

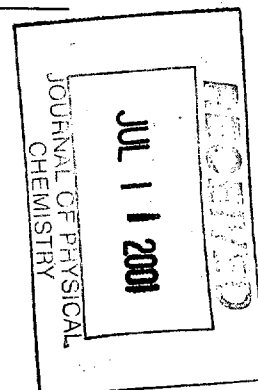
SUPPLEMENTARY MATERIAL

JP015502^TSupplementary Information "Hydrolysis, solvation and reduction of SO₃..."

Table 1.

Bond lengths (Å), bond angles (deg.), vibrational frequencies (cm⁻¹), IR intensities (km/mol), absolute and zero-point energies (H) for the SO₃ systems:

SO ₃					
D _{3h}	R ₁ (S-O): 1.463	R ₂ (O-O): 2.534	A ₁ (O-S-O): 120.0		
(Min. S)	Charge:	S: +0.882	O: -0.294		
1A ₂ "	1E'	A ₁ '	2E'		
433.2 (39)	476.3 (28)	958.9 (0)	1268. (165)		
D _{3h}	R ₁ (S-O): 1.447	R ₂ (O-O): 2.506	A ₁ (O-S-O): 120.0		
(Min. M)	Charge:	S: +0.532	O: -0.177		
1A ₂ "	1E'	A ₁ '	2E'		
441.1 (37)	495.9 (31)	1017. (0)	1329. (217)		
D _{3h}	R ₁ (S-O): 1.425	R ₂ (O-O): 2.469	A ₁ (O-S-O): 120.0		
(Min. L)	Charge:	S: +0.236	O: -0.079		
1A ₂ "	1E'	A ₁ '	2E'		
491.7 (34)	522.1 (28)	1078. (0)	1404. (204)		
D _{3h}	R ₁ (S-O): 1.426	R ₂ (O-O): 2.469	A ₁ (O-S-O): 120.0		
(Min. XL)	Charge:	S: +0.890	O: -0.297		
1A ₂ "	1E'	A ₁ '	2E'		
495.4 (33)	524.4 (26)	1075. (0)	1398. (196)		
Min. S	65 fkn.	E = -623.794001653	ZPE = 0.011117		
Min. M	96 fkn.	E = -623.856479022	ZPE = 0.011634		
Min. L	113 fkn.	E = -623.925789288	ZPE = 0.012351		
Min. XL	164 fkn.	E = -623.936318481	ZPE = 0.012339		
SO ₃ -H ₂ O					
C ₁	R ₁ (S-O ₁): 1.446	R ₆ (O ₄ -H ₂): 0.965	A ₁ (O ₁ -S-O ₂): 120.2		
(Min. M)	R ₂ (S-O ₂): 1.446	A ₂ (O ₁ -S-O ₃): 119.5	A ₃ (O ₁ -S-O ₄): 92.4		
	R ₃ (S-O ₃): 1.449	A ₄ (O ₂ -S-O ₃): 119.5	A ₅ (O ₂ -S-O ₄): 92.4		
	R ₄ (S-O ₄): 2.415	A ₆ (O ₃ -S-O ₄): 94.4	A ₇ (S-O ₄ -H ₁): 115.0		
	R ₅ (O ₄ -H ₁): 0.965	A ₈ (S-O ₄ -H ₂): 114.5	A ₉ (H ₁ -O ₄ -H ₂): 106.5		
Charge:	S: +0.489	O ₁ : -0.187	O ₂ : -0.194	O ₃ : -0.164	O ₄ : -0.535
	H ₁ : +0.296	H ₂ : +0.296			
1A	2A	3A	4A	5A	
28.5 (47)	156.5 (14)	168.1 (2)	179.5 (17)	373.8 (153)	
6A	7A	8A	9A	10A	
457.7 (155)	460.5 (1)	504.5 (54)	533.3 (43)	1021. (4)	
11A	12A	13A	14A	15A	
1324. (249)	1337. (243)	1611. (73)	3793. (61)	3897. (114)	
C ₁	R(S-O ₁): 1.423	R(O ₄ -H ₂): 0.965	A(O ₁ -S-O ₂): 119.8		
(Min. L)	R(S-O ₂): 1.427	A(O ₁ -S-O ₃): 119.8	A(O ₁ -S-O ₄): 95.0		
	R(S-O ₃): 1.427	A(O ₂ -S-O ₃): 119.4	A(O ₂ -S-O ₄): 92.1		
	R(S-O ₄): 2.374	A(O ₃ -S-O ₄): 92.2	A(S-O ₄ -H ₁): 108.7		
	R(O ₄ -H ₁): 0.965	A(S-O ₄ -H ₂): 108.7	A(H ₁ -O ₄ -H ₂): 106.6		
1A	2A	3A	4A	5A	
24.5 (55)	167.5 (6)	173.8 (12)	180.5 (20)	432.1 (152)	
6A	7A	8A	9A	10A	
488.3 (5)	489.7 (174)	534.1 (66)	559.6 (25)	1080. (5)	
11A	12A	13A	14A	15A	
1396. (234)	1411. (232)	1616. (86)	3784. (61)	3888. (115)	
Min. M	130 fkn.	E = -700.330242271	ZPE = 0.036099		
Min. L	147 fkn.	E = -700.399215631	ZPE = 0.036919		



SO ₂ (OH) ₂					
C ₂	R ₁ (S-O ₁): 1.452	R ₃ (O ₂ -H): 0.978	A ₁ (O ₁ -S-O ₂): 105.3		
(Min. S)	R ₂ (S-O ₂): 1.631	A ₂ (O ₁ -S-O ₂): 109.1	A ₃ (O ₁ -S-O ₁): 124.4		
		A ₄ (O ₂ -S-O ₂): 101.3	A ₅ (S-O ₂ -H): 114.5		
Charge:	S: +0.932	O ₁ : -0.354	O ₂ : -0.453	H: +0.431	
1A	1B	2A	3A	2B	
270.9 (98)	293.6 (117)	350.9 (12)	419.5 (54)	458.1 (63)	
4A	3B	5A	4B	6A	
494.9 (61)	499.8 (14)	727.7 (154)	793.7 (419)	1070. (150)	
5B	7A	6B	7B	8A	
1088. (51)	1135. (101)	1365. (274)	3637. (129)	3640. (58)	
C ₂	R ₁ (S-O ₁): 1.439	R ₃ (O ₂ -H): 0.970	A ₁ (O ₁ -S-O ₂): 105.3		
(Min. M)	R ₂ (S-O ₂): 1.626	A ₂ (O ₁ -S-O ₂): 108.9	A ₃ (O ₁ -S-O ₁): 124.6		
		A ₄ (O ₂ -S-O ₂): 101.6	A ₅ (S-O ₂ -H): 109.5		
Charge:	S: +0.511	O ₁ : -0.237	O ₂ : -0.315	H: +0.296	
1A	1B	2A	3A	2B	
260.7 (81)	314.4 (71)	357.7 (8)	421.2 (30)	470.2 (50)	
4A	3B	5A	4B	6A	
509.9 (48)	516.8 (20)	757.1 (129)	809.5 (353)	1127. (94)	
5B	7A	6B	7B	8A	
1137. (85)	1165. (150)	1413. (311)	3759. (199)	3763. (61)	
C ₂	R(S-O ₁): 1.420	A(O ₁ -S-O ₁): 124.1	A(O ₁ -S-O ₂): 105.5		
(Min. L)	R(S-O ₂): 1.593	A(O ₂ -S-O ₂): 102.0	A(O ₁ -S-O ₂): 108.8		
	R(O ₂ -H): 0.970		A(S-O ₂ -H): 109.4		
Charge:	S: +0.029	O ₁ : -0.151	O ₂ : -0.149	H: +0.286	
1A	1B	2A	3A	2B	
266.2 (96)	333.9 (66)	375.3 (5)	441.3 (21)	495.7 (43)	
4A	3B	5A	4B	6A	
537.3 (46)	549.5 (25)	808.7 (118)	858.5 (345)	1148. (75)	
5B	7A	6B	7B	8A	
1164. (90)	1223. (345)	1471. (301)	3766. (207)	3771. (56)	
Min. S	84 fkn.	E = -700.245208385	ZPE = 0.037009		
Min. M	130 fkn.	E = -700.338996834	ZPE = 0.038232		
Min. L	147 fkn.	E = -700.413399715	ZPE = 0.039206		

