

Supplement for

Understanding the catalytic role of oxalic acid in the SO₃ hydration to form H₂SO₄ in the atmosphere

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Table S1. Energies, enthalpies and free energies for the reaction of SO₃ with two water (in kcal mol⁻¹).

species	ΔE	$\Delta(E+ZPE)$	ΔH^a	ΔG^a
SO ₃ +2H ₂ O	0	0	0	0
SO ₃ +H ₂ O···H ₂ O	-5.32	-3.22	-3.67	2.30
SO ₃ ···H ₂ O+H ₂ O	-8.82	-6.48	-7.05	1.87
RC1	-21.00	-15.47	-17.37	2.35
TS1	-13.54	-9.74	-12.72	9.21
PC1	-34.51	-28.81	-30.91	-10.37
H ₂ SO ₄ +H ₂ O	-21.36	-17.79	-19.21	-7.85

^aThese enthalpies and free energies are obtained at 298.15 K and 1.01325 bar.

Table S2. Energies, enthalpies and free energies for the hydration of SO₃ catalyzed by cTt conformer (in kcal mol⁻¹).

species	ΔE	$\Delta(E+ZPE)$	ΔH^a	ΔG^a
SO ₃ +H ₂ O+cTt	0	0	0	0
SO ₃ ···H ₂ O+cTt	-8.82	-6.48	-7.05	1.87
SO ₃ +H ₂ O···cTt	-11.13	-9.05	-9.58	-0.52
RC _{cTt}	-24.32	-20.29	-21.47	0.54
TS _{cTt}	-20.08	-18.92	-20.80	2.99
PC _{cTt}	-37.55	-33.40	-34.71	-12.68
H ₂ SO ₄ +cCt	-18.11	-14.86	-16.19	-5.11

^aThese enthalpies and free energies are obtained at 298.15 K and 1.01325 bar.

Table S3. Energies, enthalpies and free energies for the hydration of SO₃ catalyzed by tTt conformer (in kcal mol⁻¹).

species	ΔE	$\Delta(E+ZPE)$	ΔH^a	ΔG^a
SO ₃ +H ₂ O+tTt	0	0	0	0
SO ₃ ···H ₂ O+tTt	-8.82	-6.48	-7.05	1.87
SO ₃ +H ₂ O···tTt	-10.95	-8.76	-9.31	-0.23
RC _{tTt}	-25.67	-21.58	-22.86	-0.59
TS _{tTt}	-22.77	-21.14	-23.07	0.85
PC _{tTt}	-39.73	-35.33	-36.67	-14.73
H ₂ SO ₄ +tCt	-20.80	-17.27	-18.68	-7.63

^aThese enthalpies and free energies are obtained at 298.15 K and 1.01325 bar.

Table S4. Energies, enthalpies and free energies for the hydration of SO₃ catalyzed by tCt conformer (in kcal mol⁻¹).

species	ΔE	$\Delta(E+ZPE)$	ΔH^a	ΔG^a
SO ₃ +H ₂ O+tCt	0	0	0	0
SO ₃ ···H ₂ O+tCt	-8.82	-6.48	-7.05	1.87
SO ₃ +H ₂ O···tCt	-11.15	-8.93	-9.49	-0.32
RC _{tCt}	-26.14	-22.04	-23.35	-0.68
TS _{tCt}	-23.47	-21.76	-23.70	0.57
PC _{tCt}	-40.48	-36.05	-37.39	-15.04
H ₂ SO ₄ +tTt	-21.91	-18.32	-19.74	-8.08

^aThese enthalpies and free energies are obtained at 298.15 K and 1.01325 bar.

Table S5. Energies, enthalpies and free energies for the hydration of SO₃ catalyzed by cCt conformer (in kcal mol⁻¹).

species	ΔE	$\Delta(E+ZPE)$	ΔH^a	ΔG^a
SO ₃ +H ₂ O+cCt	0	0	0	0
SO ₃ ···H ₂ O+cCt	-8.82	-6.48	-7.05	1.87
SO ₃ +H ₂ O···cCt	-12.18	-9.92	-10.54	-1.23
RC _{cCt}	-26.64	-22.53	-23.88	-1.29
TS _{cCt}	-23.88	-22.27	-24.25	-0.13
PC _{cCt}	-42.24	-37.60	-38.97	-16.81
H ₂ SO ₄ +cTt	-24.60	-20.73	-22.22	-10.60

^aThese enthalpies and free energies are obtained at 298.15 K and 1.01325 bar.

