | B17 | 12 | A16 | 10 | D15 | 0 | | | |
| H | 17 | B18 | 12 | A17 | 10 | D16 | 0 | | | |
| H | 17 | B19 | 12 | A18 | 10 | D17 | 0 | | | |
| O | 12 | B20 | 10 | A19 | 1 | D18 | 0 | | | |
| O | 12 | B21 | 10 | A20 | 1 | D19 | 0 | | | |
| O | 1 | B22 | 10 | A21 | 6 | D20 | 0 | | | |
| O | 23 | B23 | 1 | A22 | 10 | D21 | 0 | | | |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| C | 24 | B24 | 23 | A23 | 1 | D22 | 0 |
| C | 25 | B25 | 24 | A24 | 23 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 24 | D24 | 0 |
| H | 26 | B27 | 25 | A26 | 24 | D25 | 0 |
| H | 26 | B28 | 25 | A27 | 24 | D26 | 0 |
| C | 25 | B29 | 24 | A28 | 23 | D27 | 0 |
| H | 30 | B30 | 25 | A29 | 24 | D28 | 0 |
| H | 30 | B31 | 25 | A30 | 24 | D29 | 0 |
| H | 30 | B32 | 25 | A31 | 24 | D30 | 0 |
| O | 25 | B33 | 24 | A32 | 23 | D31 | 0 |
| O | 34 | B34 | 25 | A33 | 24 | D32 | 0 |
| H | 35 | B35 | 34 | A34 | 25 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.52273924 |
| B2 | 1.08892690 |
| B3 | 1.08953765 |
| B4 | 1.08833210 |
| B5 | 1.51741728 |
| B6 | 1.08840973 |
| B7 | 1.09067946 |
| B8 | 1.08940207 |
| B9 | 1.38980252 |
| B10 | 0.98411234 |
| B11 | 3.06958751 |
| B12 | 1.48312208 |
| B13 | 1.09148356 |
| B14 | 1.09097335 |
| B15 | 1.08576888 |
| B16 | 1.47296373 |
| B17 | 1.09388032 |
| B18 | 1.09026640 |
| B19 | 1.08593259 |
| B20 | 2.24727700 |
| B21 | 1.24924983 |
| B22 | 1.42267467 |
| B23 | 1.42452070 |
| B24 | 1.41190134 |
| B25 | 1.51765364 |
| B26 | 1.08606270 |
| B27 | 1.08802211 |
| B28 | 1.08778151 |
| B29 | 1.51757123 |
| B30 | 1.08782588 |
| B31 | 1.08609357 |

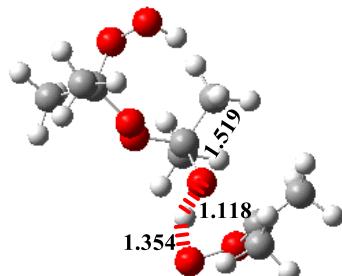
| | |
|-----|---------------|
| B32 | 1.08789906 |
| B33 | 1.41520018 |
| B34 | 1.41454686 |
| B35 | 0.96524603 |
| A1 | 108.75446983 |
| A2 | 109.58876811 |
| A3 | 110.86394040 |
| A4 | 112.75067188 |
| A5 | 109.64707462 |
| A6 | 109.77276708 |
| A7 | 109.21666106 |
| A8 | 107.64602743 |
| A9 | 108.88215335 |
| A10 | 134.49147623 |
| A11 | 121.99119623 |
| A12 | 108.63716713 |
| A13 | 109.43529171 |
| A14 | 111.13428815 |
| A15 | 78.39352075 |
| A16 | 108.11531518 |
| A17 | 108.75699048 |
| A18 | 110.82229869 |
| A19 | 58.30923998 |
| A20 | 71.18809167 |
| A21 | 110.92889986 |
| A22 | 109.14084912 |
| A23 | 108.23959772 |
| A24 | 104.15385882 |
| A25 | 110.87716472 |
| A26 | 108.88549462 |
| A27 | 109.21436365 |
| A28 | 112.92377168 |
| A29 | 109.17737088 |
| A30 | 110.60768188 |
| A31 | 109.00983418 |
| A32 | 110.48691813 |
| A33 | 109.95013923 |
| A34 | 102.12326460 |
| D1 | 118.67779047 |
| D2 | -120.20832908 |
| D3 | -59.20768823 |
| D4 | -53.54669227 |
| D5 | 66.10555658 |
| D6 | -171.80991086 |

| | |
|-----|---------------|
| D7 | 123.53661697 |
| D8 | -171.35414114 |
| D9 | -105.43751914 |
| D10 | 60.23688442 |
| D11 | 39.10323737 |
| D12 | 155.86559376 |
| D13 | -82.18127696 |
| D14 | -177.99674119 |
| D15 | -10.88169015 |
| D16 | 104.27739444 |
| D17 | -131.77039215 |
| D18 | -83.25790190 |
| D19 | -49.20812591 |
| D20 | -122.23756293 |
| D21 | 63.80217318 |
| D22 | 141.47682763 |
| D23 | 166.79850843 |
| D24 | 46.88547658 |
| D25 | 166.75360974 |
| D26 | -73.55855581 |
| D27 | 44.00654089 |
| D28 | 166.90186655 |
| D29 | -72.70423306 |
| D30 | 47.15757891 |
| D31 | -72.04043939 |
| D32 | -69.14704749 |
| D33 | 84.89837234 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 11.91 | 21.26 | 36.54 | 44.46 | 75.84 | 93.07 | 100.30 | 112.86 | 145.53 | 158.31 | 182.15 |
| 195.30 | 213.81 | 217.36 | 227.87 | 237.90 | 257.47 | 278.09 | 287.54 | 324.86 | 332.74 | |
| 341.54 | 361.43 | 367.50 | 377.42 | 380.82 | 416.23 | 457.46 | 464.78 | 497.86 | 544.83 | |
| 594.04 | 605.50 | 611.53 | 619.89 | 813.67 | 827.31 | 844.73 | 870.47 | 904.52 | 918.75 | |
| 922.34 | 941.58 | 958.23 | 959.02 | 974.76 | 990.99 | 1019.06 | 1020.93 | 1031.52 | 1053.95 | |
| 1065.10 | 1092.43 | 1108.81 | 1203.80 | 1224.66 | 1232.75 | 1251.41 | 1284.77 | 1316.79 | | |
| 1319.33 | 1384.29 | 1391.88 | 1412.40 | 1412.64 | 1415.84 | 1422.30 | 1427.76 | 1454.80 | | |
| 1467.06 | 1468.90 | 1480.34 | 1481.21 | 1486.66 | 1488.12 | 1492.46 | 1495.69 | 1497.16 | | |
| 1510.18 | 1521.19 | 1529.03 | 1663.67 | 3046.57 | 3051.24 | 3055.90 | 3062.64 | 3077.08 | | |
| 3080.34 | 3116.11 | 3116.71 | 3128.66 | 3139.31 | 3142.76 | 3155.04 | 3156.62 | 3161.28 | | |
| 3168.17 | 3177.25 | 3177.75 | 3183.34 | 3386.40 | 3824.30 | | | | | |

Rotational constants (B/GHZ): 1.0443521 0.2161672 0.2111498



TS8f

| C | | B1 | | | | |
|---|----|-----|----|-----|----|-------|
| C | 1 | | | | | |
| H | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| H | 2 | B4 | 1 | A3 | 4 | D2 0 |
| C | 1 | B5 | 2 | A4 | 3 | D3 0 |
| H | 6 | B6 | 1 | A5 | 2 | D4 0 |
| H | 6 | B7 | 1 | A6 | 2 | D5 0 |
| H | 6 | B8 | 1 | A7 | 2 | D6 0 |
| O | 1 | B9 | 6 | A8 | 2 | D7 0 |
| H | 10 | B10 | 1 | A9 | 6 | D8 0 |
| C | 10 | B11 | 1 | A10 | 6 | D9 0 |
| C | 12 | B12 | 10 | A11 | 1 | D10 0 |
| H | 13 | B13 | 12 | A12 | 10 | D11 0 |
| H | 13 | B14 | 12 | A13 | 10 | D12 0 |
| H | 13 | B15 | 12 | A14 | 10 | D13 0 |
| C | 12 | B16 | 10 | A15 | 1 | D14 0 |
| H | 17 | B17 | 12 | A16 | 10 | D15 0 |
| H | 17 | B18 | 12 | A17 | 10 | D16 0 |
| H | 17 | B19 | 12 | A18 | 10 | D17 0 |
| O | 12 | B20 | 10 | A19 | 1 | D18 0 |
| O | 12 | B21 | 10 | A20 | 1 | D19 0 |
| O | 1 | B22 | 10 | A21 | 12 | D20 0 |
| O | 23 | B23 | 1 | A22 | 10 | D21 0 |
| C | 24 | B24 | 23 | A23 | 1 | D22 0 |
| C | 25 | B25 | 24 | A24 | 23 | D23 0 |
| H | 26 | B26 | 25 | A25 | 24 | D24 0 |
| H | 26 | B27 | 25 | A26 | 24 | D25 0 |
| H | 26 | B28 | 25 | A27 | 24 | D26 0 |
| C | 25 | B29 | 24 | A28 | 23 | D27 0 |
| H | 30 | B30 | 25 | A29 | 24 | D28 0 |
| H | 30 | B31 | 25 | A30 | 24 | D29 0 |
| H | 30 | B32 | 25 | A31 | 24 | D30 0 |
| O | 25 | B33 | 24 | A32 | 23 | D31 0 |
| O | 34 | B34 | 25 | A33 | 24 | D32 0 |
| H | 35 | B35 | 34 | A34 | 25 | D33 0 |

