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Supplement of

Understanding the catalytic role of oxalic acid in SO_3 hydration to form H_2SO_4 in the atmosphere

Guochun Lv et al.

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Text S1. The proof for the same rate constants for Reaction 1 and Reaction 2, as well as Reaction X1 and Reaction X2.

For Reaction 1 and Reaction 2:

$$Recation\ 1:$$

$$SO_3 + H_2O \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} SO_3 \cdots H_2O$$

$$SO_3 \cdots H_2O + H_2O \underset{k_{-2}^{w1}}{\overset{k_2^{w1}}{\rightleftarrows}} SO_3 \cdots H_2O \cdots H_2O \xrightarrow{k_{uni\_w}} H_2SO_4 \cdots H_2O$$

$$Reaction\ 2:$$

$$H_2O + H_2O \underset{k_{-1}^{w2}}{\overset{k_1^{w2}}{\rightleftarrows}} H_2O \cdots H_2O$$

$$SO_3 + H_2O \cdots H_2O \underset{k_{-2}^{w2}}{\overset{k_2^{w2}}{\rightleftarrows}} SO_3 \cdots H_2O \cdots H_2O \xrightarrow{k_{uni\_w}} H_2SO_4 \cdots H_2O$$

For reaction 1,

$$K_{eq1} = \frac{[SO_3 \cdots H_2O]}{[SO_3][H_2O]}, \quad K_{eq2}^{w1} = \frac{[SO_3 \cdots H_2O \cdots H_2O]}{[SO_3 \cdots H_2O][H_2O]}$$

$$K_{eq1} \cdot K_{eq2}^{w1} = \frac{[SO_3 \cdots H_2O \cdots H_2O]}{[SO_3][H_2O][H_2O]}$$

For reaction 2,

$$K_{eq1}^{w2} = \frac{[H_2O \cdots H_2O]}{[H_2O][H_2O]}, \quad K_{eq2}^{w2} = \frac{[SO_3 \cdots H_2O \cdots H_2O]}{[SO_3][H_2O \cdots H_2O]}$$

$$K_{eq1}^{w2} \cdot K_{eq2}^{w2} = \frac{[SO_3 \cdots H_2O \cdots H_2O]}{[SO_3][H_2O][H_2O]}$$

Thus,

$$K_{eq1} \cdot K_{eq2}^{w1} = K_{eq1}^{w2} \cdot K_{eq2}^{w2}$$

$$K_{eq1} \cdot K_{eq2}^{w1} \cdot k_{uni\_w} = K_{eq1}^{w2} \cdot K_{eq2}^{w2} \cdot k_{uni\_w}$$

$$k_{w1} = k_{w2}$$

For Reaction X1 and Reaction X2:

Reaction X1:

$$SO_3 + H_2O \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} SO_3 \cdots H_2O$$

$$SO_3 \cdots H_2O + X \underset{k_{-2}^{X1}}{\overset{k_2^{X1}}{\rightleftharpoons}} SO_3 \cdots H_2O \cdots X \xrightarrow{k_{uni\_X}} H_2SO_4 \cdots X'$$

Reaction X2:

$$H_2O + X \underset{k_{-1}^{X2}}{\overset{k_1^{X2}}{\rightleftharpoons}} H_2O \cdots X$$

$$SO_3 + H_2O \cdots X \underset{k_{-2}^{X2}}{\overset{k_2^{X2}}{\rightleftharpoons}} SO_3 \cdots H_2O \cdots X \xrightarrow{k_{uni\_X}} H_2SO_4 \cdots X'$$

For reaction X1,

$$K_{eq1} = \frac{[SO_3 \cdots H_2O]}{[SO_3][H_2O]}, \quad K_{eq2}^{X1} = \frac{[SO_3 \cdots H_2O \cdots X]}{[SO_3 \cdots H_2O][X]}$$

$$K_{eq1} \cdot K_{eq2}^{X1} = \frac{[SO_3 \cdots H_2O \cdots X]}{[SO_3][H_2O][X]}$$