Table S6. The temperature, pressure, density of air and water vapor content at different altitudes.

altitude (km)	0	0	2	4	6	8	10	12
P (bar)	1.01325	1.01325	0.795	0.617	0.472	0.357	0.265	0.194
T (K)	298.15	288.15	275.15	262.17	249.19	236.22	223.25	216.65
Density (kg m ⁻³)		1.225	1.0066	0.81935	0.66011	0.52579	0.41351	0.31194
c _{water} (ppm by mass)		4686	2843	1268	554	216	43.2	11.3
c _{water} (molecule cm ⁻³)	^a 5.18×10 ¹⁷	1.92×10 ¹⁷	9.57×10 ¹⁶	3.47×10 ¹⁶	1.22×10 ¹⁶	3.80×10 ¹⁵	5.97×10 ¹⁴	1.18×10 ¹⁴

^aThe water vapor concentration at 0 km and 298.15 K are obtained from (Torrent-Sucarrat et al., 2012). The other data are taken from U.S. Standard Atmosphere, 1976 (NASA and NOAA).

Table S7. The equilibrium constants (K_{eq} , $\text{cm}^3 \text{ molecule}^{-1}$), tunnelling corrected unimolecular rate constants (k_{uni} , s^{-1}) and Wigner correction coefficient (κ_{uni}) for the hydration of SO_3 catalyzed water and oxalic acids at different altitude heights.