SO(OH) ₄					
C ₁	R(S-O ₁): 1.486	R(O ₅ -H ₄): 0.965	A(O ₁ -S-O ₂): 95.8		
(Min. 1 M)	R(S-O ₂): 1.633	A(O ₁ -S-O ₃): 97.6	A(O ₁ -S-O ₄): 95.9		
	R(S-O ₃): 1.652	A(O ₁ -S-O ₅): 177.9	A(O ₂ -S-O ₃): 117.2		
	R(S-O ₄): 1.672	A(O ₂ -S-O ₄): 122.9	A(O ₂ -S-O ₅): 83.0		
	R(S-O ₅): 1.758	A(O ₃ -S-O ₄): 116.2	A(O ₃ -S-O ₅): 84.5		
	R(O ₁ -H ₂): 2.145	A(O ₄ -S-O ₅): 83.2	A(O ₁ -H ₂ -O ₃): 90.5		
	R(O ₁ -H ₃): 2.127	A(O ₁ -H ₃ -O ₄): 90.7	A(O ₂ -H ₁ -O ₅): 97.6		
	R(O ₂ -H ₁): 0.973	A(S-O ₁ -H ₂): 68.2	A(S-O ₁ -H ₃): 69.5		
	R(O ₃ -H ₂): 0.973	A(S-O ₂ -H ₁): 107.8	A(S-O ₃ -H ₂): 103.8		
	R(O ₄ -H ₃): 0.972	A(S-O ₄ -H ₃): 103.9	A(S-O ₅ -H ₁): 71.5		
	R(O ₅ -H ₁): 1.904	A(S-O ₅ -H ₅): 109.9	A(H ₁ -O ₅ -H ₅): 164.4		
Charge:	S: +0.648	O ₁ : -0.452	O ₂ : -0.237	O ₃ : -0.271	O ₄ : -0.298
	O ₅ : -0.554	H ₁ : +0.309	H ₂ : +0.290	H ₃ : +0.285	H ₄ : +0.281

1A	2A	3A	4A	5A
93.9 (5)	158.9 (19)	262.4 (86)	452.3 (44)	490.9 (5)
6A	7A	8A	9A	10A
508.0 (27)	528.6 (13)	537.6 (11)	560.8 (18)	589.2 (65)
11A	12A	13A	14A	15A
624.5 (93)	632.3 (31)	644.2 (65)	778.2 (438)	807.6 (351)
16A	17A	18A	19A	20A
1043. (180)	1153. (111)	1193. (109)	1224. (49)	1334. (348)
21A	22A	23A	24A	
3692. (136)	3707. (73)	3717. (99)	3819. (77)	
C ₂	R(S-O ₁): 1.469	A(S-O ₂ -H ₁): 105.6	A(O ₁ -S-O ₂): 123.4	
(Min. 2 M)	R(S-O ₂): 1.630	A(S-O ₃ -H ₁): 69.7	A(O ₁ -S-O ₃): 96.5	
	R(S-O ₃): 1.731	A(S-O ₃ -H ₂): 107.0	A(O ₂ -S-O ₃): 86.2	
	R(O ₂ -H ₁): 0.973	A(H ₁ -O ₃ -H ₂): 144.6	A(O ₂ -S-O ₃): 86.7	
	R(O ₃ -H ₁): 1.948		A(O ₃ -S-O ₃): 167.0	
	R(O ₃ -H ₂): 0.965		A(O ₁ -H ₁ -O ₂): 98.0	
A	B	B		
Frequencies --	145.2825	198.5893	283.9629	
IR Inten --	4.7175	88.8818	75.8684	
A	A	B		
Frequencies --	295.7453	462.9839	481.8358	
IR Inten --	12.3193	3.6305	15.6974	
A	B	A		
Frequencies --	484.0983	500.2359	552.4981	
IR Inten --	4.8522	13.9296	0.4804	
B	B	A		
Frequencies --	564.5255	597.8832	615.5607	
IR Inten --	88.4721	54.0223	165.0679	
B	A	B		
Frequencies --	663.3013	705.9248	830.0695	
IR Inten --	402.8942	49.4312	309.6599	
A	B	A		
Frequencies --	1088.7567	1127.5219	1232.2440	
IR Inten --	81.4317	168.8405	0.0041	
A	B	B		
Frequencies --	1235.7286	1293.2758	3692.9055	
IR Inten --	263.7231	295.4014	223.9278	
A	B	A		
Frequencies --	3698.4170	3820.6080	3821.1918	
IR Inten --	19.1287	104.2940	87.3203	
C ₂	R(S-O ₁): 1.451	A(S-O ₂ -H ₁): 106.0	A(O ₁ -S-O ₂): 123.9	
(Min. 2 L)	R(S-O ₂): 1.600	A(S-O ₃ -H ₁): 69.5	A(O ₁ -S-O ₃): 95.7	
	R(S-O ₃): 1.703	A(S-O ₃ -H ₂): 106.3	A(O ₂ -S-O ₃): 86.5	
	R(O ₂ -H ₁): 0.972	A(H ₁ -O ₃ -H ₂): 138.5	A(O ₂ -S-O ₃): 87.0	
	R(O ₃ -H ₁): 1.942		A(O ₃ -S-O ₃): 168.5	
	R(O ₃ -H ₂): 0.965		A(O ₁ -H ₁ -O ₂): 97.0	
A	B	A		
Frequencies --	192.0529	204.8436	314.0007	
IR Inten --	0.0857	47.6408	2.4339	
B	A	A		
Frc consts --	0.0848	0.5528	0.7614	
IR Inten --	111.7440	1.4640	7.3441	
B	B	A		
Frequencies --	513.0000	538.2542	578.2060	
IR Inten --	25.3567	16.3805	0.2903	
B	B	A		
Frequencies --	600.0054	622.9613	633.4190	
IR Inten --	107.1262	59.4939	155.9933	

B	A	B	
Frequencies --	690.5955	756.2470	883.7650
IR Inten --	375.4138	35.7231	327.0881
A	B	A	
Frequencies --	1125.3614	1157.6869	1251.3152
IR Inten --	69.0629	169.2267	54.5941
A	B	B	
Frequencies --	1291.7548	1313.6839	3709.8802
IR Inten --	231.2256	303.5726	207.7665
A	B	A	
Frequencies --	3715.7480	3828.9206	3829.4850
IR Inten --	16.1626	88.0247	106.1899
Min. 1 M	164 fkn.	E = -776.722150936	ZPE = 0.065044
Min. 2 M	164 fkn.	E = -776.743503367	ZPE = 0.064684
Min. 2 L	181 fkn.	E = -776.813368065	ZPE = 0.066252

SO(OH)₂-H₂O₂

C ₁	R(S-O ₁): 1.463	A(S-O ₂ -H ₁): 109.3	A(O ₁ -S-O ₂): 109.7
(Min. 1 M)	R(S-O ₂): 1.632	A(S-O ₃ -H ₂): 109.5	A(O ₁ -S-O ₃): 101.2
	R(S-O ₃): 1.730	A(S-O ₃ -H ₃): 112.7	A(O ₂ -S-O ₃): 97.5
	R(O ₄ -O ₅): 1.448	A(H ₂ -O ₃ -H ₃): 113.8	A(O ₂ -H ₁ -O ₄): 161.7
	R(O ₂ -H ₁): 0.992	A(H ₁ -O ₄ -H ₄): 115.3	A(O ₃ -H ₃ -O ₅): 161.3
	R(O ₃ -H ₂): 0.970		A(O ₄ -O ₅ -H ₃): 101.3
	R(O ₃ -H ₃): 1.914		A(O ₅ -O ₄ -H ₁): 114.5
	R(O ₄ -H ₁): 1.797		A(O ₅ -O ₄ -H ₄): 102.2
	R(O ₄ -H ₄): 0.969		
	R(O ₅ -H ₃): 0.979		
?A	?A	?A	
Frequencies --	58.1141	86.6671	148.6446
IR Inten --	16.7409	11.8287	8.0129
?A	?A	?A	
Frequencies --	183.4216	229.6789	294.6482
IR Inten --	2.7971	11.4648	101.1399
?A	?A	?A	
Frequencies --	350.6922	393.1461	416.2463
IR Inten --	77.7663	25.5915	48.4260
?A	?A	?A	
Frequencies --	485.6275	592.6915	648.3965
IR Inten --	26.7575	144.4667	54.2236
?A	?A	?A	
Frequencies --	770.8247	838.4441	941.1611
IR Inten --	204.5000	159.0531	6.2149
?A	?A	?A	
Frequencies --	1072.5282	1189.1663	1263.0331
IR Inten --	104.5396	95.9740	137.9308
?A	?A	?A	
Frequencies --	1372.0417	1519.6629	3338.3335
IR Inten --	52.8556	31.0166	607.5848
?A	?A	?A	
Frequencies --	3572.2996	3751.4082	3764.3113
IR Inten --	408.2481	54.5691	90.5108