For reaction X2,

$$K_{eq1}^{X2} = \frac{[H_2O \cdots X]}{[H_2O][X]}, \quad K_{eq2}^{X2} = \frac{[SO_3 \cdots H_2O \cdots X]}{[SO_3][H_2O \cdots X]}$$

$$K_{eq1}^{X2} \cdot K_{eq2}^{X2} = \frac{[SO_3 \cdots H_2O \cdots X]}{[SO_3][H_2O][X]}$$

Thus,

$$K_{eq1} \cdot K_{eq2}^{X1} = K_{eq1}^{X2} \cdot K_{eq2}^{X2}$$

$$K_{eq1} \cdot K_{eq2}^{X1} \cdot k_{uni\_X} = K_{eq1}^{w2} \cdot K_{eq2}^{X2} \cdot k_{uni\_X}$$

$$k_{X1} = k_{X2}$$

Table S1. Energies, enthalpies and free energies for the reaction of SO_3 with two water (in kcal mol^{-1}).

species	△E	△(E+ZPE)	△H[a]	△G[a]
SO_3+2H_2O	0.00	0.00	0.00	0.00
$SO_3+H_2O\cdots H_2O$	-5.90	-3.80	-4.25	1.71
$SO_3\cdots H_2O+H_2O$	-9.72	-7.38	-7.95	0.97
RC1	-23.45	-17.92	-19.83	-0.10
TS1	-16.55	-12.75	-15.73	6.20
PC1	-37.45	-31.75	-33.85	-13.31
$H_2SO_4+H_2O$	-23.41	-19.85	-21.26	-9.91

[a]These 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 SO_3 catalyzed by cTt conformer (in kcal mol^{-1}).

species	△E	△(E+ZPE)	△H[a]	△G[a]
SO3+H2O+cTt	0.00	0.00	0.00	0.00
$SO_3\cdots H_2O$+cTt	-9.72	-7.38	-7.95	0.97
$SO_3+H_2O\cdots$cTt	-12.33	-10.25	-10.77	-1.71
RC_{cTt}	-25.22	-21.20	-22.38	-0.37
TS_{cTt}	-21.17	-20.01	-21.89	1.89
PC_{cTt}	-38.67	-34.52	-35.83	-13.80
H_2SO_4+cCt	-19.99	-16.74	-18.07	-6.99

[a]These 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 SO_3 catalyzed by tTt conformer (in kcal mol^{-1}).

species	△E	△(E+ZPE)	△H[a]	△G[a]
SO3+H2O+tTt	0.00	0.00	0.00	0.00
$SO_3\cdots H_2O$+tTt	-9.72	-7.38	-7.95	0.97
$SO_3+H_2O\cdots$tTt	-12.10	-9.92	-10.47	-1.38
RC_{tTt}	-26.61	-22.51	-23.80	-1.52
TS_{tTt}	-23.90	-22.27	-24.20	-0.28
PC_{tTt}	-40.96	-36.56	-37.90	-15.97
H_2SO_4+tCt	-22.76	-19.22	-20.64	-9.58

[a]These 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 SO_3 catalyzed by tCt conformer (in kcal mol^{-1}).

species	△E	△(E+ZPE)	△H[a]	△G[a]
SO3+H2O+tCt	0.00	0.00	0.00	0.00
$SO_3\cdots H_2O$+tCt	-9.72	-7.38	-7.95	0.97
$SO_3+H_2O\cdots$tCt	-12.30	-10.09	-10.65	-1.47
RC_{tCt}	-27.11	-23.01	-24.33	-1.65
TS_{tCt}	-24.67	-22.96	-24.90	-0.63
PC_{tCt}	-41.89	-37.45	-38.79	-16.45
H_2SO_4+tTt	-24.06	-20.47	-21.89	-10.23

[a]These 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 SO_3 catalyzed by cCt conformer (in kcal mol^{-1}).

species	△E	△(E+ZPE)	△H[a]	△G[a]
SO3+H2O+cCt	0.00	0.00	0.00	0.00
$SO_3\cdots H_2O$+cCt	-9.72	-7.38	-7.95	0.97
$SO_3+H_2O\cdots$cCt	-13.36	-11.10	-11.72	-2.41
RC_{cCt}	-27.59	-23.48	-24.83	-2.24
TS_{cCt}	-25.10	-23.49	-25.47	-1.35
PC_{cCt}	-43.74	-39.10	-40.47	-18.30
H_2SO_4+cTt	-26.83	-22.95	-24.45	-12.82