altitude (km)	0	0	2	4	6	8	10	12
P (bar)	1.01325	1.01325	0.795	0.617	0.472	0.357	0.265	0.194
T (K)	298.15	288.15	275.15	262.17	249.19	236.22	223.25	216.65
$K_{\text{eq}1}$	1.80×10^{-20}	3.18×10^{-20}	7.10×10^{-20}	1.72×10^{-19}	4.54×10^{-19}	1.34×10^{-18}	4.50×10^{-18}	8.83×10^{-18}
$K_{\text{eq}2}$	3.71×10^{-20}	8.00×10^{-20}	2.36×10^{-19}	7.75×10^{-19}	2.88×10^{-18}	1.23×10^{-17}	6.26×10^{-17}	1.54×10^{-16}
k_{uni_w}	8.42×10^7	6.32×10^7	4.21×10^7	2.69×10^7	1.64×10^7	9.39×10^6	5.03×10^6	3.55×10^6
κ_{uni_w}	1.45	1.48	1.52	1.58	1.64	1.71	1.80	1.85
$K_{\text{eq}_c\text{Tt}1}$	3.83×10^{-19}	8.64×10^{-19}	2.71×10^{-18}	9.52×10^{-18}	3.82×10^{-17}	1.79×10^{-16}	1.00×10^{-15}	2.61×10^{-15}
$K_{\text{eq}2_c\text{Tt}2}$	6.84×10^{-21}	1.33×10^{-20}	3.39×10^{-20}	9.49×10^{-20}	2.96×10^{-19}	1.05×10^{-18}	4.32×10^{-18}	9.46×10^{-18}
$k_{\text{uni}_c\text{Tt}}$	1.53×10^{11}	1.46×10^{11}	1.36×10^{11}	1.25×10^{11}	1.15×10^{11}	1.04×10^{11}	9.31×10^{10}	8.74×10^{10}
$\kappa_{\text{uni}_c\text{Tt}}$	1.53	1.57	1.62	1.69	1.76	1.85	1.95	2.01
$K_{\text{eq}_t\text{Tt}1}$	2.56×10^{-18}	6.25×10^{-18}	2.20×10^{-17}	8.73×10^{-17}	4.03×10^{-16}	2.19×10^{-15}	1.46×10^{-14}	4.16×10^{-14}
$K_{\text{eq}2_t\text{Tt}2}$	7.49×10^{-20}	1.60×10^{-19}	4.67×10^{-19}	1.52×10^{-18}	5.58×10^{-18}	2.37×10^{-17}	1.19×10^{-16}	2.92×10^{-16}
$k_{\text{uni}_t\text{Tt}}$	7.60×10^{11}	7.74×10^{11}	7.71×10^{11}	7.67×10^{11}	7.63×10^{11}	7.58×10^{11}	7.52×10^{11}	7.49×10^{11}
$\kappa_{\text{uni}_t\text{Tt}}$	1.41	1.43	1.48	1.52	1.58	1.65	1.72	1.77
$K_{\text{eq}_c\text{Ct}1}$	2.99×10^{-18}	7.52×10^{-18}	2.75×10^{-17}	1.14×10^{-16}	5.54×10^{-16}	3.18×10^{-15}	2.25×10^{-14}	6.64×10^{-14}
$K_{\text{eq}2_c\text{Ct}2}$	7.49×10^{-20}	1.64×10^{-19}	4.90×10^{-19}	1.64×10^{-18}	6.19×10^{-18}	2.72×10^{-17}	1.42×10^{-16}	3.56×10^{-16}
$k_{\text{uni}_c\text{Ct}}$	1.04×10^{12}	1.04×10^{12}	1.05×10^{12}	1.05×10^{12}	1.06×10^{12}	1.07×10^{12}	1.08×10^{12}	1.08×10^{12}
$\kappa_{\text{uni}_c\text{Ct}}$	1.37	1.40	1.44	1.48	1.53	1.60	1.67	1.71
$K_{\text{eq}_c\text{Ct}1}$	8.40×10^{-18}	2.18×10^{-17}	8.32×10^{-17}	3.62×10^{-16}	1.85×10^{-15}	1.13×10^{-14}	8.48×10^{-14}	2.60×10^{-13}
$K_{\text{eq}2_c\text{Ct}2}$	4.53×10^{-20}	9.55×10^{-20}	2.74×10^{-19}	8.73×10^{-19}	3.15×10^{-18}	1.31×10^{-17}	6.41×10^{-17}	1.55×10^{-16}
$k_{\text{uni}_c\text{Ct}}$	1.21×10^{12}	1.22×10^{12}	1.23×10^{12}	1.24×10^{12}	1.25×10^{12}	1.27×10^{12}	1.28×10^{12}	1.29×10^{12}
$\kappa_{\text{uni}_c\text{Ct}}$	1.39	1.42	1.46	1.51	1.56	1.63	1.70	1.75

Table S8. The Gibbs free energy (in Hartree) of oxalic acid conformers at G4 level at different altitudes.

altitude (km)	0	0	2	4	6	8	10	12
P (bar)	1.01325	1.01325	0.795	0.617	0.472	0.357	0.265	0.194
T (K)	298.15	288.15	275.15	262.17	249.19	236.22	223.25	216.65
cTc	-378.23881	-378.23764	-378.23634	-378.23506	-378.23378	-378.23251	-378.23125	-378.23072
cTt	-378.23527	-378.23409	-378.23277	-378.23147	-378.23017	-378.22889	-378.22761	-378.22707
tTt	-378.23417	-378.23294	-378.23158	-378.23023	-378.22889	-378.22755	-378.22622	-378.22566
tCt	-378.23381	-378.23257	-378.23119	-378.22982	-378.22846	-378.22711	-378.22577	-378.22520
cCt	-378.23123	-378.23003	-378.22869	-378.22736	-378.22604	-378.22473	-378.22343	-378.22288

Text S1.

In order to obtain the mole fractions for oxalic acid conformers at different altitudes with different temperature and pressure, the Boltzmann distribution are used in this paper. The equation to calculate the conformational population is as follows:

$$p_i = \frac{e^{-\Delta G_i/RT}}{\sum_j e^{-\Delta G_j/RT}}$$

where p_i represents the population of conformer i ; ΔG represents the Gibbs free energy difference between a conformer and the most stable conformer (G_{\min}). The denominator also includes $e^{-(G_{\min}-G_{\min})/RT}$ which is equal to 1.