C ₁ (Min. 2 M)	R(S-O ₁): 1.490 R(S-O ₂): 1.645 R(S-O ₃): 1.653 R(O ₄ -O ₅): 1.450 R(O ₁ -H ₁): 1.824 R(O ₂ -H ₂): 0.980 R(O ₃ -H ₃): 0.979 R(O ₄ -H ₁): 0.987 R(O ₄ -H ₃): 2.144 R(O ₅ -H ₂): 1.970 R(O ₅ -H ₄): 0.967	A(S-O ₁ -H ₁): 111.5 A(S-O ₂ -H ₂): 110.4 A(S-O ₃ -H ₃): 110.5 A(H ₁ -O ₄ -H ₃): 138.6 A(H ₂ -O ₅ -H ₄): 83.0	A(O ₁ -S-O ₂): 109.7 A(O ₁ -S-O ₃): 101.2 A(O ₂ -S-O ₃): 97.5 A(O ₁ -H ₁ -O ₄): 145.8 A(O ₂ -H ₂ -O ₅): 154.5 A(O ₃ -H ₃ -O ₄): 143.6 A(O ₄ -O ₅ -H ₂): 109.4 A(O ₄ -O ₅ -H ₄): 102.3 A(O ₅ -O ₄ -H ₁): 96.6 A(O ₅ -O ₄ -H ₃): 101.1
?A	?A	?A	
Frequencies --	80.4876	111.0274	150.1906
IR Inten --	7.9656	11.9168	8.9668
?A	?A	?A	
Frequencies --	166.7402	226.5646	253.5840
IR Inten --	1.9908	122.0012	17.6704
?A	?A	?A	
Frequencies --	349.4058	386.1316	497.7560
IR Inten --	2.0280	1.2534	30.7986
?A	?A	?A	
Frequencies --	527.0615	615.1309	721.8192
IR Inten --	53.8920	137.4281	267.1515
?A	?A	?A	
Frequencies --	738.3067	796.9576	941.1686
IR Inten --	192.9529	283.6328	7.0130
?A	?A	?A	
Frequencies --	1088.8233	1160.6156	1260.8744
IR Inten --	137.5504	79.1001	60.6738
?A	?A	?A	
Frequencies --	1349.7955	1518.9058	3419.1758
IR Inten --	83.1054	16.6336	234.7523
?A	?A	?A	
Frequencies --	3562.5987	3594.5347	3782.2102
IR Inten --	119.2294	539.5740	62.4588
C ₁ (Min. 2 L)	R(S-O ₁): 1.470 R(S-O ₂): 1.612 R(S-O ₃): 1.622 R(O ₄ -O ₅): 1.450 R(O ₁ -H ₁): 1.824 R(O ₂ -H ₂): 0.982 R(O ₃ -H ₃): 0.979 R(O ₄ -H ₁): 0.987 R(O ₄ -H ₃): 2.184 R(O ₅ -H ₂): 1.935 R(O ₅ -H ₄): 0.968	A(S-O ₁ -H ₁): 111.2 A(S-O ₂ -H ₂): 110.4 A(S-O ₃ -H ₃): 110.6 A(H ₁ -O ₄ -H ₃): 79.4 A(H ₂ -O ₅ -H ₄): 135.2	A(O ₁ -S-O ₂): 106.3 A(O ₁ -S-O ₃): 106.0 A(O ₂ -S-O ₃): 101.2 A(O ₁ -H ₁ -O ₄): 148.6 A(O ₂ -H ₂ -O ₅): 156.9 A(O ₃ -H ₃ -O ₄): 143.5 A(O ₄ -O ₅ -H ₂): 107.9 A(O ₄ -O ₅ -H ₄): 102.3 A(O ₅ -O ₄ -H ₁): 101.0 A(O ₅ -O ₄ -H ₃): 96.8
?A	?A	?A	
Frequencies --	74.3487	106.5688	152.5480
IR Inten --	7.5304	7.1559	9.9613
?A	?A	?A	
Frequencies --	170.0509	244.9565	277.9504
IR Inten --	2.6492	35.2038	100.1897
?A	?A	?A	
Frequencies --	374.9035	391.9046	515.3445
IR Inten --	4.5619	2.1037	70.6614
?A	?A	?A	
Frequencies --	523.9447	613.1909	755.8619
IR Inten --	35.6624	112.2678	192.6570

?A	?A	?A	
Frequencies --	770.6773	806.3713	939.1857
IR Inten --	285.3029	233.2932	4.4116
?A	?A	?A	
Frequencies --	1124.3047	1166.8378	1270.9301
IR Inten --	107.0661	88.5929	82.8257
?A	?A	?A	
Frequencies --	1351.6714	1508.4392	3415.5658
IR Inten --	78.5110	14.3849	227.9229
?A	?A	?A	
Frequencies --	3529.0298	3598.8647	3777.4852
IR Inten --	346.9905	388.2445	61.9212
Min. 1 M	164 fkn.	E = -776.734866052	ZPE = 0.062151
Min. 2 M	164 fkn.	E = -776.738436775	ZPE = 0.062194
Min. 2 L	181 fkn.	E = -776.783601478	ZPE = 0.062561

SO₃:2 H₂O

C ₁	R(S-O ₁): 1.443	A(S-O ₃ -H ₁): 124.0	A(O ₁ -S-O ₂): 120.0
(Min. M)	R(S-O ₂): 1.449	A(S-O ₄ -H ₂): 107.2	A(O ₁ -S-O ₃): 119.0
	R(S-O ₃): 1.456	A(S-O ₄ -H ₃): 110.7	A(O ₁ -S-O ₄): 96.5
	R(S-O ₄): 2.234	A(H ₁ -O ₅ -H ₂): 98.6	A(O ₂ -S-O ₃): 118.5
	R(O ₃ -H ₁): 2.083	A(H ₁ -O ₅ -H ₄): 107.0	A(O ₂ -S-O ₄): 95.3
	R(O ₄ -H ₂): 0.989	A(H ₂ -O ₄ -H ₃): 107.9	A(O ₃ -S-O ₄): 93.5
	R(O ₄ -H ₃): 0.965	A(H ₂ -O ₅ -H ₄): 131.7	A(O ₃ -H ₁ -O ₅): 134.3
	R(O ₅ -H ₁): 0.969		A(O ₄ -H ₂ -O ₅): 158.4
	R(O ₅ -H ₂): 1.733		
	R(O ₅ -H ₄): 0.962		

Charge:	S: +0.448	O ₁ : -0.175	O ₂ : -0.310	O ₃ : -0.132	O ₄ : -0.598
	O ₅ : -0.595	H ₁ : +0.328	H ₂ : +0.292	H ₃ : +0.438	H ₄ : +0.304
1A	2A	3A	4A	5A	
22.3 (3)	136.9 (1)	181.9 (24)	186.5 (68)	200.6 (54)	
6A	7A	8A	9A	10A	
235.2 (71)	289.2 (8)	303.7 (64)	429.8 (167)	480.1 (189)	
11A	12A	13A	14A	15A	
491.5 (53)	500.9 (35)	510.1 (48)	646.9 (149)	918.1 (86)	
16A	17A	18A	19A	20A	
1017. (20)	1302. (290)	1339. (267)	1619. (82)	1643. (53)	
21A	22A	23A	24A		
3368. (832)	3744. (124)	3842. (121)	3898. (130)		

C ₁	R(S-O ₁): 1.422	A(S-O ₃ -H ₁): 123.7	A(O ₁ -S-O ₂): 119.8
(Min. L)	R(S-O ₂): 1.429	A(S-O ₄ -H ₂): 106.5	A(O ₁ -S-O ₃): 119.0
	R(S-O ₃): 1.434	A(S-O ₄ -H ₃): 107.5	A(O ₁ -S-O ₄): 96.7
	R(S-O ₄): 2.166	A(H ₁ -O ₅ -H ₂): 98.8	A(O ₂ -S-O ₃): 118.5
	R(O ₃ -H ₁): 2.125	A(H ₁ -O ₅ -H ₄): 107.0	A(O ₂ -S-O ₄): 95.3
	R(O ₄ -H ₂): 0.992	A(H ₂ -O ₄ -H ₃): 108.0	A(O ₃ -S-O ₄): 94.6
	R(O ₄ -H ₃): 0.966	A(H ₂ -O ₅ -H ₄): 130.7	A(O ₃ -H ₁ -O ₅): 131.3
	R(O ₅ -H ₁): 0.969		A(O ₄ -H ₂ -O ₅): 161.2
	R(O ₅ -H ₂): 1.712		
	R(O ₅ -H ₄): 0.962		

?A	?A	?A	
Frequencies --	20.9569	133.4073	182.4636
IR Inten --	3.2417	4.6607	14.8241
?A	?A	?A	
Frequencies --	191.1673	222.8135	241.4203
IR Inten --	128.5149	10.1281	65.2034
?A	?A	?A	
Frequencies --	305.1763	308.5088	445.7203
IR Inten --	53.1653	14.6651	254.5246