[a]These 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} (molecules 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}

[a]The 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}, cm^3 $molecule^{-1}$), tunnelling corrected unimolecular rate constants (k_{uni}, s^{-1}) and Wigner correction coefficient ($\boldsymbol{\kappa_{uni}}$) 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_{eq1}	7.95×10^{-21}	1.23×10^{-20}	2.26×10^{-20}	4.45×10^{-20}	9.40×10^{-20}	2.17×10^{-19}	5.55×10^{-19}	9.37×10^{-19}
K_{eq2}^{w1}	2.47×10^{-19}	4.78×10^{-19}	1.22×10^{-18}	3.39×10^{-18}	1.05×10^{-17}	3.69×10^{-17}	1.46×10^{-16}	3.26×10^{-16}
K_{eq1}^{w2}	2.25×10^{-21}	2.79×10^{-21}	3.79×10^{-21}	5.32×10^{-21}	7.81×10^{-21}	1.20×10^{-20}	1.95×10^{-20}	2.56×10^{-20}
K_{eq2}^{w2}	8.77×10^{-19}	2.11×10^{-18}	7.26×10^{-18}	2.82×10^{-17}	1.26×10^{-16}	6.66×10^{-16}	4.26×10^{-15}	1.19×10^{-14}
k_{uni_w}	2.14×10^{8}	1.66×10^{8}	1.16×10^{8}	7.80×10^{7}	5.01×10^{7}	3.06×10^{7}	1.75×10^{7}	1.28×10^{7}
κ_{uni_w}	1.45	1.48	1.52	1.58	1.64	1.71	1.80	1.85
K_{eq2}^{cTt1}	3.85×10^{-19}	8.68×10^{-19}	2.72×10^{-18}	9.56×10^{-18}	3.85×10^{-17}	1.80×10^{-16}	1.01×10^{-15}	2.64×10^{-15}
K_{eq1}^{cTt2}	7.33×10^{-19}	1.33×10^{-18}	3.10×10^{-18}	7.86×10^{-18}	2.21×10^{-17}	6.98×10^{-17}	2.52×10^{-16}	5.15×10^{-16}
K_{eq2}^{cTt2}	4.16×10^{-21}	7.96×10^{-21}	1.98×10^{-20}	5.40×10^{-20}	1.63×10^{-19}	5.61×10^{-19}	2.22×10^{-18}	4.79×10^{-18}
k_{uni_cTt}	2.11×10^{11}	2.03×10^{11}	1.92×10^{11}	1.80×10^{11}	1.68×10^{11}	1.56×10^{11}	1.42×10^{11}	1.36×10^{11}
κ_{uni_cTt}	1.53	1.57	1.62	1.69	1.76	1.85	1.95	2.01
K_{eq2}^{tTt1}	2.71×10^{-18}	6.61×10^{-18}	2.34×10^{-17}	9.34×10^{-17}	4.30×10^{-16}	2.36×10^{-15}	1.57×10^{-14}	4.52×10^{-14}
K_{eq1}^{tTt2}	4.20×10^{-19}	7.48×10^{-19}	1.70×10^{-18}	4.20×10^{-18}	1.14×10^{-17}	3.46×10^{-17}	1.21×10^{-16}	2.42×10^{-16}
K_{eq2}^{tTt2}	5.15×10^{-20}	1.09×10^{-19}	3.11×10^{-19}	9.89×10^{-19}	3.54×10^{-18}	1.47×10^{-17}	7.22×10^{-17}	1.74×10^{-16}
k_{uni_tTt}	1.08×10^{12}	1.09×10^{12}	1.10×10^{12}	1.11×10^{12}	1.13×10^{12}	1.15×10^{12}	1.16×10^{12}	1.17×10^{12}
κ_{uni_tTt}	1.41	1.43	1.48	1.52	1.58	1.65	1.72	1.77
K_{eq2}^{tCt1}	3.38×10^{-18}	8.52×10^{-18}	3.14×10^{-17}	1.31×10^{-16}	6.40×10^{-16}	3.72×10^{-15}	2.64×10^{-14}	7.87×10^{-14}
K_{eq1}^{tCt2}	4.90×10^{-19}	8.80×10^{-19}	2.03×10^{-18}	5.07×10^{-18}	1.41×10^{-17}	4.37×10^{-17}	1.56×10^{-16}	3.17×10^{-16}