Variables:

| | |
|-----|--------------|
| B1 | 1.52292891 |
| B2 | 1.08774116 |
| B3 | 1.08850336 |
| B4 | 1.08823772 |
| B5 | 1.51881122 |
| B6 | 1.08865399 |
| B7 | 1.09087755 |
| B8 | 1.08958795 |
| B9 | 1.40296657 |
| B10 | 1.11823038 |
| B11 | 1.98463547 |
| B12 | 1.48997617 |
| B13 | 1.08754584 |
| B14 | 1.09169300 |
| B15 | 1.08595709 |
| B16 | 1.49309639 |
| B17 | 1.08560001 |
| B18 | 1.08242306 |
| B19 | 1.09365751 |
| B20 | 2.21460198 |
| B21 | 1.28634824 |
| B22 | 1.41604706 |
| B23 | 1.42456963 |
| B24 | 1.41430839 |
| B25 | 1.51724101 |
| B26 | 1.08601902 |
| B27 | 1.08794484 |
| B28 | 1.08773845 |
| B29 | 1.51732738 |
| B30 | 1.08768798 |
| B31 | 1.08598038 |
| B32 | 1.08782364 |
| B33 | 1.41464185 |
| B34 | 1.41450970 |
| B35 | 0.96473408 |
| A1 | 110.01225807 |
| A2 | 109.93129696 |
| A3 | 109.69695735 |
| A4 | 112.64478361 |
| A5 | 110.03235749 |
| A6 | 109.44286386 |
| A7 | 109.36894348 |
| A8 | 108.80518114 |

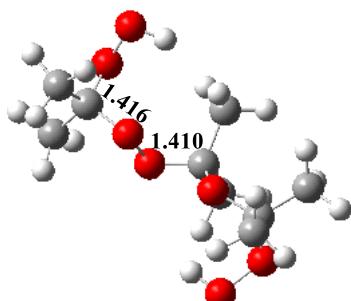
| | |
|-----|---------------|
| A9 | 109.94489217 |
| A10 | 126.58062816 |
| A11 | 110.27152375 |
| A12 | 109.39542719 |
| A13 | 108.26521946 |
| A14 | 111.37860712 |
| A15 | 91.41440307 |
| A16 | 110.09189151 |
| A17 | 111.57211418 |
| A18 | 106.08417925 |
| A19 | 69.03750650 |
| A20 | 93.52167679 |
| A21 | 108.39359476 |
| A22 | 109.40623556 |
| A23 | 108.24518331 |
| A24 | 104.10401668 |
| A25 | 110.96564270 |
| A26 | 108.82564669 |
| A27 | 109.22609893 |
| A28 | 112.89171662 |
| A29 | 109.12456871 |
| A30 | 110.65795043 |
| A31 | 109.05598258 |
| A32 | 110.44056820 |
| A33 | 110.01330653 |
| A34 | 102.19987485 |
| D1 | 119.23860208 |
| D2 | 120.82171425 |
| D3 | 60.22757490 |
| D4 | -51.69084916 |
| D5 | 67.32620798 |
| D6 | -170.79679304 |
| D7 | 126.05873743 |
| D8 | -169.66488206 |
| D9 | -82.20148917 |
| D10 | 45.02347720 |
| D11 | 47.69495530 |
| D12 | 165.10662643 |
| D13 | -74.92638000 |
| D14 | 165.50907104 |
| D15 | -63.87812597 |
| D16 | 59.44332394 |
| D17 | 178.41398401 |
| D18 | -101.38322835 |

| | |
|-----|--------------|
| D19 | -72.56013583 |
| D20 | 156.31976267 |
| D21 | 64.16378371 |
| D22 | 139.92163431 |
| D23 | 166.19139878 |
| D24 | 47.17617989 |
| D25 | 167.01288101 |
| D26 | -73.34276878 |
| D27 | 43.40949485 |
| D28 | 167.41114105 |
| D29 | -72.21392791 |
| D30 | 47.74044689 |
| D31 | -72.61888122 |
| D32 | -70.02219485 |
| D33 | 87.35763461 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 26.54 | 39.48 | 53.93 | 103.89 | 114.95 | 127.38 | 137.77 | 156.40 | 176.68 | 182.84 | 219.51 |
| 224.03 | 227.48 | 247.26 | 258.40 | 276.27 | 280.11 | 296.91 | 335.03 | 341.14 | 359.53 | |
| 371.28 | 379.59 | 389.11 | 398.30 | 421.25 | 434.32 | 470.48 | 530.96 | 566.13 | 576.82 | |
| 609.38 | 623.07 | 628.91 | 778.72 | 823.09 | 847.92 | 900.88 | 919.31 | 927.66 | 939.49 | |
| 945.18 | 964.46 | 970.52 | 982.35 | 995.72 | 1017.69 | 1032.84 | 1052.39 | 1062.76 | 1076.10 | |
| 1081.99 | 1134.28 | 1213.30 | 1234.95 | 1252.15 | 1260.02 | 1276.90 | 1313.96 | 1318.47 | | |
| 1393.33 | 1406.53 | 1414.38 | 1419.18 | 1423.26 | 1423.50 | 1425.10 | 1445.79 | 1455.22 | | |
| 1473.39 | 1478.24 | 1484.19 | 1489.31 | 1491.12 | 1496.31 | 1499.25 | 1501.18 | 1510.23 | | |
| 1519.06 | 1530.06 | 1581.11 | 1909.28 | 3050.51 | 3055.46 | 3068.20 | 3074.70 | 3078.63 | | |
| 3084.12 | 3137.81 | 3140.48 | 3148.19 | 3149.72 | 3154.78 | 3159.81 | 3165.18 | 3167.34 | | |
| 3171.61 | 3173.41 | 3180.07 | 3208.00 | 3831.39 | | | | | | |

Rotational constants (B/GHZ): 1.0009495 0.2692170 0.2600291



P8f

| | | | | | | | | |
|---|---|--|----|---|----|---|----|---|
| C | | | | | | | | |
| C | 1 | | B1 | | | | | |
| H | 2 | | B2 | 1 | A1 | | | |
| H | 2 | | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 2 | | B4 | 1 | A3 | 4 | D2 | 0 |
| C | 1 | | B5 | 2 | A4 | 3 | D3 | 0 |
| H | 6 | | B6 | 1 | A5 | 2 | D4 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 6 | B7 | 1 | A6 | 2 | D5 | 0 |
| H | 6 | B8 | 1 | A7 | 2 | D6 | 0 |
| O | 1 | B9 | 6 | A8 | 2 | D7 | 0 |
| H | 10 | B10 | 1 | A9 | 6 | D8 | 0 |
| C | 10 | B11 | 1 | A10 | 6 | D9 | 0 |
| C | 12 | B12 | 10 | A11 | 1 | D10 | 0 |
| H | 13 | B13 | 12 | A12 | 10 | D11 | 0 |
| H | 13 | B14 | 12 | A13 | 10 | D12 | 0 |
| H | 13 | B15 | 12 | A14 | 10 | D13 | 0 |
| C | 12 | B16 | 10 | A15 | 1 | D14 | 0 |
| H | 17 | B17 | 12 | A16 | 10 | D15 | 0 |
| H | 17 | B18 | 12 | A17 | 10 | D16 | 0 |
| H | 17 | B19 | 12 | A18 | 10 | D17 | 0 |
| O | 12 | B20 | 10 | A19 | 1 | D18 | 0 |
| O | 21 | B21 | 12 | A20 | 10 | D19 | 0 |
| O | 1 | B22 | 10 | A21 | 12 | D20 | 0 |
| O | 23 | B23 | 1 | A22 | 10 | D21 | 0 |
| C | 24 | B24 | 23 | A23 | 1 | D22 | 0 |
| C | 25 | B25 | 24 | A24 | 23 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 24 | D24 | 0 |
| H | 26 | B27 | 25 | A26 | 24 | D25 | 0 |
| H | 26 | B28 | 25 | A27 | 24 | D26 | 0 |
| C | 25 | B29 | 24 | A28 | 23 | D27 | 0 |
| H | 30 | B30 | 25 | A29 | 24 | D28 | 0 |
| H | 30 | B31 | 25 | A30 | 24 | D29 | 0 |
| H | 30 | B32 | 25 | A31 | 24 | D30 | 0 |
| O | 25 | B33 | 24 | A32 | 23 | D31 | 0 |
| O | 34 | B34 | 25 | A33 | 24 | D32 | 0 |
| H | 35 | B35 | 34 | A34 | 25 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.52323570 |
| B2 | 1.08462549 |
| B3 | 1.08821815 |
| B4 | 1.08863244 |
| B5 | 1.52252559 |
| B6 | 1.08690584 |
| B7 | 1.09100579 |
| B8 | 1.08935748 |
| B9 | 1.41972855 |
| B10 | 2.26696523 |
| B11 | 1.40982482 |
| B12 | 1.52080138 |
| B13 | 1.08825513 |
| B14 | 1.08777496 |