Table S9. Concentrations (in molecule cm^{-3}) of oxalic acid including all conformers at different altitudes.

altitude (km)	0	0	2	4	6	8	10	12
P (bar)	1.01325	1.01325	0.795	0.617	0.472	0.357	0.265	0.194
T (K)	298.15	288.15	275.15	262.17	249.19	236.22	223.25	216.65
concentration	2.02×10^9	2.09×10^9	1.72×10^9	1.39×10^9	1.13×10^9	8.98×10^8	7.06×10^8	5.32×10^8

Table S10. Relative rate of SO₃ hydration reaction catalyzed by oxalic acid conformers (cTt, tTt, tCt and cCt) and by water at different altitudes.

altitude (km)	0	0	2	4	6	8	10	12
P (bar)	1.01325	1.01325	0.795	0.617	0.472	0.357	0.265	0.194
T (K)	298.15	288.15	275.15	262.17	249.19	236.22	223.25	216.65
$V_{\text{SO}_3 \cdots \text{H}_2\text{O} + \text{cT}}$								
$\sqrt[4]{V_{\text{SO}_3 \cdots \text{H}_2\text{O} + \text{H}_2\text{O}}}$	3.44×10^{-6}	1.35×10^{-5}	3.56×10^{-5}	1.35×10^{-4}	5.54×10^{-4}	2.70×10^{-3}	2.80×10^{-2}	1.60×10^{-1}
$V_{\text{SO}_3 \cdots \text{H}_2\text{O} + \text{tT}}$								
$\sqrt[4]{V_{\text{SO}_3 \cdots \text{H}_2\text{O} + \text{H}_2\text{O}}}$	3.61×10^{-5}	1.48×10^{-4}	4.18×10^{-4}	1.70×10^{-3}	7.59×10^{-3}	4.06×10^{-2}	4.66×10^{-1}	2.81
$V_{\text{SO}_3 \cdots \text{H}_2\text{O} + \text{tC}}$								
$\sqrt[4]{V_{\text{SO}_3 \cdots \text{H}_2\text{O} + \text{H}_2\text{O}}}$	3.84×10^{-5}	1.59×10^{-4}	4.55×10^{-4}	1.88×10^{-3}	8.49×10^{-3}	4.61×10^{-2}	5.39×10^{-1}	3.29
$V_{\text{SO}_3 \cdots \text{H}_2\text{O} + \text{cC}}$								
$\sqrt[4]{V_{\text{SO}_3 \cdots \text{H}_2\text{O} + \text{H}_2\text{O}}}$	8.24×10^{-6}	3.32×10^{-5}	9.15×10^{-5}	3.62×10^{-4}	1.56×10^{-3}	8.05×10^{-3}	8.91×10^{-2}	5.26×10^{-1}

Table S11. Optimized geometries of SO₃, H₂O, oxalic acid (cTc, cTt, tTt, tCt and cCt) and H₂SO₄ at M06-2X/6-311++G(3df,3pd).

SO₃

S	0.00000	-0.00002	0.00000
O	1.22411	-0.70687	0.00000
O	-1.22431	-0.70653	0.00000
O	0.00020	1.41343	0.00000

H₂O

O	0.00000	0.00000	0.11665
H	0.00000	0.76086	-0.46658
H	0.00000	-0.76086	-0.46658

cTc

C	0.75266	0.17015	0.00000
O	1.12628	1.30445	-0.00001
O	1.52979	-0.89110	0.00001
C	-0.75266	-0.17015	0.00000
O	-1.12629	-1.30445	-0.00001
O	-1.52978	0.89109	0.00001
H	-0.96242	1.67957	0.00000
H	0.96240	-1.67955	0.00002

cTt

C	-0.72460	0.13091	-0.00009
O	-1.11274	1.26546	-0.00018
O	-1.48394	-0.94545	0.00018
H	-2.40969	-0.66590	0.00029
C	0.78432	-0.19701	-0.00011
O	1.21467	-1.30178	-0.00013
O	1.52197	0.90532	0.00019
H	0.93172	1.67414	0.00039