K_{eq2}^{tCt2}	5.52×10^{-20}	1.19×10^{-19}	3.50×10^{-19}	1.15×10^{-18}	4.27×10^{-18}	1.84×10^{-17}	9.40×10^{-17}	2.32×10^{-16}
k_{uni_tCt}	1.52×10^{12}	1.55×10^{12}	1.59×10^{12}	1.63×10^{12}	1.68×10^{12}	1.74×10^{12}	1.80×10^{12}	1.83×10^{12}
κ_{uni_tCt}	1.37	1.40	1.44	1.48	1.53	1.60	1.67	1.71
K_{eq2}^{cCt1}	9.14×10^{-18}	2.37×10^{-17}	9.12×10^{-17}	3.98×10^{-16}	2.04×10^{-15}	1.25×10^{-14}	9.47×10^{-14}	2.91×10^{-13}
K_{eq1}^{cCt2}	2.39×10^{-18}	4.58×10^{-18}	1.16×10^{-17}	3.19×10^{-17}	9.84×10^{-17}	3.43×10^{-16}	1.40×10^{-15}	3.05×10^{-15}
K_{eq2}^{cCt2}	3.04×10^{-20}	6.33×10^{-20}	1.78×10^{-19}	5.54×10^{-19}	1.95×10^{-18}	7.90×10^{-18}	3.76×10^{-17}	8.95×10^{-17}
k_{uni_cCt}	1.92×10^{12}	1.96×10^{12}	2.02×10^{12}	2.09×10^{12}	2.17×10^{12}	2.26×10^{12}	2.37×10^{12}	2.43×10^{12}
κ_{uni_cCt}	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 S2.

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 molecules 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 SO_3 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
ν_{cTt1}/ν_{w1}	1.36×10^{-7}	4.77×10^{-7}	1.07×10^{-6}	3.42×10^{-6}	1.16×10^{-5}	4.57×10^{-5}	3.72×10^{-4}	1.87×10^{-3}
ν_{tTt1}/ν_{w1}	1.51×10^{-6}	5.55×10^{-6}	1.35×10^{-5}	4.63×10^{-5}	1.70×10^{-4}	7.40×10^{-4}	6.71×10^{-3}	3.58×10^{-2}
ν_{tCt1}/ν_{w1}	1.82×10^{-6}	6.78×10^{-6}	1.67×10^{-5}	5.85×10^{-5}	2.20×10^{-4}	9.82×10^{-4}	9.13×10^{-3}	4.94×10^{-2}
ν_{cCt1}/ν_{w1}	4.06×10^{-7}	1.47×10^{-6}	3.50×10^{-6}	1.17×10^{-5}	4.23×10^{-5}	1.80×10^{-4}	1.59×10^{-3}	8.29×10^{-3}

Table S11. Optimized geometries of SO_3, H_2O, oxalic acid (cTc, cTt, tTt, tCt and cCt) and H_2SO_4 at M06-2X/6-311++G(3df,3pd).

SO_3

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

H_2O

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

H_2SO_4

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 SO_3 hydration catalyzed by water at M06-2X/6-311++G(3df,3pd).

$SO_3\cdots H_2O$

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

$H_2O\cdots H_2O$

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 SO_3 hydration catalyzed by oxalic acid at M06-2X/6-311++G(3df,3pd).

SO_3···H_2O

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···H_2O

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_{cTc}

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···H_2O

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_{cTt}

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_{cTt}

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···H_2O

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_{tTt}

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_{tTt}

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···H_2O

O	-3.13567	-0.10507	-0.07384

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···H_2O

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

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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