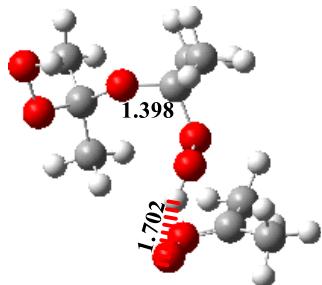
| | |
|-----|--------------|
| B15 | 1.08694670 |
| B16 | 1.51846699 |
| B17 | 1.08826994 |
| B18 | 1.08553843 |
| B19 | 1.08821535 |
| B20 | 2.31265431 |
| B21 | 1.41410261 |
| B22 | 1.41022553 |
| B23 | 1.42399169 |
| B24 | 1.41604005 |
| B25 | 1.51737491 |
| B26 | 1.08604708 |
| B27 | 1.08790671 |
| B28 | 1.08763825 |
| B29 | 1.51708388 |
| B30 | 1.08761042 |
| B31 | 1.08607505 |
| B32 | 1.08782948 |
| B33 | 1.41363539 |
| B34 | 1.41415447 |
| B35 | 0.96508446 |
| A1 | 111.55367028 |
| A2 | 110.66116666 |
| A3 | 108.14972104 |
| A4 | 112.32907726 |
| A5 | 110.89932161 |
| A6 | 108.60203229 |
| A7 | 109.47687648 |
| A8 | 110.99120760 |
| A9 | 101.56890624 |
| A10 | 124.54656174 |
| A11 | 115.40338212 |
| A12 | 109.22186334 |
| A13 | 108.85536360 |
| A14 | 112.21242925 |
| A15 | 105.05282363 |
| A16 | 109.42384384 |
| A17 | 110.34185917 |
| A18 | 109.34421582 |
| A19 | 90.20219656 |
| A20 | 35.28236338 |
| A21 | 104.57376450 |
| A22 | 109.59625653 |
| A23 | 108.36075782 |

| | |
|-----|---------------|
| A24 | 103.97156694 |
| A25 | 110.96793453 |
| A26 | 108.84490399 |
| A27 | 109.24775055 |
| A28 | 112.89310615 |
| A29 | 109.01917383 |
| A30 | 110.74594179 |
| A31 | 109.11393009 |
| A32 | 110.41064844 |
| A33 | 110.08050208 |
| A34 | 102.33085284 |
| D1 | 120.57574930 |
| D2 | 119.20701844 |
| D3 | 63.45308665 |
| D4 | -49.94534562 |
| D5 | 69.01527944 |
| D6 | -169.71740223 |
| D7 | 130.77809170 |
| D8 | -169.12418787 |
| D9 | -85.30612839 |
| D10 | 49.32201141 |
| D11 | 53.35693515 |
| D12 | 172.21135225 |
| D13 | -68.20450785 |
| D14 | 172.13098980 |
| D15 | -69.04283053 |
| D16 | 50.81040881 |
| D17 | 170.96261062 |
| D18 | -97.72722464 |
| D19 | 125.03390516 |
| D20 | 154.90226086 |
| D21 | 64.34663352 |
| D22 | 139.09039004 |
| D23 | 165.80616169 |
| D24 | 46.06274937 |
| D25 | 165.89127130 |
| D26 | -74.41057639 |
| D27 | 43.10664219 |
| D28 | 167.29556928 |
| D29 | -72.44074115 |
| D30 | 47.72235712 |
| D31 | -72.96806768 |
| D32 | -71.06835049 |
| D33 | 87.04093739 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 35.47 | 50.66 | 59.60 | 97.09 | 123.89 | 155.80 | 173.47 | 187.11 | 201.54 | 214.32 | 217.52 |
| 234.65 | 242.67 | 260.76 | 267.56 | 279.87 | 289.69 | 291.18 | 319.90 | 345.63 | 354.00 | |
| 372.13 | 376.80 | 379.05 | 390.74 | 398.17 | 425.93 | 436.68 | 496.83 | 533.62 | 550.47 | |
| 594.88 | 614.02 | 624.51 | 643.70 | 754.66 | 825.24 | 852.65 | 898.33 | 919.68 | 925.12 | |
| 939.42 | 947.80 | 963.56 | 969.41 | 980.40 | 1018.73 | 1021.83 | 1030.82 | 1052.43 | 1057.83 | |
| 1065.24 | 1073.37 | 1192.74 | 1214.04 | 1235.74 | 1246.30 | 1252.58 | 1262.57 | 1274.03 | | |
| 1305.90 | 1320.98 | 1402.53 | 1409.09 | 1414.83 | 1418.57 | 1422.21 | 1423.27 | 1428.65 | | |
| 1458.31 | 1474.49 | 1482.57 | 1483.23 | 1486.44 | 1487.08 | 1494.25 | 1497.55 | 1499.73 | | |
| 1507.11 | 1507.55 | 1514.32 | 1531.37 | 3054.27 | 3073.41 | 3074.80 | 3077.38 | 3079.38 | | |
| 3082.47 | 3138.82 | 3151.43 | 3151.86 | 3156.02 | 3156.53 | 3159.49 | 3163.15 | 3163.56 | | |
| 3167.95 | 3173.02 | 3177.96 | 3180.86 | 3757.38 | 3823.75 | | | | | |

Rotational constants (B/GHZ): 0.9827454 0.2863241 0.2751025



IM8g

| C | | | | | | | |
|---|----|--|-----|---|-----|---|-------|
| O | 1 | | B1 | | | | |
| O | 1 | | B2 | 2 | A1 | | |
| H | 2 | | B3 | 1 | A2 | 3 | D1 0 |
| C | 3 | | B4 | 1 | A3 | 2 | D2 0 |
| C | 5 | | B5 | 3 | A4 | 1 | D3 0 |
| H | 6 | | B6 | 5 | A5 | 3 | D4 0 |
| H | 6 | | B7 | 5 | A6 | 3 | D5 0 |
| H | 6 | | B8 | 5 | A7 | 3 | D6 0 |
| C | 5 | | B9 | 3 | A8 | 1 | D7 0 |
| H | 10 | | B10 | 5 | A9 | 3 | D8 0 |
| H | 10 | | B11 | 5 | A10 | 3 | D9 0 |
| H | 10 | | B12 | 5 | A11 | 3 | D10 0 |
| O | 5 | | B13 | 3 | A12 | 1 | D11 0 |
| O | 5 | | B14 | 3 | A13 | 1 | D12 0 |
| C | 1 | | B15 | 3 | A14 | 2 | D13 0 |
| H | 16 | | B16 | 1 | A15 | 3 | D14 0 |
| H | 16 | | B17 | 1 | A16 | 3 | D15 0 |
| H | 16 | | B18 | 1 | A17 | 3 | D16 0 |
| C | 1 | | B19 | 3 | A18 | 2 | D17 0 |
| H | 20 | | B20 | 1 | A19 | 3 | D18 0 |
| H | 20 | | B21 | 1 | A20 | 3 | D19 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 20 | B22 | 1 | A21 | 3 | D20 | 0 |
| O | 1 | B23 | 3 | A22 | 2 | D21 | 0 |
| C | 24 | B24 | 1 | A23 | 3 | D22 | 0 |
| C | 25 | B25 | 24 | A24 | 1 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 24 | D24 | 0 |
| H | 26 | B27 | 25 | A26 | 24 | D25 | 0 |
| H | 26 | B28 | 25 | A27 | 24 | D26 | 0 |
| C | 25 | B29 | 24 | A28 | 1 | D27 | 0 |
| H | 30 | B30 | 25 | A29 | 24 | D28 | 0 |
| H | 30 | B31 | 25 | A30 | 24 | D29 | 0 |
| H | 30 | B32 | 25 | A31 | 24 | D30 | 0 |
| O | 25 | B33 | 24 | A32 | 1 | D31 | 0 |
| O | 34 | B34 | 25 | A33 | 24 | D32 | 0 |
| H | 35 | B35 | 34 | A34 | 25 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 2.31853844 |
| B2 | 1.41828594 |
| B3 | 0.99408782 |
| B4 | 2.78739122 |
| B5 | 1.48250182 |
| B6 | 1.08606723 |
| B7 | 1.09246637 |
| B8 | 1.09018543 |
| B9 | 1.47262944 |
| B10 | 1.09393184 |
| B11 | 1.09045301 |
| B12 | 1.08571693 |
| B13 | 2.25215948 |
| B14 | 1.24795013 |
| B15 | 1.51928968 |
| B16 | 1.08845269 |
| B17 | 1.08843900 |
| B18 | 1.08604480 |
| B19 | 1.52389330 |
| B20 | 1.08857806 |
| B21 | 1.08847642 |
| B22 | 1.08785285 |
| B23 | 1.39828603 |
| B24 | 1.42439799 |
| B25 | 1.52310456 |
| B26 | 1.08885652 |
| B27 | 1.08682775 |
| B28 | 1.08704711 |
| B29 | 1.51668841 |