?A	?A	?A	
Frequencies --	488.1841	515.1466	523.5691
IR Inten --	58.8646	104.9063	42.6283
?A	?A	?A	
Frequencies --	529.5275	688.0618	956.0902
IR Inten --	34.0410	154.8281	79.0063
?A	?A	?A	
Frequencies --	1076.5356	1371.6463	1409.4968
IR Inten --	21.0446	280.3208	260.0880
?A	?A	?A	
Frequencies --	1614.5392	1655.7835	3318.7213
IR Inten --	76.4753	62.2519	932.2224
?A	?A	?A	
Frequencies --	3751.5813	3831.5675	3896.5924
IR Inten --	104.0682	122.3484	130.8925
Min. M	164 fkn.	E = -776.807308990	ZPE = 0.062208
Min. L	181 fkn.	E = -776.876192860	ZPE = 0.063057

SO₂(OH)₂-H₂O

C ₁	R(S-O ₁): 1.440	R(O ₅ -H ₃): 0.968	A(O ₁ -S-O ₂): 123.0
(Min. M)	R(S-O ₂): 1.449	R(O ₅ -H ₄): 0.962	A(O ₁ -S-O ₃): 107.3
	R(S-O ₃): 1.596	A(O ₁ -S-O ₄): 108.5	A(O ₂ -S-O ₃): 109.3
	R(S-O ₄): 1.631	A(O ₂ -S-O ₄): 104.4	A(O ₃ -S-O ₄): 102.4
	R(O ₂ -H ₃): 2.242	A(O ₂ -H ₃ -O ₅): 122.0	A(O ₃ -H ₁ -O ₅): 163.0
	R(O ₃ -H ₁): 1.000	A(S-O ₂ -H ₃): 110.8	A(S-O ₃ -H ₁): 109.2
	R(O ₄ -H ₂): 0.970	A(S-O ₄ -H ₂): 109.2	A(H ₁ -O ₅ -H ₃): 100.6
	R(O ₅ -H ₁): 1.691	A(H ₁ -O ₅ -H ₄): 126.8	A(H ₃ -O ₅ -H ₄): 107.0
Charge:	S: +0.485	O ₁ : -0.206	O ₂ : -0.319
	O ₅ : -0.550	H ₁ : +0.442	H ₂ : +0.298
			O ₃ : -0.412
			O ₄ : -0.311
			H ₃ : +0.286
			H ₄ : +0.288
1A	2A	3A	4A
44.4 (3)	121.2 (18)	199.9 (104)	220.8 (47)
6A	7A	8A	9A
324.2 (94)	358.8 (5)	410.2 (67)	486.1 (78)
11A	12A	13A	14A
516.6 (30)	524.7 (56)	762.7 (103)	827.9 (113)
16A	17A	18A	19A
1131. (149)	1154. (128)	1311. (104)	1418. (330)
21A	22A	23A	24A
3202. (1217)	3759. (68)	3767. (120)	3895. (121)
C ₁	R(S-O ₁): 1.421	R(O ₅ -H ₃): 0.968	A(O ₁ -S-O ₂): 122.6
(Min. L)	R(S-O ₂): 1.429	R(O ₅ -H ₄): 0.962	A(O ₁ -S-O ₃): 107.5
	R(S-O ₃): 1.564	A(O ₁ -S-O ₄): 108.3	A(O ₂ -S-O ₃): 109.2
	R(S-O ₄): 1.600	A(O ₂ -S-O ₄): 104.6	A(O ₃ -S-O ₄): 102.8
	R(O ₂ -H ₃): 2.264	A(O ₂ -H ₃ -O ₅): 121.5	A(O ₃ -H ₁ -O ₅): 164.4
	R(O ₃ -H ₁): 1.000	A(S-O ₂ -H ₃): 110.9	A(S-O ₃ -H ₁): 109.6
	R(O ₄ -H ₂): 0.969	A(S-O ₄ -H ₂): 109.0	A(H ₁ -O ₅ -H ₃): 99.6
	R(O ₅ -H ₁): 1.676	A(H ₁ -O ₅ -H ₄): 126.2	A(H ₃ -O ₅ -H ₄): 107.0
?A	?A	?A	
Frequencies --	45.6785	118.7829	195.6809
IR Inten --	2.9450	20.4903	80.2618
?A	?A	?A	
Frequencies --	224.6805	272.7066	322.3493
IR Inten --	51.9984	35.6909	106.5629
?A	?A	?A	
Frequencies --	375.9440	432.3328	481.9573
IR Inten --	6.9523	87.8585	135.8178
?A	?A	?A	
Frequencies --	524.3914	545.1774	557.5964

IR Inten	--	21.4232	31.3841	57.4088
?A		?A	?A	
Frequencies	--	810.6816	848.5523	905.2227
IR Inten	--	74.6873	165.7127	313.5258
?A		?A	?A	
Frequencies	--	1157.0256	1209.3353	1342.7034
IR Inten	--	96.0465	174.7791	84.6326
?A		?A	?A	
Frequencies	--	1463.0851	1617.3360	3182.8719
IR Inten	--	358.7152	55.4123	1287.1079
?A		?A	?A	
Frequencies	--	3762.4748	3775.3404	3894.2535
IR Inten	--	65.0166	121.2904	121.4465
Min. M		164 fkn.	E = -776.817282402	ZPE = 0.063031
Min. L		181 fkn.	E = -776.891569778	ZPE = 0.063939

SO₂(OH)₂·2 H₂O

C ₂	R(S-O ₁): 1.451	A(S-O ₁ -H ₃): 110.6	A(O ₁ -S-O ₁): 121.7
(Min. 1 M)	R(S-O ₂): 1.600	A(S-O ₂ -H ₁): 109.8	A(O ₁ -S-O ₂): 106.3
	R(O ₁ -H ₂): 2.187	A(H ₁ -O ₃ -H ₂): 98.3	A(O ₁ -S-O ₂): 108.8
	R(O ₂ -H ₁): 0.997	A(H ₁ -O ₃ -H ₃): 125.8	A(O ₂ -S-O ₂): 103.4
	R(O ₃ -H ₁): 1.711	A(H ₂ -O ₃ -H ₃): 106.9	A(O ₁ -H ₂ -O ₃): 125.4
	R(O ₃ -H ₂): 0.969		A(O ₂ -H ₁ -O ₃): 161.8
	R(O ₃ -H ₃): 0.962		

Charge:	S: +0.461	O ₁ : -0.293	O ₂ : -0.403	O ₃ : -0.545
	H ₁ : +0.445	H ₂ : +0.283	H ₃ : +0.283	

1A	1B	2A	2B	3A
31.5 (3)	44.7 (8)	129.9 (3)	132.4 (44)	215.0 (13)
3B	4A	4B	5A	5B
215.6 (123)	219.1 (29)	228.9 (92)	322.1 (65)	326.4 (55)
6A	7A	6B	7B	8A
360.0 (6)	410.4 (6)	507.4 (309)	517.2 (154)	523.9 (30)
8B	9A	10A	9B	11A
532.0 (101)	534.6 (8)	795.1 (29)	817.0 (5)	824.6 (199)
10B	12A	11B	13A	12B
873.3 (429)	1136. (224)	1269. (126)	1340. (53)	1419. (368)
14A	13B	14B	15A	15B
1617. (0)	1618. (122)	3228. (2143)	3247. (166)	3744. (99)
16A	16B	17A		
3745. (77)	3891. (69)	3892. (163)		

C ₂	R(S-O ₁): 1.431	A(S-O ₁ -H ₃): 110.8	A(O ₁ -S-O ₁): 121.2
(Min. 1 L)	R(S-O ₂): 1.569	A(S-O ₂ -H ₁): 109.5	A(O ₁ -S-O ₂): 106.5
	R(O ₁ -H ₂): 2.220	A(H ₁ -O ₃ -H ₂): 97.0	A(O ₁ -S-O ₂): 108.8
	R(O ₂ -H ₁): 0.997	A(H ₁ -O ₃ -H ₃): 125.0	A(O ₂ -S-O ₂): 103.6
	R(O ₃ -H ₁): 1.696	A(H ₂ -O ₃ -H ₃): 106.8	A(O ₁ -H ₂ -O ₃): 125.2
	R(O ₃ -H ₂): 0.969		A(O ₂ -H ₁ -O ₃): 163.0
	R(O ₃ -H ₃): 0.962		

A	B	A	
Frequencies	--	29.5294	43.5433
IR Inten	--	2.9531	7.6643
B		B	A
Frequencies	--	128.5596	211.3631
IR Inten	--	50.4814	108.6770
A		B	A
Frequencies	--	218.8671	230.0197
IR Inten	--	21.2543	67.1735
B		A	A
Frequencies	--	324.0674	378.6920