tTt

C	0.75184	0.16672	-0.00003
O	1.18464	1.27557	-0.00033
O	1.47494	-0.94732	0.00033

H	2.40670	-0.69104	0.00020
C	-0.75185	-0.16677	-0.00003
O	-1.18467	-1.27558	-0.00033
O	-1.47491	0.94735	0.00032
H	-2.40669	0.69111	0.00022

tCt

C	-0.77088	-0.12624	-0.00001
O	-1.28348	1.10297	0.00008
O	-1.39798	-1.13545	-0.00008
C	0.77088	-0.12623	0.00001
O	1.39797	-1.13545	0.00008
O	1.28348	1.10296	-0.00008
H	2.24653	1.01727	-0.00006
H	-2.24652	1.01728	0.00007

cCt

C	0.74011	-0.17258	-0.00014
O	1.26767	1.06677	0.00063
O	1.36925	-1.17536	-0.00058
C	-0.80742	-0.12211	-0.00003
O	-1.44803	-1.11694	0.00064
O	-1.33684	1.10121	-0.00058
H	2.23115	0.99050	0.00060
H	-0.64362	1.77219	-0.00043

H₂SO₄

H	1.69009	-0.00859	1.10291
S	0.00000	0.00001	-0.15403
O	1.02989	-0.66200	0.83621
O	0.63954	1.06897	-0.81993
O	-0.63945	-1.06888	-0.82011
O	-1.03000	0.66191	0.83616
H	-1.69009	0.00841	1.10291

Table S12. Optimized geometries of SO₃ hydration catalyzed by water at M06-2X/6-311++G(3df,3pd).

SO₃···H₂O

S	0.40953	0.00000	-0.03606
O	0.37189	1.22270	-0.75173
O	0.37189	-1.22269	-0.75174
O	0.75839	-0.00001	1.33189
O	-1.79060	0.00000	0.28875
H	-2.12250	-0.77385	-0.18016
H	-2.12250	0.77385	-0.18016

H₂O...H₂O

H	-1.68941	0.78219	-0.34132
O	-1.38500	-0.0054	0.11504
H	-1.70183	-0.74313	-0.41082
H	0.55220	-0.00717	0.06948
O	1.49852	0.00602	-0.12125
H	1.93083	-0.03688	0.73237

RC1

S	-0.72222	-0.21215	-0.01647
O	-0.58086	-0.75716	1.28257
O	0.03797	-0.81049	-1.06976
O	-1.88227	0.520400	-0.36453
H	2.04043	-0.76247	-0.52733
O	2.56701	-0.08822	-0.07285
H	2.94841	-0.51544	0.69832
H	1.38567	0.95583	0.18673
O	0.46574	1.35399	0.27027
H	0.32024	1.96837	-0.45986

TS1

S	-0.64877	-0.14450	-0.01812
O	-0.82763	-0.75895	1.24708
O	0.24385	-0.86516	-0.92499
O	-1.72050	0.54435	-0.64319
H	1.69398	-0.63244	-0.53547
O	2.3985	-0.02392	-0.08777
H	2.7892	-0.48706	0.66183
H	1.58775	0.72198	0.24281

O	0.42181	1.19864	0.41650
H	0.181	1.94996	-0.14027

PC1

S	-0.57356	-0.07575	0.12162
O	0.21842	0.29741	1.24427
O	0.33927	-0.72817	-0.94377
O	-1.73078	-0.87759	0.25513
H	1.29069	-0.46446	-0.77614
O	2.66277	0.10624	-0.10916
H	3.38120	-0.49556	0.09731
H	2.25822	0.35711	0.73311
O	-0.99047	1.28661	-0.55439
H	-1.74680	1.13898	-1.13677

Table S13. Optimized geometries of SO₃ hydration catalyzed by oxalic acid at M06-2X/6-311++G(3df,3pd).