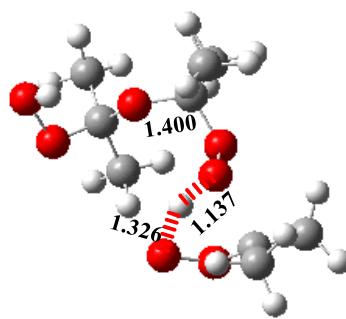
| | |
|-----|--------------|
| B30 | 1.08700260 |
| B31 | 1.08787657 |
| B32 | 1.08898064 |
| B33 | 1.41270178 |
| B34 | 1.41411684 |
| B35 | 0.96632749 |
| A1 | 35.39701443 |
| A2 | 123.39208814 |
| A3 | 155.63149642 |
| A4 | 100.17279658 |
| A5 | 111.00168193 |
| A6 | 107.63720103 |
| A7 | 110.09414549 |
| A8 | 90.36040851 |
| A9 | 108.11610179 |
| A10 | 108.67641230 |
| A11 | 110.80685276 |
| A12 | 74.48041482 |
| A13 | 78.49651031 |
| A14 | 110.80310733 |
| A15 | 109.87803335 |
| A16 | 109.41046141 |
| A17 | 109.54937119 |
| A18 | 102.86686799 |
| A19 | 109.15550229 |
| A20 | 111.39677123 |
| A21 | 109.56158283 |
| A22 | 112.32176818 |
| A23 | 125.36751287 |
| A24 | 111.53900694 |
| A25 | 108.56790299 |
| A26 | 110.29429350 |
| A27 | 111.28177260 |
| A28 | 114.64191989 |
| A29 | 110.99997089 |
| A30 | 110.74060395 |
| A31 | 108.21426067 |
| A32 | 103.65906677 |
| A33 | 109.53162590 |
| A34 | 101.44787439 |
| D1 | -55.77706272 |
| D2 | 165.81927776 |
| D3 | 19.23014080 |
| D4 | -84.77776431 |

| | |
|-----|---------------|
| D5 | 35.49337289 |
| D6 | 152.58071343 |
| D7 | 142.86109003 |
| D8 | 6.64142460 |
| D9 | 121.60018803 |
| D10 | -114.54392638 |
| D11 | -128.99304855 |
| D12 | -95.15201306 |
| D13 | 53.53964410 |
| D14 | 52.04904216 |
| D15 | 172.20518153 |
| D16 | -67.98070988 |
| D17 | 172.70364417 |
| D18 | -66.73981256 |
| D19 | 53.18896654 |
| D20 | 174.04251048 |
| D21 | -63.36827522 |
| D22 | -66.54062301 |
| D23 | -83.06597635 |
| D24 | -161.42384972 |
| D25 | -42.35124530 |
| D26 | 79.25164638 |
| D27 | 47.25467762 |
| D28 | -68.61741084 |
| D29 | 52.36682363 |
| D30 | 172.05643725 |
| D31 | 158.52462700 |
| D32 | 61.42543371 |
| D33 | -76.68264449 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 39.46 | 40.92 | 66.54 | 75.64 | 94.93 | 111.47 | 128.11 | 133.60 | 152.44 | 179.44 | 194.76 |
| 206.61 | 209.89 | 222.88 | 241.77 | 274.71 | 298.65 | 324.71 | 328.15 | 328.88 | 335.53 | |
| 338.39 | 360.21 | 373.35 | 378.54 | 390.91 | 407.13 | 414.46 | 485.07 | 501.60 | 536.55 | |
| 557.60 | 598.89 | 602.09 | 637.28 | 754.66 | 785.13 | 831.81 | 849.79 | 902.61 | 915.90 | |
| 924.30 | 940.25 | 946.28 | 956.00 | 973.17 | 990.14 | 1020.82 | 1023.84 | 1056.88 | 1066.23 | |
| 1077.33 | 1091.50 | 1110.38 | 1201.45 | 1232.76 | 1249.27 | 1263.11 | 1280.17 | 1303.03 | | |
| 1318.02 | 1395.52 | 1405.59 | 1410.24 | 1410.77 | 1417.89 | 1427.07 | 1443.41 | 1450.91 | | |
| 1468.08 | 1477.98 | 1480.72 | 1482.65 | 1490.82 | 1491.13 | 1494.74 | 1499.61 | 1504.56 | | |
| 1517.38 | 1521.01 | 1620.56 | 1673.43 | 3048.56 | 3060.79 | 3066.12 | 3075.49 | 3079.30 | | |
| 3084.41 | 3114.73 | 3127.24 | 3143.47 | 3148.73 | 3155.47 | 3162.60 | 3164.79 | 3168.52 | | |
| 3170.76 | 3172.61 | 3174.38 | 3176.72 | 3203.82 | 3803.72 | | | | | |

Rotational constants (B/GHZ): 0.7920870 0.3283419 0.3053114



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C

| | | | | | | |
|---|----|-----|----|-----|----|-------|
| O | 1 | B1 | | | | |
| O | 2 | B2 | 1 | A1 | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 0 |
| C | 2 | B4 | 1 | A3 | 3 | D2 0 |
| C | 5 | B5 | 2 | A4 | 1 | D3 0 |
| H | 6 | B6 | 5 | A5 | 2 | D4 0 |
| H | 6 | B7 | 5 | A6 | 2 | D5 0 |
| H | 6 | B8 | 5 | A7 | 2 | D6 0 |
| C | 5 | B9 | 2 | A8 | 1 | D7 0 |
| H | 10 | B10 | 5 | A9 | 2 | D8 0 |
| H | 10 | B11 | 5 | A10 | 2 | D9 0 |
| H | 10 | B12 | 5 | A11 | 2 | D10 0 |
| O | 5 | B13 | 2 | A12 | 1 | D11 0 |
| O | 5 | B14 | 2 | A13 | 1 | D12 0 |
| C | 1 | B15 | 3 | A14 | 2 | D13 0 |
| H | 16 | B16 | 1 | A15 | 3 | D14 0 |
| H | 16 | B17 | 1 | A16 | 3 | D15 0 |
| H | 16 | B18 | 1 | A17 | 3 | D16 0 |
| C | 1 | B19 | 3 | A18 | 2 | D17 0 |
| H | 20 | B20 | 1 | A19 | 3 | D18 0 |
| H | 20 | B21 | 1 | A20 | 3 | D19 0 |
| H | 20 | B22 | 1 | A21 | 3 | D20 0 |
| O | 1 | B23 | 3 | A22 | 2 | D21 0 |
| C | 24 | B24 | 1 | A23 | 3 | D22 0 |
| C | 25 | B25 | 24 | A24 | 1 | D23 0 |
| H | 26 | B26 | 25 | A25 | 24 | D24 0 |
| H | 26 | B27 | 25 | A26 | 24 | D25 0 |
| H | 26 | B28 | 25 | A27 | 24 | D26 0 |
| C | 25 | B29 | 24 | A28 | 1 | D27 0 |
| H | 30 | B30 | 25 | A29 | 24 | D28 0 |
| H | 30 | B31 | 25 | A30 | 24 | D29 0 |
| H | 30 | B32 | 25 | A31 | 24 | D30 0 |
| O | 25 | B33 | 24 | A32 | 1 | D31 0 |
| O | 34 | B34 | 25 | A33 | 24 | D32 0 |

| H | 35 | B35 | 34 | A34 | 25 | D33 | 0 |
|------------|----|--------------|----|-----|----|-----|---|
| Variables: | | | | | | | |
| B1 | | 2.32210448 | | | | | |
| B2 | | 1.41592847 | | | | | |
| B3 | | 1.13656547 | | | | | |
| B4 | | 2.05629839 | | | | | |
| B5 | | 1.48482728 | | | | | |
| B6 | | 1.08561491 | | | | | |
| B7 | | 1.09064008 | | | | | |
| B8 | | 1.08945983 | | | | | |
| B9 | | 1.48929130 | | | | | |
| B10 | | 1.08644313 | | | | | |
| B11 | | 1.08269620 | | | | | |
| B12 | | 1.09389284 | | | | | |
| B13 | | 2.21323193 | | | | | |
| B14 | | 1.28136631 | | | | | |
| B15 | | 1.51985831 | | | | | |
| B16 | | 1.08859619 | | | | | |
| B17 | | 1.08847567 | | | | | |
| B18 | | 1.08560528 | | | | | |
| B19 | | 1.52289209 | | | | | |
| B20 | | 1.08801294 | | | | | |
| B21 | | 1.08668351 | | | | | |
| B22 | | 1.08758830 | | | | | |
| B23 | | 1.40019361 | | | | | |
| B24 | | 1.42952427 | | | | | |
| B25 | | 1.52422844 | | | | | |
| B26 | | 1.08867271 | | | | | |
| B27 | | 1.08683934 | | | | | |
| B28 | | 1.08683289 | | | | | |
| B29 | | 1.51756572 | | | | | |
| B30 | | 1.08632739 | | | | | |
| B31 | | 1.08770826 | | | | | |
| B32 | | 1.08916914 | | | | | |
| B33 | | 1.41139928 | | | | | |
| B34 | | 1.41454750 | | | | | |
| B35 | | 0.96618600 | | | | | |
| A1 | | 35.20319587 | | | | | |
| A2 | | 106.45019894 | | | | | |
| A3 | | 136.95684885 | | | | | |
| A4 | | 107.40000050 | | | | | |
| A5 | | 110.69825837 | | | | | |
| A6 | | 107.08932879 | | | | | |
| A7 | | 110.19837405 | | | | | |