IR Inten	--	89.1466	1.0579	5.7739	
B		A	B		
Frequencies	--	494.4529	525.1117	543.7353	
IR Inten	--	472.5093	5.5277	9.4394	
A		B	A		
Frequencies	--	552.1363	566.6420	828.8720	
IR Inten	--	26.9103	84.0918	87.5068	
B		A	B		
Frequencies	--	836.4200	853.5714	920.7590	
IR Inten	--	37.8436	136.5615	393.8831	
A		B	A		
Frequencies	--	1194.8175	1310.6895	1354.1905	
IR Inten	--	207.0447	93.7143	68.5996	
B		A	B		
Frequencies	--	1455.0633	1618.5034	1620.2262	
IR Inten	--	406.9287	0.1759	108.8637	
B		A	B		
Frequencies	--	3210.4822	3232.0542	3746.8036	
IR Inten	--	2279.2690	160.7961	99.6573	
A		B	A		
Frequencies	--	3747.7036	3890.4128	3890.9832	
IR Inten	--	75.1032	68.4037	164.8574	
C ₁		R(S-O ₁): 1.441	A(S-O ₂ -H ₁): 138.4	A(O ₁ -S-O ₂): 121.6	
(Min. 2 M)		R(S-O ₂): 1.453	A(S-O ₃ -H ₂): 108.9	A(O ₁ -S-O ₃): 108.7	
		R(S-O ₃): 1.634	A(S-O ₄ -H ₃): 113.4	A(O ₁ -S-O ₄): 107.6	
		R(S-O ₄): 1.577	A(H ₁ -O ₆ -H ₄): 99.3	A(O ₂ -S-O ₃): 103.8	
		R(O ₂ -H ₁): 1.892	A(H ₁ -O ₆ -H ₆): 106.7	A(O ₂ -S-O ₄): 110.5	
		R(O ₃ -H ₂): 0.970	A(H ₃ -O ₅ -H ₄): 110.2	A(O ₃ -S-O ₄): 103.0	
		R(O ₄ -H ₃): 1.023	A(H ₃ -O ₅ -H ₅): 119.6	A(O ₂ -H ₁ -O ₆): 156.2	
		R(O ₅ -H ₃): 1.550	A(H ₄ -O ₅ -H ₅): 107.4	A(O ₄ -H ₃ -O ₅): 177.2	
		R(O ₅ -H ₄): 0.987	A(H ₄ -O ₆ -H ₆): 125.5	A(O ₅ -H ₄ -O ₆): 162.3	
		R(O ₅ -H ₅): 0.962			
		R(O ₆ -H ₁): 0.973			
		R(O ₆ -H ₄): 1.732			
		R(O ₆ -H ₆): 0.962			
?A		?A	?A		
Frequencies	--	36.0685	52.7938	112.5460	
IR Inten	--	2.9026	0.5134	2.5956	
?A		?A	?A		
Frequencies	--	165.1230	225.5567	233.3277	
IR Inten	--	9.4571	72.6010	119.6279	
?A		?A	?A		
Frequencies	--	256.4610	283.7127	311.0367	
IR Inten	--	63.4015	7.0486	113.5483	
?A		?A	?A		
Frequencies	--	364.3891	375.8126	409.6295	
IR Inten	--	16.7167	20.2210	56.7332	
?A		?A	?A		
Frequencies	--	479.3380	516.2834	523.3246	
IR Inten	--	88.2575	21.1882	36.6756	
?A		?A	?A		
Frequencies	--	529.5674	624.9634	766.3305	
IR Inten	--	35.9753	170.6531	171.2459	
?A		?A	?A		
Frequencies	--	885.1956	903.3768	1054.3744	
IR Inten	--	156.1609	286.5435	68.0857	
?A		?A	?A		
Frequencies	--	1131.1905	1156.0076	1330.6677	

IR Inten	--	161.9052	192.8223	215.8225	
?A		?A	?A		
Frequencies	--	1415.2522	1630.1610	1661.7656	
IR Inten	--	227.3145	80.1464	16.1861	
?A		?A	?A		
Frequencies	--	2753.6785	3398.9679	3670.8016	
IR Inten	--	2151.4232	731.8435	475.7620	
?A		?A	?A		
Frequencies	--	3767.6152	3878.4029	3888.3242	
IR Inten	--	115.6804	93.2268	125.6452	
C ₁		R(S-O ₁): 1.422	A(S-O ₂ -H ₁): 139.9	A(O ₁ -S-O ₂): 121.2	
(Min. 2 L)		R(S-O ₂): 1.432	A(S-O ₃ -H ₂): 108.9	A(O ₁ -S-O ₃): 108.6	
		R(S-O ₃): 1.600	A(S-O ₄ -H ₃): 113.5	A(O ₁ -S-O ₄): 107.7	
		R(S-O ₄): 1.548	A(H ₁ -O ₆ -H ₄): 99.4	A(O ₂ -S-O ₃): 104.0	
		R(O ₂ -H ₁): 1.917	A(H ₁ -O ₆ -H ₆): 106.7	A(O ₂ -S-O ₄): 110.5	
		R(O ₃ -H ₂): 0.969	A(H ₃ -O ₅ -H ₄): 109.8	A(O ₃ -S-O ₄): 103.2	
		R(O ₄ -H ₃): 1.023	A(H ₃ -O ₅ -H ₅): 119.7	A(O ₂ -H ₁ -O ₆): 154.3	
		R(O ₅ -H ₃): 1.548	A(H ₄ -O ₆ -H ₅): 107.3	A(O ₄ -H ₃ -O ₆): 177.0	
		R(O ₅ -H ₄): 0.987	A(H ₄ -O ₆ -H ₆): 125.4	A(O ₆ -H ₄ -O ₆): 162.9	
		R(O ₅ -H ₅): 0.962			
		R(O ₆ -H ₁): 0.973			
		R(O ₆ -H ₄): 1.731			
		R(O ₆ -H ₆): 0.962			
?A		?A	?A		
Frequencies	--	31.6197	52.3073	110.8765	
IR Inten	--	2.9009	0.5494	2.1370	
?A		?A	?A		
Frequencies	--	159.0952	223.6739	232.2877	
IR Inten	--	9.5373	79.0880	99.6794	
?A		?A	?A		
Frequencies	--	270.3919	286.5522	309.6201	
IR Inten	--	90.7845	2.9595	113.5234	
?A		?A	?A		
Frequencies	--	356.7996	389.2262	431.7150	
IR Inten	--	20.7188	3.1411	57.7711	
?A		?A	?A		
Frequencies	--	484.0690	539.5290	551.4486	
IR Inten	--	105.6722	19.6494	20.3924	
?A		?A	?A		
Frequencies	--	554.2695	600.5546	814.6250	
IR Inten	--	48.7733	165.2615	165.7161	
?A		?A	?A		
Frequencies	--	900.0703	941.0038	1055.6019	
IR Inten	--	144.7112	284.4197	79.7329	
?A		?A	?A		
Frequencies	--	1156.9876	1211.7992	1361.6901	
IR Inten	--	110.8987	232.6128	139.8025	
?A		?A	?A		
Frequencies	--	1449.0539	1624.1343	1662.4715	
IR Inten	--	309.2891	76.8481	17.5785	
?A		?A	?A		
Frequencies	--	2759.1020	3401.7883	3681.0690	
IR Inten	--	2161.5351	741.6633	434.0943	
?A		?A	?A		
Frequencies	--	3775.7746	3878.8139	3889.1179	
IR Inten	--	116.7609	92.8144	127.6334	
Min. 2 S	122 fkn.	E = -853.148337716		ZPE = 0.085847	
Min. 1 M	198 fkn.	E = -853.295075360		ZPE = 0.088179	

Min. 2 M	198 fkn.	E = -853.296950839	ZPE = 0.088375
Min. 1 L	215 fkn.	E = -853.369164277	ZPE = 0.088958
Min. 2 L	215 fkn.	E = -853.370748162	ZPE = 0.089184