SO₃···H₂O

S	0.40953	0.00000	-0.03606
O	0.37189	1.22270	-0.75173
O	0.37189	-1.22269	-0.75174
O	0.75839	-0.00001	1.33189
O	-1.79060	0.00000	0.28875
H	-2.12250	-0.77385	-0.18016
H	-2.12250	0.77385	-0.18016

cTc···H₂O

C	-0.58924	-0.74807	0.00286
O	0.39782	-1.42484	0.01504
O	-1.81118	-1.23189	-0.00543
C	-0.58028	0.80529	0.00193
O	-1.64115	1.36845	0.00784
O	0.57622	1.39776	0.00031
O	2.76585	-0.07515	-0.09311
H	3.43614	-0.00665	0.58946
H	2.33393	-0.93268	0.01156
H	1.36752	0.79404	-0.01728
H	-2.42090	-0.47266	-0.00962

RC_{cTe}

C	-1.67827	0.76452	-0.20426
O	-0.82883	1.14720	-0.9647
O	-2.38364	1.55161	0.56249
C	-2.07464	-0.72369	-0.06393
O	-3.04223	-0.98836	0.59020
O	-1.33638	-1.58636	-0.70391
S	1.76210	-0.33161	0.23458
O	1.39039	-0.98907	-0.97379
O	0.74170	-0.14087	1.20885
O	3.11578	-0.31790	0.63420
O	1.73160	1.50807	-0.54127
H	1.96094	2.14140	0.15091
H	0.78823	1.64455	-0.79004
H	-0.50750	-1.19565	-1.04346
H	-3.02488	0.99579	1.04198

cTt···H₂O

C	-0.05433	0.02603	-0.00411
O	-0.53883	1.13589	0.00039
O	-0.70255	-1.10025	-0.01317
H	-1.67320	-0.90424	-0.01639
C	1.48236	-0.13882	0.00434
O	2.02917	-1.19100	0.01419
O	2.10217	1.03556	0.00164
O	-3.11875	-0.00329	-0.07379
H	-3.82437	-0.01697	0.57575
H	-2.67063	0.84853	0.01075
H	1.43028	1.73417	-0.00561

RC_{cTt}

C	-1.57123	-0.09074	-0.17416
O	-0.98321	0.98039	-0.25277
O	-1.06757	-1.26253	-0.28677
H	-0.08239	-1.23569	-0.45349
C	-3.09655	-0.08274	0.08392

O	-3.73479	-1.07641	0.16657
O	-3.58639	1.14532	0.19597
S	2.25859	-0.21557	0.14015
O	1.50400	-1.0492	-0.75504
O	1.79359	-0.13615	1.47822
O	3.61635	0.02013	-0.15895
O	1.52093	1.43742	-0.51017
H	1.80060	2.15322	0.07611
H	0.51769	1.31394	-0.42958
H	-2.87006	1.78675	0.08959

TS_{eff}

C	-1.48241	-0.09864	-0.17084
O	-0.93245	1.02462	-0.26343
O	-0.94363	-1.22280	-0.26312
H	0.11836	-1.20975	-0.44149
C	-3.00971	-0.09551	0.07822
O	-3.62588	-1.10212	0.15444
O	-3.52591	1.12109	0.18790
S	2.17056	-0.14566	0.13857
O	1.45800	-1.10005	-0.70868
O	1.70337	-0.09195	1.48093
O	3.54120	0.03037	-0.14903
O	1.43799	1.30021	-0.54176
H	1.79035	2.07364	-0.08010
H	0.24797	1.16762	-0.40768
H	-2.83440	1.78891	0.08978

PC_{eff}

C	-1.64537	0.05965	-0.09954
O	-1.23413	-1.18164	-0.14337
O	-0.9534	1.04328	-0.16217
H	0.61251	1.21544	-0.38749
C	-3.18227	0.17489	0.05164
O	-3.71130	1.23189	0.11308
O	-3.82466	-0.98788	0.10463
S	2.25785	-0.07248	-0.06797