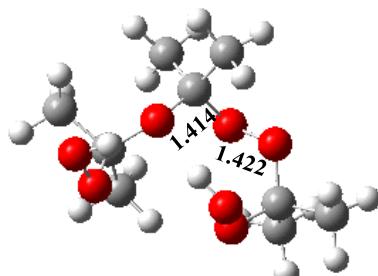
| | |
|-----|--------------|
| A8 | 90.98183625 |
| A9 | 109.61461942 |
| A10 | 111.88785221 |
| A11 | 106.30250244 |
| A12 | 67.71480690 |
| A13 | 90.97640390 |
| A14 | 111.22881191 |
| A15 | 109.78299764 |
| A16 | 109.10323845 |
| A17 | 110.12483942 |
| A18 | 103.18592891 |
| A19 | 108.69572466 |
| A20 | 111.87768147 |
| A21 | 109.51047365 |
| A22 | 111.07844750 |
| A23 | 124.94060005 |
| A24 | 111.69789769 |
| A25 | 108.27906484 |
| A26 | 110.59975367 |
| A27 | 111.18836855 |
| A28 | 114.64747914 |
| A29 | 111.09753033 |
| A30 | 110.26150076 |
| A31 | 108.08616627 |
| A32 | 103.29184706 |
| A33 | 109.50353012 |
| A34 | 101.51795860 |
| D1 | -93.24753495 |
| D2 | -7.60476205 |
| D3 | 48.53986448 |
| D4 | -95.04524278 |
| D5 | 23.78551328 |
| D6 | 141.59935625 |
| D7 | 169.80344290 |
| D8 | -67.12587435 |
| D9 | 56.46320559 |
| D10 | 175.56604397 |
| D11 | -97.17945785 |
| D12 | -67.52221967 |
| D13 | 48.14996969 |
| D14 | 49.72754848 |
| D15 | 169.56973472 |
| D16 | -70.51500502 |
| D17 | 167.00506191 |

| | |
|-----|---------------|
| D18 | -66.52233343 |
| D19 | 53.15991507 |
| D20 | 174.54391476 |
| D21 | -68.67370834 |
| D22 | -73.07142732 |
| D23 | -79.81703988 |
| D24 | -157.52244561 |
| D25 | -38.54249103 |
| D26 | 83.42478458 |
| D27 | 50.55552095 |
| D28 | -64.58098663 |
| D29 | 56.36092132 |
| D30 | 176.06185134 |
| D31 | 161.80059164 |
| D32 | 63.24565856 |
| D33 | -76.83444381 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-----------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 764.48 <i>i</i> | 30.41 | 45.26 | 83.37 | 88.13 | 116.58 | 119.94 | 134.91 | 154.44 | 179.36 | 194.44 |
| 214.08 | 226.50 | 228.49 | 255.67 | 265.53 | 280.87 | 293.57 | 311.91 | 322.98 | 343.85 | |
| 356.90 | 367.78 | 374.63 | 383.64 | 391.11 | 414.19 | 427.89 | 482.96 | 533.45 | 545.56 | |
| 554.32 | 575.87 | 624.66 | 637.38 | 752.89 | 808.23 | 848.80 | 879.67 | 902.09 | 922.09 | |
| 943.62 | 945.06 | 948.99 | 961.03 | 973.21 | 982.53 | 1019.96 | 1023.32 | 1054.68 | 1069.06 | |
| 1081.78 | 1082.71 | 1120.45 | 1205.52 | 1227.88 | 1247.91 | 1259.95 | 1280.15 | 1303.90 | | |
| 1313.61 | 1402.33 | 1407.58 | 1408.78 | 1418.75 | 1421.21 | 1429.94 | 1441.62 | 1448.56 | | |
| 1458.61 | 1472.61 | 1477.04 | 1484.70 | 1489.48 | 1493.18 | 1496.87 | 1497.43 | 1501.80 | | |
| 1512.33 | 1516.81 | 1582.38 | 1612.79 | 1784.91 | 3051.91 | 3072.68 | 3073.11 | 3075.43 | | |
| 3076.23 | 3080.81 | 3144.78 | 3147.92 | 3149.71 | 3151.04 | 3154.73 | 3159.15 | 3165.67 | | |
| 3171.62 | 3172.73 | 3179.56 | 3184.04 | 3209.60 | 3805.94 | | | | | |

Rotational constants (B/GHZ): 0.8198346 0.3409872 0.3016902



P8g

| | | | | | | | |
|---|---|----|----|----|---|----|---|
| C | | | | | | | |
| O | 1 | | B1 | | | | |
| O | 1 | B2 | 2 | A1 | | | |
| H | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| C | 2 | B4 | 1 | A3 | 3 | D2 | 0 |
| C | 5 | B5 | 2 | A4 | 1 | D3 | 0 |
| H | 6 | B6 | 5 | A5 | 2 | D4 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 6 | B7 | 5 | A6 | 2 | D5 | 0 |
| H | 6 | B8 | 5 | A7 | 2 | D6 | 0 |
| C | 5 | B9 | 2 | A8 | 1 | D7 | 0 |
| H | 10 | B10 | 5 | A9 | 2 | D8 | 0 |
| H | 10 | B11 | 5 | A10 | 2 | D9 | 0 |
| H | 10 | B12 | 5 | A11 | 2 | D10 | 0 |
| O | 5 | B13 | 2 | A12 | 1 | D11 | 0 |
| O | 5 | B14 | 2 | A13 | 1 | D12 | 0 |
| C | 1 | B15 | 3 | A14 | 2 | D13 | 0 |
| H | 16 | B16 | 1 | A15 | 3 | D14 | 0 |
| H | 16 | B17 | 1 | A16 | 3 | D15 | 0 |
| H | 16 | B18 | 1 | A17 | 3 | D16 | 0 |
| C | 1 | B19 | 3 | A18 | 2 | D17 | 0 |
| H | 20 | B20 | 1 | A19 | 3 | D18 | 0 |
| H | 20 | B21 | 1 | A20 | 3 | D19 | 0 |
| H | 20 | B22 | 1 | A21 | 3 | D20 | 0 |
| O | 1 | B23 | 3 | A22 | 2 | D21 | 0 |
| C | 24 | B24 | 1 | A23 | 3 | D22 | 0 |
| C | 25 | B25 | 24 | A24 | 1 | D23 | 0 |
| H | 26 | B26 | 25 | A25 | 24 | D24 | 0 |
| H | 26 | B27 | 25 | A26 | 24 | D25 | 0 |
| H | 26 | B28 | 25 | A27 | 24 | D26 | 0 |
| C | 25 | B29 | 24 | A28 | 1 | D27 | 0 |
| H | 30 | B30 | 25 | A29 | 24 | D28 | 0 |
| H | 30 | B31 | 25 | A30 | 24 | D29 | 0 |
| H | 30 | B32 | 25 | A31 | 24 | D30 | 0 |
| O | 25 | B33 | 24 | A32 | 1 | D31 | 0 |
| O | 34 | B34 | 25 | A33 | 24 | D32 | 0 |
| H | 35 | B35 | 34 | A34 | 25 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 2.32158435 |
| B2 | 1.42022542 |
| B3 | 2.64911617 |
| B4 | 1.41310944 |
| B5 | 1.51631171 |
| B6 | 1.08685373 |
| B7 | 1.08802861 |
| B8 | 1.08783284 |
| B9 | 1.51793281 |
| B10 | 1.08769932 |
| B11 | 1.08644205 |
| B12 | 1.08802661 |
| B13 | 2.30820016 |
| B14 | 1.40780521 |

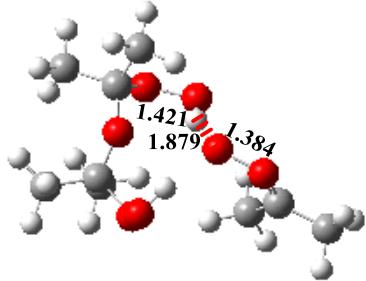
| | |
|-----|--------------|
| B15 | 1.51981948 |
| B16 | 1.08788338 |
| B17 | 1.08829814 |
| B18 | 1.08636329 |
| B19 | 1.52252668 |
| B20 | 1.08752177 |
| B21 | 1.08670405 |
| B22 | 1.08715216 |
| B23 | 1.41426041 |
| B24 | 1.43578929 |
| B25 | 1.52346863 |
| B26 | 1.08856740 |
| B27 | 1.08656004 |
| B28 | 1.08620012 |
| B29 | 1.51805972 |
| B30 | 1.08671291 |
| B31 | 1.08617830 |
| B32 | 1.08874064 |
| B33 | 1.41052186 |
| B34 | 1.41504141 |
| B35 | 0.96508612 |
| A1 | 35.26321706 |
| A2 | 68.08487571 |
| A3 | 127.65520861 |
| A4 | 112.69575386 |
| A5 | 110.39109228 |
| A6 | 109.07805534 |
| A7 | 109.49573294 |
| A8 | 103.38811872 |
| A9 | 109.99500913 |
| A10 | 110.19505770 |
| A11 | 108.52677048 |
| A12 | 90.36764045 |
| A13 | 111.07515571 |
| A14 | 112.04002922 |
| A15 | 109.91841814 |
| A16 | 108.73127151 |
| A17 | 110.46372841 |
| A18 | 103.29026199 |
| A19 | 108.05507898 |
| A20 | 112.24055157 |
| A21 | 109.88623948 |
| A22 | 111.10050208 |
| A23 | 124.81501055 |