SO(OH)₄H₂O

C ₁ (Min. 1 M)	R(S-O ₁): 1.502	R(O ₆ -H ₆): 0.962	A(O ₁ -S-O ₂): 98.7
	R(S-O ₂): 1.629	A(O ₁ -S-O ₃): 94.5	A(O ₁ -S-O ₄): 95.5
	R(S-O ₃): 1.634	A(O ₁ -S-O ₅): 176.4	A(O ₂ -S-O ₃): 120.3
	R(S-O ₄): 1.657	A(O ₂ -S-O ₄): 116.0	A(O ₂ -S-O ₅): 84.8
	R(S-O ₅): 1.763	A(O ₃ -S-O ₄): 120.0	A(O ₃ -S-O ₅): 82.8
	R(O ₁ -H ₃): 2.100	A(O ₄ -S-O ₅): 83.8	A(O ₁ -H ₃ -O ₄): 91.7
	R(O ₁ -H ₅): 1.913	A(O ₁ -H ₅ -O ₆): 134.7	A(O ₂ -H ₁ -O ₆): 167.5
	R(O ₂ -H ₁): 1.000	A(O ₄ -H ₃ -O ₆): 98.3	A(S-O ₁ -H ₃): 68.4
	R(O ₃ -H ₂): 0.974	A(S-O ₁ -H ₅): 120.7	A(S-O ₂ -H ₁): 109.2
	R(O ₄ -H ₃): 0.973	A(S-O ₃ -H ₂): 103.5	A(S-O ₄ -H ₃): 107.4
	R(O ₅ -H ₂): 1.892	A(S-O ₅ -H ₃): 71.5	A(S-O ₅ -H ₄): 109.6
	R(O ₅ -H ₄): 0.965	A(H ₁ -O ₆ -H ₅): 86.8	A(H ₁ -O ₆ -H ₆): 126.0
	R(O ₆ -H ₁): 1.698	A(H ₂ -O ₁ -H ₅): 131.6	A(H ₃ -O ₅ -H ₄): 164.9
	R(O ₆ -H ₅): 0.975	A(H ₅ -O ₆ -H ₆): 107.3	

Charge:	S: +0.669	O ₁ : -0.546	O ₂ : -0.461	O ₃ : -0.237	O ₄ : -0.269
	O ₅ : -0.535	O ₆ : -0.610	H ₁ : +0.495	H ₂ : +0.312	H ₃ : +0.285
	H ₄ : +0.275	H ₅ : +0.340	H ₆ : +0.282		

1A	2A	3A	4A	5A
56.6 (9)	68.2 (17)	186.5 (13)	193.5 (46)	193.9 (15)
6A	7A	8A	9A	10A
250.3 (59)	291.9 (135)	379.4 (71)	455.2 (47)	502.5 (9)
11A	12A	13A	14A	15A
538.9 (38)	542.8 (34)	554.0 (5)	566.9 (25)	621.9 (81)
16A	17A	18A	19A	20A
638.7 (280)	643.8 (104)	662.1 (3)	802.6 (287)	829.6 (348)
21A	22A	23A	24A	25A
933.8 (206)	1010. (241)	1151. (120)	1223. (73)	1292. (208)
26A	27A	28A	29A	30A
1434. (187)	1623. (54)	3171. (1177)	3635. (328)	3687. (115)
31A	32A	33A		
3711. (75)	3824. (72)	3887. (101)		

C ₁ (Min. 2 M)	R(S-O ₁): 1.479	A(S-O ₁ -H ₁): 118.8	A(O ₁ -S-O ₂): 122.5
	R(S-O ₂): 1.630	A(S-O ₂ -H ₂): 105.2	A(O ₁ -S-O ₃): 122.6
	R(S-O ₃): 1.633	A(S-O ₃ -H ₃): 105.6	A(O ₁ -S-O ₄): 98.0
	R(S-O ₄): 1.693	A(S-O ₄ -H ₂): 70.4	A(O ₁ -S-O ₅): 95.0
	R(S-O ₅): 1.744	A(S-O ₄ -H ₄): 110.0	A(O ₂ -S-O ₃): 114.7
	R(O ₁ -H ₁): 2.065	A(S-O ₅ -H ₃): 70.0	A(O ₂ -S-O ₄): 86.8
	R(O ₂ -H ₂): 0.974	A(S-O ₅ -H ₅): 107.0	A(O ₂ -S-O ₅): 86.0
	R(O ₃ -H ₃): 0.974	A(H ₁ -O ₆ -H ₄): 89.2	A(O ₃ -S-O ₄): 87.7
	R(O ₄ -H ₂): 1.945	A(H ₁ -O ₆ -H ₆): 106.7	A(O ₃ -S-O ₅): 85.3
	R(O ₄ -H ₄): 0.984	A(H ₂ -O ₄ -H ₄): 149.8	A(O ₄ -S-O ₅): 166.9
	R(O ₅ -H ₃): 1.930	A(H ₃ -O ₅ -H ₅): 146.9	A(O ₁ -H ₁ -O ₆): 133.0
	R(O ₅ -H ₅): 0.965	A(H ₅ -O ₆ -H ₆): 126.7	A(O ₂ -H ₂ -O ₄): 97.3
	R(O ₆ -H ₁): 0.970		A(O ₃ -H ₃ -O ₅): 98.6
	R(O ₆ -H ₄): 1.800		A(O ₄ -H ₄ -O ₆): 162.0
	R(O ₆ -H ₆): 0.962		

?A	?A	?A	
Frequencies --	42.7921	132.9523	152.5093
IR Inten --	1.9726	13.8131	31.1651
?A	?A	?A	
Frequencies --	188.6810	241.9882	254.9284
IR Inten --	42.7800	70.0096	49.2196
?A	?A	?A	

Frequencies --	272.4025	295.4623	469.6358	
IR Inten --	46.4462	54.0838	14.8625	
?A	?A	?A		
Frequencies --	483.3724	493.5120	507.0244	
IR Inten --	101.3718	28.2046	50.6957	
?A	?A	?A		
Frequencies --	541.3234	567.2960	575.0036	
IR Inten --	186.6058	57.4294	45.7951	
?A	?A	?A		
Frequencies --	611.2368	626.8271	688.6270	
IR Inten --	78.4681	111.5676	261.6228	
?A	?A	?A		
Frequencies --	709.1252	761.2526	835.7455	
IR Inten --	104.0228	68.1890	360.6099	
?A	?A	?A		
Frequencies --	1086.5917	1176.9000	1235.5431	
IR Inten --	149.5434	230.1736	35.1279	
?A	?A	?A		
Frequencies --	1298.2918	1327.2543	1612.3328	
IR Inten --	314.6517	132.1044	60.6251	
?A	?A	?A		
Frequencies --	3460.1264	3686.9642	3692.2045	
IR Inten --	769.4074	209.4199	19.9584	
?A	?A	?A		
Frequencies --	3730.8410	3825.6749	3893.0135	
IR Inten --	171.2968	87.0663	107.6485	
C ₁	R(S-O ₁): 1.459	A(S-O ₁ -H ₁): 121.0	A(O ₁ -S-O ₂): 123.0	
(Min. 2 L)	R(S-O ₂): 1.600	A(S-O ₂ -H ₂): 105.7	A(O ₁ -S-O ₃): 122.9	
	R(S-O ₃): 1.603	A(S-O ₃ -H ₃): 105.9	A(O ₁ -S-O ₄): 97.5	
	R(S-O ₄): 1.666	A(S-O ₄ -H ₂): 70.3	A(O ₁ -S-O ₅): 94.4	
	R(S-O ₅): 1.716	A(S-O ₄ -H ₄): 110.0	A(O ₂ -S-O ₃): 113.9	
	R(O ₁ -H ₁): 2.079	A(S-O ₅ -H ₃): 69.8	A(O ₂ -S-O ₄): 87.4	
	R(O ₂ -H ₂): 0.972	A(S-O ₅ -H ₅): 106.3	A(O ₂ -S-O ₅): 85.9	
	R(O ₃ -H ₃): 0.972	A(H ₁ -O ₆ -H ₄): 88.0	A(O ₃ -S-O ₄): 87.6	
	R(O ₄ -H ₂): 1.935	A(H ₁ -O ₆ -H ₆): 106.7	A(O ₃ -S-O ₅): 86.0	
	R(O ₄ -H ₄): 0.983	A(H ₂ -O ₄ -H ₄): 146.0	A(O ₄ -S-O ₅): 168.0	
	R(O ₅ -H ₃): 1.924	A(H ₃ -O ₅ -H ₅): 140.6	A(O ₁ -H ₁ -O ₅): 131.7	
	R(O ₅ -H ₅): 0.964	A(H ₅ -O ₆ -H ₆): 125.8	A(O ₂ -H ₂ -O ₄): 96.7	
	R(O ₆ -H ₁): 0.969		A(O ₃ -H ₃ -O ₅): 97.6	
	R(O ₆ -H ₄): 1.798		A(O ₄ -H ₄ -O ₆): 165.0	
	R(O ₆ -H ₆): 0.962			
?A	?A	?A		
Frequencies --	39.6411	135.5763	165.2400	
IR Inten --	2.0577	25.9920	6.9038	
?A	?A	?A		
Frequencies --	195.0146	236.3032	249.8470	
IR Inten --	49.0409	79.5967	24.7575	
?A	?A	?A		
Frequencies --	275.0735	311.6086	490.4556	
IR Inten --	59.3975	52.8736	276.2440	
?A	?A	?A		
Frequencies --	497.3255	516.9410	535.2704	
IR Inten --	30.0740	12.6670	28.7537	
?A	?A	?A		
Frequencies --	557.0035	589.2297	611.2003	
IR Inten --	41.7938	44.3104	57.2703	
?A	?A	?A		
Frequencies --	631.9830	642.9245	716.2910	