O	1.60945	1.24558	-0.51421
O	1.37242	-1.16156	-0.35947
O	3.59137	-0.09356	-0.52371
O	2.23848	0.01811	1.50269
H	2.96510	0.57594	1.81232
H	-0.24153	-1.22996	-0.22791
H	-3.20183	-1.72288	0.03825

tTt...H₂O

C	0.0811	-0.06515	-0.00227
O	0.59433	-1.15114	0.01939
O	0.70102	1.08845	-0.02972
H	1.67267	0.91546	-0.02966
C	-1.44904	0.12148	0.00557
O	-1.98717	1.18295	0.03281
O	-2.06747	-1.05551	-0.01818
H	-3.0182	-0.88343	-0.01085
O	3.14442	-0.00458	-0.07693
H	3.82642	-0.02151	0.59693
H	2.6458	-0.82980	0.00484

RC_{tTt}

C	-1.54953	-0.06702	-0.18124
O	-0.94982	0.98339	-0.30698
O	-1.06262	-1.25641	-0.2411
H	-0.07749	-1.24497	-0.40647
C	-3.07046	-0.07241	0.07117
O	-3.71836	-1.06762	0.11258
O	-3.52610	1.16532	0.22409
H	-4.47909	1.11174	0.37697
S	2.26539	-0.19867	0.14626
O	1.51365	-1.07672	-0.70972
O	1.81423	-0.08347	1.48753
O	3.62316	0.02491	-0.16672
O	1.52268	1.40267	-0.54855
H	1.78909	2.14039	0.01665
H	0.50664	1.27149	-0.47587

TS_{tt}

C	-1.47741	-0.07324	-0.17632
O	-0.91577	1.0215	-0.32485
O	-0.95673	-1.2211	-0.20850
H	0.08271	-1.22015	-0.38425
C	-2.99945	-0.08412	0.06548
O	-3.63283	-1.08789	0.08993
O	-3.46400	1.14738	0.22852
H	-4.41776	1.08907	0.37650
S	2.19155	-0.14352	0.14308
O	1.47176	-1.11839	-0.66675
O	1.73776	-0.04046	1.48793
O	3.56106	0.02707	-0.15773
O	1.45679	1.28981	-0.57833
H	1.78361	2.07361	-0.11549
H	0.28342	1.154670	-0.46296

PC_{tt}

C	-1.64291	0.00968	-0.09471
O	-1.24097	-1.22307	-0.10662
O	-0.95273	0.99856	-0.17648
H	0.59679	1.16868	-0.39938
C	-3.17014	0.17405	0.04585
O	-3.68064	1.24417	0.12173
O	-3.80104	-0.99508	0.06829
H	-4.74765	-0.81836	0.15531
S	2.27734	-0.07322	-0.06977
O	1.59480	1.22173	-0.53216
O	1.40512	-1.18302	-0.30892
O	3.60125	-0.08049	-0.55648
O	2.30078	0.06125	1.49925
H	3.03232	0.63240	1.76951
H	-0.25308	-1.26604	-0.18478

tCt···H₂O

O	-3.13567	-0.10507	-0.07384
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H	-3.82180	-0.09104	0.59587
H	-2.68484	0.75045	-0.03447
C	-0.08374	0.14079	-0.00543
O	-0.63584	-1.05050	0.02082
O	-0.66174	1.19106	-0.03251
C	1.45841	0.10156	0.00617
O	2.11554	1.09214	0.03563
O	1.93914	-1.14029	-0.02097
H	2.90374	-1.07781	-0.01468
H	-1.61659	-0.93438	0.01579

RC_{tCt}

S	2.25495	-0.22863	0.13651
O	1.48077	-1.04114	-0.76458
O	1.80243	-0.17245	1.4812
O	3.62065	-0.03403	-0.16085
O	1.56632	1.42105	-0.47586
H	1.85037	2.12233	0.12622
H	0.54354	1.31748	-0.41737
C	-1.54294	0.03479	-0.18553
O	-1.09074	-1.16720	-0.29471
O	-0.91233	1.06876	-0.27136
C	-3.05965	0.12524	0.08149
O	-3.60732	1.16932	0.22815
O	-3.63207	-1.07174	0.12084
H	-4.57516	-0.94481	0.29235
H	-0.10418	-1.17753	-0.46381