| | |
|-----|---------------|
| A24 | 112.20939126 |
| A25 | 108.06581592 |
| A26 | 110.95904285 |
| A27 | 111.13399794 |
| A28 | 114.09979369 |
| A29 | 110.92784598 |
| A30 | 109.78191471 |
| A31 | 108.29743922 |
| A32 | 103.15395489 |
| A33 | 109.84998723 |
| A34 | 102.38554809 |
| D1 | -121.15436441 |
| D2 | -71.85217268 |
| D3 | 86.46636630 |
| D4 | -65.19704925 |
| D5 | 54.77521231 |
| D6 | 174.45547251 |
| D7 | -150.74901670 |
| D8 | -65.88193068 |
| D9 | 55.00452859 |
| D10 | 174.36852136 |
| D11 | -59.42185252 |
| D12 | -30.26898840 |
| D13 | 36.82466006 |
| D14 | 48.45958330 |
| D15 | 168.38205868 |
| D16 | -71.71979843 |
| D17 | 155.79598382 |
| D18 | -66.64491941 |
| D19 | 52.43441143 |
| D20 | 174.49264228 |
| D21 | -80.19009417 |
| D22 | -76.78326004 |
| D23 | -76.56902352 |
| D24 | -154.02023340 |
| D25 | -35.08671776 |
| D26 | 87.15965277 |
| D27 | 53.60682935 |
| D28 | -62.40320359 |
| D29 | 58.20166096 |
| D30 | 178.08389873 |
| D31 | 164.64656410 |
| D32 | 70.01985496 |
| D33 | -88.18945459 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 23.87 | 61.52 | 90.32 | 117.11 | 130.85 | 133.62 | 148.00 | 174.33 | 180.32 | 202.26 | 219.87 |
| 228.57 | 232.74 | 254.29 | 273.52 | 276.02 | 287.07 | 298.26 | 307.72 | 322.82 | 340.87 | |
| 356.25 | 377.32 | 380.19 | 383.38 | 427.70 | 446.06 | 501.10 | 504.26 | 547.58 | 554.47 | |
| 589.95 | 597.63 | 631.85 | 640.56 | 750.53 | 831.09 | 853.23 | 895.23 | 913.31 | 928.43 | |
| 945.59 | 948.34 | 951.43 | 965.43 | 975.31 | 1019.67 | 1021.40 | 1030.53 | 1042.03 | 1057.02 | |
| 1066.07 | 1072.59 | 1174.89 | 1217.48 | 1230.64 | 1247.96 | 1249.10 | 1259.18 | 1283.94 | | |
| 1297.79 | 1317.47 | 1409.15 | 1410.12 | 1412.96 | 1416.74 | 1419.35 | 1424.44 | 1427.12 | | |
| 1471.60 | 1477.90 | 1479.99 | 1485.43 | 1487.45 | 1489.99 | 1493.45 | 1497.80 | 1503.50 | | |
| 1504.82 | 1514.74 | 1517.27 | 1519.46 | 3069.10 | 3071.26 | 3072.55 | 3075.58 | 3081.78 | | |
| 3085.94 | 3149.66 | 3151.50 | 3151.59 | 3156.22 | 3157.00 | 3158.10 | 3162.58 | 3168.45 | | |
| 3169.81 | 3173.10 | 3176.29 | 3177.93 | 3710.63 | 3832.86 | | | | | |

Rotational constants (B/GHZ): 0.7707336 0.4206507 0.3623053



IM8h

| C | | | | | | | |
|---|----|--|-----|----|-----|----|-------|
| C | 1 | | B1 | | | | |
| O | 2 | | B2 | 1 | A1 | | |
| O | 3 | | B3 | 2 | A2 | 1 | D1 0 |
| H | 3 | | B4 | 2 | A3 | 1 | D2 0 |
| C | 3 | | B5 | 2 | A4 | 1 | D3 0 |
| C | 6 | | B6 | 3 | A5 | 2 | D4 0 |
| H | 7 | | B7 | 6 | A6 | 3 | D5 0 |
| H | 7 | | B8 | 6 | A7 | 3 | D6 0 |
| H | 7 | | B9 | 6 | A8 | 3 | D7 0 |
| O | 6 | | B10 | 3 | A9 | 2 | D8 0 |
| O | 6 | | B11 | 3 | A10 | 2 | D9 0 |
| H | 1 | | B12 | 2 | A11 | 4 | D10 0 |
| H | 1 | | B13 | 2 | A12 | 4 | D11 0 |
| H | 1 | | B14 | 2 | A13 | 4 | D12 0 |
| O | 2 | | B15 | 1 | A14 | 4 | D13 0 |
| C | 16 | | B16 | 2 | A15 | 1 | D14 0 |
| C | 17 | | B17 | 16 | A16 | 2 | D15 0 |
| H | 18 | | B18 | 17 | A17 | 16 | D16 0 |
| H | 18 | | B19 | 17 | A18 | 16 | D17 0 |
| H | 18 | | B20 | 17 | A19 | 16 | D18 0 |
| O | 17 | | B21 | 16 | A20 | 2 | D19 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| O | 22 | B22 | 17 | A21 | 16 | D20 | 0 |
| H | 23 | B23 | 22 | A22 | 17 | D21 | 0 |
| C | 6 | B24 | 3 | A23 | 2 | D22 | 0 |
| H | 25 | B25 | 6 | A24 | 3 | D23 | 0 |
| H | 25 | B26 | 6 | A25 | 3 | D24 | 0 |
| H | 25 | B27 | 6 | A26 | 3 | D25 | 0 |
| C | 2 | B28 | 1 | A27 | 16 | D26 | 0 |
| H | 29 | B29 | 2 | A28 | 1 | D27 | 0 |
| H | 29 | B30 | 2 | A29 | 1 | D28 | 0 |
| H | 29 | B31 | 2 | A30 | 1 | D29 | 0 |
| C | 17 | B32 | 16 | A31 | 2 | D30 | 0 |
| H | 33 | B33 | 17 | A32 | 16 | D31 | 0 |
| H | 33 | B34 | 17 | A33 | 16 | D32 | 0 |
| H | 33 | B35 | 17 | A34 | 16 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.51757346 |
| B2 | 2.33124472 |
| B3 | 1.41232900 |
| B4 | 0.98229453 |
| B5 | 3.87534454 |
| B6 | 1.46983004 |
| B7 | 1.09561361 |
| B8 | 1.09504700 |
| B9 | 1.08551692 |
| B10 | 2.25308028 |
| B11 | 1.25008227 |
| B12 | 1.08884807 |
| B13 | 1.08892004 |
| B14 | 1.08722879 |
| B15 | 1.41881719 |
| B16 | 1.40995222 |
| B17 | 1.52134576 |
| B18 | 1.08729468 |
| B19 | 1.08828145 |
| B20 | 1.08831320 |
| B21 | 1.41103678 |
| B22 | 1.42113531 |
| B23 | 0.98078727 |
| B24 | 1.48352230 |
| B25 | 1.09119925 |
| B26 | 1.09103232 |
| B27 | 1.08559750 |
| B28 | 1.52245523 |
| B29 | 1.08902441 |

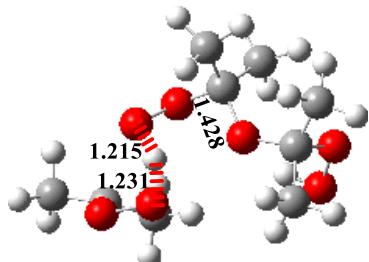
| | |
|-----|---------------|
| B30 | 1.08489540 |
| B31 | 1.08712097 |
| B32 | 1.52097894 |
| B33 | 1.08612564 |
| B34 | 1.08818976 |
| B35 | 1.08813734 |
| A1 | 93.41099525 |
| A2 | 34.74323489 |
| A3 | 94.86131564 |
| A4 | 100.03218726 |
| A5 | 74.16746429 |
| A6 | 109.07054232 |
| A7 | 108.93647042 |
| A8 | 110.78946552 |
| A9 | 43.96847222 |
| A10 | 62.36383670 |
| A11 | 110.27931618 |
| A12 | 109.81402251 |
| A13 | 109.13845780 |
| A14 | 109.27090144 |
| A15 | 125.38965377 |
| A16 | 104.67252562 |
| A17 | 110.58982293 |
| A18 | 109.26491566 |
| A19 | 109.21800086 |
| A20 | 109.89564676 |
| A21 | 110.22178497 |
| A22 | 105.50092919 |
| A23 | 138.14031110 |
| A24 | 108.85921965 |
| A25 | 109.00226767 |
| A26 | 111.21570886 |
| A27 | 113.42667137 |
| A28 | 107.51911212 |
| A29 | 112.10750224 |
| A30 | 110.45023751 |
| A31 | 114.67621786 |
| A32 | 112.31318442 |
| A33 | 108.87900767 |
| A34 | 109.00543121 |
| D1 | 121.87692637 |
| D2 | -136.90676523 |
| D3 | 178.19168689 |
| D4 | -33.71324886 |