IR Inten	--	82.8079	97.0885	286.6859
?A		?A	?A	
Frequencies	--	754.3452	762.9815	883.4961
IR Inten	--	81.4818	77.1270	351.0575
?A		?A	?A	
Frequencies	--	1122.0637	1221.1461	1254.9528
IR Inten	--	123.4227	253.3669	41.2375
?A		?A	?A	
Frequencies	--	1317.9119	1348.3099	1611.5911
IR Inten	--	320.2339	143.2592	59.9674
?A		?A	?A	
Frequencies	--	3471.1085	3704.9599	3711.2682
IR Inten	--	795.7003	187.9282	20.2175
?A		?A	?A	
Frequencies	--	3738.5875	3833.9157	3893.2485
IR Inten	--	161.8369	86.7745	110.4201
Min. 1 M	198 fkn.	E = -853.199314524	ZPE = 0.090128	
Min. 2 M	198 fkn.	E = -853.216707404	ZPE = 0.089936	
Min. 2 L	215 fkn.	E = -853.285784204	ZPE = 0.091188	

S(OH) ₆				
Ci	R(S-O): 1.702	A(O-S-O): 180.0	A(O-S-O): 88.6	
(Min. M)	R(O-H): 0.967	A(S-O-H): 106.3	A(O-S-O): 91.4	
Charge:	S: +0.908	O: -0.445	H: +0.294	
1A _u	2A _u	3A _u	1A _g	2A _g
177.7 (75)	195.2 (69)	308.5 (50)	334.9 (0)	345.5 (0)
4A _u	5A _u	3A _g	6A _u	4A _g
358.1 (22)	363.3 (24)	387.3 (0)	452.0 (14)	457.1 (0)
5A _g	6A _g	7A _u	8A _u	9A _u
459.1 (0)	476.1 (0)	505.3 (32)	506.1 (30)	536.1 (70)
7A _g	8A _g	9A _g	10A _u	11A _u
536.6 (0)	536.9 (0)	629.8 (0)	714.7 (336)	714.9 (336)
12A _u	10A _g	11A _g	12A _g	13A _u
777.5 (735)	1174. (0)	1179. (0)	1184 (0)	1214. (60)
14A _u	15A _u	16A _u	13A _g	17A _u
1239. (337)	1244. (336)	3788. (170)	3789. (0)	3789. (171)
14A _g	18A _u	15A _g		
3790. (0)	3791. (176)	3793. (0)		
Ci	R(S-O): 1.675	A(O-S-O): 180.0	A(O-S-O): 88.6	
(Min. L)	R(O-H): 0.967	A(S-O-H): 106.3	A(O-S-O): 91.4	
Charge:	S: +0.079	O: -0.297	H: +0.283	
1A _u	2A _u	3A _u	1A _g	2A _g
191.8 (85)	212.2 (79)	324.0 (53)	330.4 (0)	343.3 (0)
4A _u	5A _u	3A _g	6A _u	4A _g
364.8 (14)	369.5 (16)	404.1 (0)	470.6 (23)	488.2 (0)
5A _g	6A _g	7A _u	8A _u	7A _g
490.0 (0)	506.0 (0)	547.0 (29)	547.6 (30)	561.9 (0)
8A _g	9A _u	9A _g	10A _u	11A _u
562.5 (0)	574.9 (60)	678.3 (0)	748.3 (338)	748.5 (338)
12A _u	10A _g	11A _g	12A _g	13A _u
802.4 (711)	1196. (0)	1204. (0)	1210 (0)	1242. (66)
14A _u	15A _u	16A _u	17A _u	13A _g
1263. (352)	1267. (349)	3797. (157)	3798. (158)	3798. (0)
18A _u	14A _g	15A _g		
3799. (168)	3799. (0)	3802. (0)		
Min. M	198 fkn.	E = -853.178085555	ZPE = 0.090550	
Min. L	215 fkn.	E = -853.246524514	ZPE = 0.092131	

SO ₂ (OH) ₂ ·3 H ₂ O			
C ₁	R(S-O ₁): 1.459	A(S-O ₂ -H ₁): 131.4	A(O ₁ -S-O ₂): 117.5
(Min. 1 M)	R(S-O ₂): 1.480	A(S-O ₃ -H ₂): 126.9	A(O ₁ -S-O ₃): 115.8
	R(S-O ₃): 1.487	A(S-O ₄ -H ₃): 107.6	A(O ₁ -S-O ₄): 103.6
	R(S-O ₄): 1.754	A(S-O ₄ -H ₄): 113.8	A(O ₂ -S-O ₃): 113.9
	R(O ₂ -H ₁): 1.741	A(H ₁ -O ₆ -H ₅): 101.3	A(O ₂ -S-O ₄): 99.9
	R(O ₃ -H ₂): 1.722	A(H ₁ -O ₆ -H ₇): 107.0	A(O ₃ -S-O ₄): 102.7
	R(O ₄ -H ₃): 0.974	A(H ₂ -O ₇ -H ₅): 102.0	A(O ₂ -H ₁ -O ₆): 162.3
	R(O ₄ -H ₄): 1.640	A(H ₂ -O ₇ -H ₆): 107.5	A(O ₃ -H ₂ -O ₇): 162.7
	R(O ₅ -H ₄): 1.014	A(H ₃ -O ₄ -H ₄): 125.4	A(O ₄ -H ₄ -O ₅): 161.6
	R(O ₅ -H ₅): 1.043	A(H ₄ -O ₅ -H ₅): 104.2	A(O ₅ -H ₅ -O ₆): 165.6
	R(O ₅ -H ₆): 1.043	A(H ₄ -O ₅ -H ₆): 104.7	A(O ₅ -H ₆ -O ₇): 165.9
	R(O ₆ -H ₁): 0.994	A(H ₅ -O ₆ -H ₇): 118.6	
	R(O ₆ -H ₅): 1.517	A(H ₆ -O ₇ -H ₆): 120.0	
	R(O ₆ -H ₇): 0.970		
	R(O ₇ -H ₂): 0.997		
	R(O ₇ -H ₆): 1.515		
	R(O ₇ -H ₈): 0.969		
?A	?A	?A	
Frequencies --	46.8488	79.3387	81.6339
IR Inten --	0.1179	6.1559	2.7461
?A	?A	?A	
Frequencies --	110.8656	174.8109	188.2564
IR Inten --	9.1545	67.1047	29.0390
?A	?A	?A	
Frequencies --	193.0508	249.5829	282.8309
IR Inten --	3.2835	44.9654	12.9378
?A	?A	?A	
Frequencies --	311.5190	327.2772	360.2863
IR Inten --	128.4604	135.2610	76.4538
?A	?A	?A	
Frequencies --	380.1425	397.8892	488.5762
IR Inten --	26.4820	9.6967	27.0225
?A	?A	?A	
Frequencies --	491.6153	510.4987	540.2306
IR Inten --	11.2587	89.1282	25.7391
?A	?A	?A	
Frequencies --	563.2415	631.8854	717.0822
IR Inten --	70.0721	277.4937	29.7472
?A	?A	?A	
Frequencies --	786.5278	820.6453	903.9130
IR Inten --	164.2385	23.8117	163.7866
?A	?A	?A	
Frequencies --	1003.3375	1071.4800	1107.3858
IR Inten --	54.7117	83.5484	85.9163
?A	?A	?A	
Frequencies --	1187.1661	1300.5238	1484.7483
IR Inten --	325.8077	388.8865	452.8510
?A	?A	?A	
Frequencies --	1640.0258	1653.3909	1738.6586
IR Inten --	84.9699	11.9354	44.7167
?A	?A	?A	
Frequencies --	1789.6691	2462.6532	2638.7628
IR Inten --	71.5130	2297.7424	1012.3782
?A	?A	?A	
Frequencies --	3103.6607	3337.4083	3387.1095
IR Inten --	819.8525	836.0469	1508.8599
?A	?A	?A	