TS_{tCt}

S	2.19069	-0.17903	0.12954
O	1.43626	-1.06248	-0.75074
O	1.74814	-0.17136	1.48184
O	3.56298	-0.02675	-0.16799
O	1.49728	1.33047	-0.46918
H	1.84098	2.06447	0.05872
H	0.32598	1.22118	-0.37122
C	-1.47904	0.03106	-0.1768

O	-0.99379	-1.1308	-0.2896
O	-0.88290	1.11146	-0.24790
C	-2.99831	0.11132	0.07349
O	-3.56006	1.15074	0.19257
O	-3.54605	-1.09410	0.13056
H	-4.49355	-0.98631	0.29104
H	0.04480	-1.14660	-0.46798

PC_{tct}

S	-2.27869	0.04815	-0.07356
O	-1.55120	-1.2403	-0.48495
O	-1.43418	1.17382	-0.33404
O	-3.59441	0.00063	-0.58020
O	-2.32553	-0.03998	1.49822
H	-3.05642	-0.60949	1.77343
H	0.22718	1.31291	-0.21052
C	1.65181	0.08350	-0.09059
O	0.99125	-0.92999	-0.14331
O	1.21478	1.30050	-0.13311
C	3.18627	0.02668	0.04606
O	3.87041	0.99581	0.12383
O	3.60937	-1.2316	0.06418
H	4.57196	-1.21755	0.15048
H	-0.55614	-1.14841	-0.35427

cCt...H₂O

O	3.09381	0.10046	-0.07544
H	3.79737	0.12665	0.57594
H	2.69058	-0.77772	-0.02446
C	0.05693	-0.18900	-0.00226
O	0.62614	1.00951	0.00657
O	0.63495	-1.23461	-0.01222
C	-1.48877	-0.09379	0.00406
O	-2.16700	-1.06464	0.01662
O	-1.97093	1.14836	-0.00471
H	1.61147	0.89115	0.00520
H	-1.24411	1.78403	-0.01413

RC_{cct}

S	2.22860	-0.23242	0.13431
O	1.44806	-1.01469	-0.79139
O	1.75986	-0.19844	1.47350
O	3.59920	-0.05881	-0.14808
O	1.57611	1.43851	-0.45359
H	1.87753	2.12900	0.15305
H	0.55412	1.35813	-0.39709
C	-1.54690	0.08151	-0.18257
O	-1.08737	-1.12698	-0.31681
O	-0.91359	1.10976	-0.25348
C	-3.07088	0.12425	0.08990
O	-3.63659	1.15579	0.22028
O	-3.65553	-1.06624	0.15920
H	-0.09480	-1.14278	-0.49273
H	-3.00900	-1.77145	0.02669

TS_{cct}

S	2.17077	-0.17986	0.12859
O	1.40684	-1.04360	-0.76905
O	1.71969	-0.19047	1.47683
O	3.54389	-0.04415	-0.16637
O	1.49727	1.34389	-0.45339
H	1.85262	2.07157	0.07638
H	0.33239	1.25339	-0.35836
C	-1.48622	0.07301	-0.17217
O	-0.99609	-1.09523	-0.2982
O	-0.8867	1.14691	-0.23541
C	-3.01265	0.11037	0.08150
O	-3.58861	1.13813	0.19220
O	-3.57908	-1.08608	0.15551
H	0.05859	-1.11902	-0.48708
H	-2.92052	-1.78365	0.03858

PC_{cct}

S	2.26880	-0.05194	-0.07549
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O	1.54266	1.24778	-0.46475
O	1.41240	-1.16615	-0.34587
O	3.57868	-0.00294	-0.59444
O	2.32866	0.01649	1.49507
H	3.08180	0.55479	1.77382
H	-0.23138	-1.32188	-0.20779
C	-1.67534	-0.11601	-0.08509
O	-1.02578	0.91564	-0.13788
O	-1.22091	-1.31808	-0.12682
C	-3.21307	-0.02724	0.04965
O	-3.90701	-0.98469	0.11681
O	-3.64447	1.22680	0.08097
H	0.55302	1.15252	-0.34154
H	-2.88766	1.82637	0.01124

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