| | |
|-----|---------------|
| D5 | -9.07370884 |
| D6 | 105.49957591 |
| D7 | -132.91647803 |
| D8 | 70.95554472 |
| D9 | 105.79596058 |
| D10 | -177.70479024 |
| D11 | -57.56257245 |
| D12 | 62.24906627 |
| D13 | -115.35959741 |
| D14 | -97.13033404 |
| D15 | 176.11726054 |
| D16 | 48.97727829 |
| D17 | 169.64275749 |
| D18 | -70.46332555 |
| D19 | -63.42705496 |
| D20 | -61.95462750 |
| D21 | 33.59558227 |
| D22 | -155.86585644 |
| D23 | 44.37192781 |
| D24 | 160.93710725 |
| D25 | -77.25460418 |
| D26 | -131.72966213 |
| D27 | -60.78390532 |
| D28 | 58.55573637 |
| D29 | 179.71344320 |
| D30 | 54.19287541 |
| D31 | -66.25256140 |
| D32 | 54.88780737 |
| D33 | 173.61597745 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|---------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 25.10 | 43.77 | 67.81 | 87.71 | 94.80 | 112.07 | 132.92 | 136.58 | 154.59 | 171.32 | 193.69 |
| 211.31 | 228.78 | 242.75 | 257.30 | 267.25 | 272.43 | 291.80 | 303.29 | 332.85 | 338.95 | |
| 349.99 | 358.25 | 376.55 | 385.62 | 387.66 | 407.58 | 475.76 | 506.95 | 522.65 | 565.57 | |
| 597.79 | 608.02 | 636.52 | 662.01 | 752.33 | 773.09 | 832.25 | 847.80 | 893.53 | 914.40 | |
| 925.77 | 938.27 | 951.71 | 958.90 | 973.09 | 995.00 | 1019.67 | 1024.46 | 1058.25 | 1070.18 | |
| 1078.10 | 1096.48 | 1106.07 | 1194.96 | 1228.46 | 1248.08 | 1261.41 | 1270.76 | 1305.89 | | |
| 1320.42 | 1397.15 | 1405.55 | 1411.24 | 1413.01 | 1423.59 | 1428.19 | 1452.13 | 1466.16 | | |
| 1472.64 | 1477.84 | 1484.33 | 1487.50 | 1489.02 | 1491.70 | 1501.38 | 1503.26 | 1509.00 | | |
| 1516.15 | 1518.04 | 1548.57 | 1663.14 | 3027.98 | 3056.04 | 3068.90 | 3069.71 | 3081.23 | | |
| 3082.98 | 3088.85 | 3117.08 | 3147.86 | 3149.39 | 3159.68 | 3162.07 | 3162.81 | 3163.44 | | |
| 3166.36 | 3171.44 | 3182.07 | 3191.66 | 3476.22 | 3561.38 | | | | | |

Rotational constants (B/GHZ): 0.7665196 0.3543521 0.3034123



TS8h

| C | | B1 | | | | |
|---|----|-----|----|-----|----|-------|
| C | 1 | | | | | |
| O | 2 | B2 | 1 | A1 | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 0 |
| H | 3 | B4 | 2 | A3 | 1 | D2 0 |
| C | 3 | B5 | 2 | A4 | 1 | D3 0 |
| C | 6 | B6 | 3 | A5 | 2 | D4 0 |
| H | 7 | B7 | 6 | A6 | 3 | D5 0 |
| H | 7 | B8 | 6 | A7 | 3 | D6 0 |
| H | 7 | B9 | 6 | A8 | 3 | D7 0 |
| O | 6 | B10 | 3 | A9 | 2 | D8 0 |
| O | 6 | B11 | 3 | A10 | 2 | D9 0 |
| H | 1 | B12 | 2 | A11 | 4 | D10 0 |
| H | 1 | B13 | 2 | A12 | 4 | D11 0 |
| H | 1 | B14 | 2 | A13 | 4 | D12 0 |
| O | 2 | B15 | 1 | A14 | 4 | D13 0 |
| C | 16 | B16 | 2 | A15 | 1 | D14 0 |
| C | 17 | B17 | 16 | A16 | 2 | D15 0 |
| H | 18 | B18 | 17 | A17 | 16 | D16 0 |
| H | 18 | B19 | 17 | A18 | 16 | D17 0 |
| H | 18 | B20 | 17 | A19 | 16 | D18 0 |
| O | 17 | B21 | 16 | A20 | 2 | D19 0 |
| O | 22 | B22 | 17 | A21 | 16 | D20 0 |
| H | 23 | B23 | 22 | A22 | 17 | D21 0 |
| C | 6 | B24 | 3 | A23 | 2 | D22 0 |
| H | 25 | B25 | 6 | A24 | 3 | D23 0 |
| H | 25 | B26 | 6 | A25 | 3 | D24 0 |
| H | 25 | B27 | 6 | A26 | 3 | D25 0 |
| C | 2 | B28 | 1 | A27 | 4 | D26 0 |
| H | 29 | B29 | 2 | A28 | 1 | D27 0 |
| H | 29 | B30 | 2 | A29 | 1 | D28 0 |
| H | 29 | B31 | 2 | A30 | 1 | D29 0 |
| C | 17 | B32 | 16 | A31 | 2 | D30 0 |
| H | 33 | B33 | 17 | A32 | 16 | D31 0 |
| H | 33 | B34 | 17 | A33 | 16 | D32 0 |
| H | 33 | B35 | 17 | A34 | 16 | D33 0 |

Variables:

| | |
|-----|--------------|
| B1 | 1.52214374 |
| B2 | 2.31717819 |
| B3 | 1.40702772 |
| B4 | 1.21538070 |
| B5 | 2.18173445 |
| B6 | 1.48202667 |
| B7 | 1.08745813 |
| B8 | 1.08378641 |
| B9 | 1.09474741 |
| B10 | 2.21506623 |
| B11 | 1.27670481 |
| B12 | 1.08704920 |
| B13 | 1.08856099 |
| B14 | 1.08698123 |
| B15 | 1.42802621 |
| B16 | 1.40557612 |
| B17 | 1.51785276 |
| B18 | 1.08611283 |
| B19 | 1.08839303 |
| B20 | 1.08836856 |
| B21 | 1.42245047 |
| B22 | 1.41341199 |
| B23 | 0.96789261 |
| B24 | 1.48263146 |
| B25 | 1.09155715 |
| B26 | 1.08877019 |
| B27 | 1.08591517 |
| B28 | 1.51969064 |
| B29 | 1.08851704 |
| B30 | 1.08550282 |
| B31 | 1.08950605 |
| B32 | 1.51995501 |
| B33 | 1.08721488 |
| B34 | 1.08799453 |
| B35 | 1.08790100 |
| A1 | 88.25195254 |
| A2 | 110.76724924 |
| A3 | 87.76799474 |
| A4 | 130.69427858 |
| A5 | 92.26585079 |
| A6 | 109.41622023 |
| A7 | 111.85823211 |
| A8 | 106.02153260 |

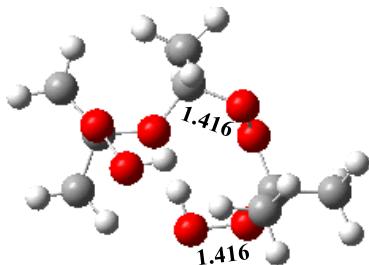
| | |
|-----|---------------|
| A9 | 65.27424690 |
| A10 | 85.47738294 |
| A11 | 111.02255228 |
| A12 | 108.54691651 |
| A13 | 110.35363259 |
| A14 | 111.54551172 |
| A15 | 125.87645966 |
| A16 | 104.90071180 |
| A17 | 110.23895157 |
| A18 | 109.62295746 |
| A19 | 109.31670739 |
| A20 | 109.46466357 |
| A21 | 109.59429181 |
| A22 | 102.24809777 |
| A23 | 107.25813143 |
| A24 | 106.27063379 |
| A25 | 110.62829646 |
| A26 | 110.95548113 |
| A27 | 112.79268129 |
| A28 | 108.52721685 |
| A29 | 111.40250144 |
| A30 | 110.58192226 |
| A31 | 115.70649291 |
| A32 | 111.89947362 |
| A33 | 109.40072628 |
| A34 | 108.69873420 |
| D1 | 27.16715611 |
| D2 | -96.21172856 |
| D3 | -158.36588189 |
| D4 | -14.99733485 |
| D5 | -64.02825920 |
| D6 | 58.70514099 |
| D7 | 179.07880507 |
| D8 | 76.43731584 |
| D9 | 108.43609377 |
| D10 | -163.89656671 |
| D11 | -44.40046395 |
| D12 | 74.61495498 |
| D13 | -114.39805188 |
| D14 | -80.22560658 |
| D15 | 169.43959361 |
| D16 | 51.79226484 |
| D17 | 172.25535975 |
| D18 | -67.25728397 |

| | |
|-----|---------------|
| D19 | -70.42212057 |
| D20 | -58.95171516 |
| D21 | 66.45836935 |
| D22 | -137.34011218 |
| D23 | 23.38759829 |
| D24 | 140.82975446 |
| D25 | -95.26654255 |
| D26 | 115.54500795 |
| D27 | -55.30191837 |
| D28 | 65.16543147 |
| D29 | -174.24454646 |
| D30 | 46.03137277 |
| D31 | -67.21817865 |
| D32 | 54.29780671 |
| D33 | 173.26256522 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|------------------|---------|---------|---------|---------|---------|---------|---------|---------|---------|--------|
| 1128.63 <i>i</i> | 39.70 | 45.29 | 62.24 | 82.79 | 87.04 | 108.54 | 133.22 | 172.25 | 179.08 | 196.24 |
| 219.59 | 236.88 | 243.35 | 255.02 | 264.38 | 281.23 | 286.69 | 311.31 | 314.57 | 321.12 | |
| 351.14 | 356.61 | 371.17 | 382.74 | 390.16 | 400.75 | 407.55 | 481.68 | 497.67 | 539.63 | |
| 563.85 | 579.17 | 605.31 | 641.80 | 690.65 | 754.71 | 821.67 | 848.37 | 901.16 | 922.16 | |
| 939.51 | 945.11 | 949.00 | 954.46 | 971.16 | 989.39 | 1019.70 | 1025.24 | 1055.31 | 1068.43 | |
| 1085.53 | 1090.84 | 1100.98 | 1195.79 | 1228.46 | 1250.58 | 1262.97 | 1276.21 | 1306.26 | | |
| 1318.44 | 1396.04 | 1404.40 | 1407.87 | 1413.28 | 1421.35 | 1425.74 | 1426.89 | 1447.30 | | |
| 1452.11 | 1460.75 | 1472.85 | 1473.77 | 1481.92 | 1484.31 | 1491.74 | 1493.95 | 1494.34 | | |
| 1503.09 | 1511.91 | 1517.54 | 1598.95 | 1917.55 | 3051.54 | 3068.76 | 3070.91 | 3072.63 | | |
| 3080.21 | 3081.03 | 3141.51 | 3143.67 | 3146.21 | 3146.49 | 3157.16 | 3157.61 | 3163.40 | | |
| 3168.69 | 3173.36 | 3178.81 | 3179.44 | 3203.44 | 3763.71 | | | | | |

Rotational constants (B/GHZ): 0.8060942 0.3540877 0.3256465



P8h

C

| | | | | | | | |
|---|---|----|---|----|---|----|---|
| C | 1 | B1 | | | | | |
| O | 2 | B2 | 1 | A1 | | | |
| O | 2 | B3 | 1 | A2 | 3 | D1 | 0 |
| H | 3 | B4 | 2 | A3 | 1 | D2 | 0 |
| C | 3 | B5 | 2 | A4 | 1 | D3 | 0 |
| C | 6 | B6 | 3 | A5 | 2 | D4 | 0 |
| H | 7 | B7 | 6 | A6 | 3 | D5 | 0 |

| | | | | | | | |
|---|----|-----|----|-----|----|-----|---|
| H | 7 | B8 | 6 | A7 | 3 | D6 | 0 |
| H | 7 | B9 | 6 | A8 | 3 | D7 | 0 |
| O | 6 | B10 | 3 | A9 | 2 | D8 | 0 |
| O | 6 | B11 | 3 | A10 | 2 | D9 | 0 |
| H | 1 | B12 | 2 | A11 | 4 | D10 | 0 |
| H | 1 | B13 | 2 | A12 | 4 | D11 | 0 |
| H | 1 | B14 | 2 | A13 | 4 | D12 | 0 |
| O | 2 | B15 | 1 | A14 | 4 | D13 | 0 |
| C | 16 | B16 | 2 | A15 | 1 | D14 | 0 |
| C | 17 | B17 | 16 | A16 | 2 | D15 | 0 |
| H | 18 | B18 | 17 | A17 | 16 | D16 | 0 |
| H | 18 | B19 | 17 | A18 | 16 | D17 | 0 |
| H | 18 | B20 | 17 | A19 | 16 | D18 | 0 |
| O | 17 | B21 | 16 | A20 | 2 | D19 | 0 |
| O | 22 | B22 | 17 | A21 | 16 | D20 | 0 |
| H | 23 | B23 | 22 | A22 | 17 | D21 | 0 |
| C | 6 | B24 | 3 | A23 | 2 | D22 | 0 |
| H | 25 | B25 | 6 | A24 | 3 | D23 | 0 |
| H | 25 | B26 | 6 | A25 | 3 | D24 | 0 |
| H | 25 | B27 | 6 | A26 | 3 | D25 | 0 |
| C | 2 | B28 | 1 | A27 | 4 | D26 | 0 |
| H | 29 | B29 | 2 | A28 | 1 | D27 | 0 |
| H | 29 | B30 | 2 | A29 | 1 | D28 | 0 |
| H | 29 | B31 | 2 | A30 | 1 | D29 | 0 |
| C | 17 | B32 | 16 | A31 | 2 | D30 | 0 |
| H | 33 | B33 | 17 | A32 | 16 | D31 | 0 |
| H | 33 | B34 | 17 | A33 | 16 | D32 | 0 |
| H | 33 | B35 | 17 | A34 | 16 | D33 | 0 |

Variables:

| | |
|-----|------------|
| B1 | 1.51999581 |
| B2 | 2.29522116 |
| B3 | 1.41556679 |
| B4 | 2.28713178 |
| B5 | 1.44588786 |
| B6 | 1.51433628 |
| B7 | 1.08685310 |
| B8 | 1.08582546 |
| B9 | 1.08853031 |
| B10 | 2.30925084 |
| B11 | 1.40176235 |
| B12 | 1.08737252 |
| B13 | 1.08869800 |
| B14 | 1.08693495 |
| B15 | 1.42481102 |

| | |
|-----|--------------|
| B16 | 1.41522728 |
| B17 | 1.51828429 |
| B18 | 1.08662810 |
| B19 | 1.08797701 |
| B20 | 1.08935088 |
| B21 | 1.41521147 |
| B22 | 1.41253459 |
| B23 | 0.96812056 |
| B24 | 1.51524259 |
| B25 | 1.08826708 |
| B26 | 1.08798102 |
| B27 | 1.08799065 |
| B28 | 1.52078442 |
| B29 | 1.08833138 |
| B30 | 1.08480836 |
| B31 | 1.08808921 |
| B32 | 1.51978639 |
| B33 | 1.08697238 |
| B34 | 1.08811677 |
| B35 | 1.08788261 |
| A1 | 88.56171736 |
| A2 | 110.79604196 |
| A3 | 80.49879843 |
| A4 | 130.70650365 |
| A5 | 113.70270571 |
| A6 | 110.45495516 |
| A7 | 111.01977024 |
| A8 | 107.33182437 |
| A9 | 91.40603833 |
| A10 | 103.75099985 |
| A11 | 110.44016013 |
| A12 | 109.29193947 |
| A13 | 110.09684267 |
| A14 | 110.52691367 |
| A15 | 125.40396453 |
| A16 | 104.81368279 |
| A17 | 110.50343310 |
| A18 | 109.30832305 |
| A19 | 109.56453143 |
| A20 | 109.79837054 |
| A21 | 109.76400100 |
| A22 | 102.78518548 |
| A23 | 107.72689666 |
| A24 | 108.82358199 |

| | |
|-----|---------------|
| A25 | 110.38882289 |
| A26 | 109.55844724 |
| A27 | 112.66646058 |
| A28 | 107.83215332 |
| A29 | 111.53210941 |
| A30 | 111.23109769 |
| A31 | 114.82670349 |
| A32 | 112.09336152 |
| A33 | 109.29534534 |
| A34 | 108.81021247 |
| D1 | 28.76269698 |
| D2 | -97.71851434 |
| D3 | -159.49353719 |
| D4 | -20.11371846 |
| D5 | -67.05643783 |
| D6 | 54.99859512 |
| D7 | 173.69444424 |
| D8 | 69.56426844 |
| D9 | 102.86218371 |
| D10 | -170.31182382 |
| D11 | -50.68645443 |
| D12 | 68.94319471 |
| D13 | -115.31728114 |
| D14 | -88.59573692 |
| D15 | 174.41321122 |
| D16 | 50.87068470 |
| D17 | 171.19641539 |
| D18 | -69.12402057 |
| D19 | -65.19706597 |
| D20 | -61.54204653 |
| D21 | 71.47897466 |
| D22 | -146.45114451 |
| D23 | 62.95557980 |
| D24 | -176.79626185 |
| D25 | -56.22728661 |
| D26 | 113.88389951 |
| D27 | -58.42611579 |
| D28 | 61.33383115 |
| D29 | -177.48525925 |
| D30 | 51.60507161 |
| D31 | -67.60680992 |
| D32 | 53.83922160 |
| D33 | 172.79408537 |

Harmonic Vibrational Frequencies (cm⁻¹):

| | | | | | | | | | | |
|-------------------------------|---------|---------|---------|---------|-----------|-----------|-----------|---------|---------|--------|
| 16.99 | 54.47 | 66.92 | 81.98 | 108.22 | 158.33 | 174.37 | 185.84 | 202.66 | 217.77 | 222.99 |
| 237.82 | 255.89 | 264.67 | 274.20 | 285.72 | 296.95 | 301.70 | 319.79 | 328.96 | 354.34 | |
| 362.15 | 364.64 | 377.67 | 394.57 | 402.89 | 457.47 | 471.50 | 486.44 | 529.52 | 535.50 | |
| 582.90 | 600.14 | 611.41 | 640.29 | 757.56 | 797.53 | 851.15 | 892.58 | 909.10 | 925.83 | |
| 940.47 | 946.61 | 948.26 | 973.15 | 981.43 | 1017.99 | 1021.41 | 1027.70 | 1055.08 | 1065.38 | |
| 1070.09 | 1084.81 | 1179.05 | 1205.81 | 1231.63 | 1248.42 | 1258.38 | 1265.49 | 1278.32 | | |
| 1305.56 | 1310.53 | 1409.65 | 1411.14 | 1415.24 | 1417.71 | 1420.29 | 1428.67 | 1439.63 | | |
| 1466.36 | 1471.05 | 1480.92 | 1483.37 | 1486.40 | 1488.26 | 1493.88 | 1500.25 | 1501.20 | | |
| 1506.86 | 1508.76 | 1510.83 | 1521.06 | 3068.51 | 3070.02 | 3076.16 | 3079.27 | 3079.83 | | |
| 3083.36 | 3148.42 | 3149.24 | 3154.02 | 3157.16 | 3159.16 | 3160.93 | 3162.16 | 3163.41 | | |
| 3164.57 | 3167.57 | 3171.65 | 3182.81 | 3700.88 | 3760.83 | | | | | |
| Rotational constants (B/GHZ): | | | | | 0.8003076 | 0.3916650 | 0.3507378 | | | |