Frequencies --	3810.9270	3878.7939	3882.5990
IR Inten --	106.6473	122.8783	103.8692
C ₁	R(S-O ₁): 1.431	A(S-O ₂ -H ₁): 131.6	A(O ₁ -S-O ₂): 117.0
(Min. 1 L)	R(S-O ₂): 1.453	A(S-O ₃ -H ₂): 128.7	A(O ₁ -S-O ₃): 115.8
	R(S-O ₃): 1.457	A(S-O ₄ -H ₃): 107.9	A(O ₁ -S-O ₄): 103.6
	R(S-O ₄): 1.708	A(S-O ₄ -H ₄): 114.5	A(O ₂ -S-O ₃): 113.5
	R(O ₂ -H ₁): 1.715	A(H ₁ -O ₆ -H ₅): 102.2	A(O ₂ -S-O ₄): 100.8
	R(O ₃ -H ₂): 1.700	A(H ₁ -O ₆ -H ₇): 107.9	A(O ₃ -S-O ₄): 102.9
	R(O ₄ -H ₃): 0.966	A(H ₂ -O ₇ -H ₆): 102.7	A(O ₂ -H ₁ -O ₆): 161.3
	R(O ₄ -H ₄): 1.662	A(H ₂ -O ₇ -H ₈): 108.2	A(O ₃ -H ₂ -O ₇): 161.9
	R(O ₅ -H ₄): 1.002	A(H ₃ -O ₄ -H ₄): 130.7	A(O ₄ -H ₄ -O ₆): 159.3
	R(O ₅ -H ₅): 1.040	A(H ₄ -O ₅ -H ₅): 104.4	A(O ₅ -H ₅ -O ₆): 165.9
	R(O ₅ -H ₆): 1.040	A(H ₄ -O ₅ -H ₆): 104.6	A(O ₅ -H ₆ -O ₇): 165.9
	R(O ₆ -H ₁): 0.990	A(H ₅ -O ₆ -H ₇): 123.0	
	R(O ₆ -H ₅): 1.490	A(H ₆ -O ₇ -H ₈): 124.0	
	R(O ₆ -H ₇): 0.962		
	R(O ₇ -H ₂): 0.992		
	R(O ₇ -H ₆): 1.488		
	R(O ₇ -H ₈): 0.962		
?A	?A	?A	
Frequencies --	42.2497	71.9297	80.0187
IR Inten --	0.1405	0.5081	8.1950
?A	?A	?A	
Frequencies --	105.3259	177.0013	187.1927
IR Inten --	7.3896	26.4354	11.6514
?A	?A	?A	
Frequencies --	193.8073	248.3030	287.5267
IR Inten --	54.0402	51.2262	7.3472
?A	?A	?A	
Frequencies --	315.6621	333.4272	371.7007
IR Inten --	149.3127	150.2983	50.7327
?A	?A	?A	
Frequencies --	397.4628	413.6234	484.1208
IR Inten --	19.4713	10.8994	31.2277
?A	?A	?A	
Frequencies --	522.4489	530.0248	566.1763
IR Inten --	105.0728	1.7875	24.6090
?A	?A	?A	
Frequencies --	574.3429	663.9096	710.0573
IR Inten --	60.8996	259.1347	29.8249
?A	?A	?A	
Frequencies --	771.5767	818.5442	889.8234
IR Inten --	136.9220	27.6621	195.5903
?A	?A	?A	
Frequencies --	1059.9791	1083.5134	1129.2539
IR Inten --	57.9602	65.6289	82.2017
?A	?A	?A	
Frequencies --	1246.0190	1360.1952	1485.3105
IR Inten --	336.3808	410.6826	444.4922
?A	?A	?A	
Frequencies --	1633.6393	1648.6423	1734.5050
IR Inten --	76.2315	14.3394	43.5044
?A	?A	?A	
Frequencies --	1779.8720	2413.4370	2609.7276
IR Inten --	76.4916	2378.2348	1027.8321
?A	?A	?A	
Frequencies --	3167.1496	3319.6600	3372.8761
IR Inten --	639.1551	891.9518	1594.2184

?A	?A	?A	
Frequencies --	3811.6907	3878.8637	3881.6152
IR Inten --	106.0323	126.4398	98.7718
C ₁	R(S-O ₁): 1.424	A(S-O ₂ -H ₁): 129.6	A(O ₁ -S-O ₂): 118.8
(Min. 2 M)	R(S-O ₂): 1.477	A(S-O ₃ -H ₂): 116.5	A(O ₁ -S-O ₃): 114.0
	R(S-O ₃): 1.510	A(S-O ₄ -H ₃): 106.9	A(O ₁ -S-O ₄): 104.9
	R(S-O ₄): 1.706	A(S-O ₄ -H ₄): 117.6	A(O ₂ -S-O ₃): 112.2
	R(O ₂ -H ₁): 1.800	A(H ₁ -O ₆ -H ₅): 99.8	A(O ₂ -S-O ₄): 101.4
	R(O ₃ -H ₂): 1.453	A(H ₁ -O ₆ -H ₇): 107.0	A(O ₃ -S-O ₄): 103.0
	R(O ₄ -H ₃): 0.975	A(H ₂ -O ₅ -H ₆): 104.3	A(O ₂ -H ₁ -O ₆): 158.0
	R(O ₄ -H ₄): 1.856	A(H ₂ -O ₆ -H ₆): 103.6	A(O ₃ -H ₂ -O ₅): 170.6
	R(O ₅ -H ₂): 1.064	A(H ₃ -O ₄ -H ₄): 123.9	A(O ₄ -H ₄ -O ₇): 161.4
	R(O ₅ -H ₅): 1.025	A(H ₄ -O ₇ -H ₆): 103.5	A(O ₅ -H ₅ -O ₆): 162.9
	R(O ₅ -H ₆): 1.013	A(H ₄ -O ₇ -H ₈): 107.2	A(O ₅ -H ₆ -O ₇): 163.7
	R(O ₆ -H ₁): 0.989	A(H ₅ -O ₅ -H ₆): 107.4	
	R(O ₆ -H ₅): 1.587	A(H ₅ -O ₆ -H ₇): 120.9	
	R(O ₆ -H ₇): 0.969	A(H ₆ -O ₇ -H ₈): 119.9	
	R(O ₇ -H ₄): 0.986		
	R(O ₇ -H ₆): 1.637		
	R(O ₇ -H ₈): 0.969		
?A	?A	?A	
Frequencies --	50.6599	76.4140	101.2369
IR Inten --	1.8726	6.7484	6.6721
?A	?A	?A	
Frequencies --	124.1663	164.9426	182.7834
IR Inten --	1.1982	7.0949	3.7799
?A	?A	?A	
Frequencies --	217.8450	248.0266	271.3304
IR Inten --	55.8714	62.5186	56.8681
?A	?A	?A	
Frequencies --	300.5412	307.9765	341.0713
IR Inten --	130.2110	152.7949	29.5584
?A	?A	?A	
Frequencies --	386.1659	416.0180	443.6335
IR Inten --	10.4792	0.0424	40.4474
?A	?A	?A	
Frequencies --	500.3128	514.3123	537.9955
IR Inten --	166.4142	12.8806	30.9104
?A	?A	?A	
Frequencies --	570.0013	677.0574	713.1454
IR Inten --	75.1503	184.0812	93.9495
?A	?A	?A	
Frequencies --	765.0099	788.0826	892.7067
IR Inten --	109.6266	99.7348	95.4340
?A	?A	?A	
Frequencies --	980.0241	990.6213	1113.1059
IR Inten --	115.4250	146.4177	200.8374
?A	?A	?A	
Frequencies --	1183.0570	1296.8466	1456.8095
IR Inten --	215.2799	562.9542	417.2185
?A	?A	?A	
Frequencies --	1639.5723	1645.6153	1713.4497
IR Inten --	94.7763	38.7340	29.9709
?A	?A	?A	
Frequencies --	1781.0509	2310.7235	2820.4539
IR Inten --	97.1426	1943.6374	1652.0962
?A	?A	?A	
Frequencies --	3076.8443	3429.6641	3567.3400

IR Inten	--	829.7289	922.6331	678.4467	
?A		?A	?A		
Frequencies	--	3789.7305	3879.6269	3881.0291	
IR Inten	--	97.4121	145.5239	89.6457	
C ₁		R(S-O ₁): 1.428	A(S-O ₂ -H ₁): 129.4	A(O ₁ -S-O ₂): 116.4	
(Min. 2 L)		R(S-O ₂): 1.455	A(S-O ₃ -H ₂): 119.0	A(O ₁ -S-O ₃): 115.0	
		R(S-O ₃): 1.475	A(S-O ₄ -H ₃): 108.0	A(O ₁ -S-O ₄): 106.0	
		R(S-O ₄): 1.663	A(S-O ₄ -H ₄): 120.9	A(O ₂ -S-O ₃): 112.6	
		R(O ₂ -H ₁): 1.764	A(H ₁ -O ₆ -H ₅): 101.0	A(O ₂ -S-O ₄): 104.6	
		R(O ₃ -H ₂): 1.420	A(H ₁ -O ₆ -H ₇): 107.7	A(O ₃ -S-O ₄): 99.8	
		R(O ₄ -H ₃): 0.968	A(H ₂ -O ₅ -H ₅): 104.5	A(O ₂ -H ₁ -O ₆): 160.2	
		R(O ₄ -H ₄): 1.893	A(H ₂ -O ₅ -H ₆): 103.0	A(O ₃ -H ₂ -O ₆): 170.8	
		R(O ₅ -H ₂): 1.063	A(H ₃ -O ₄ -H ₄): 125.6	A(O ₄ -H ₄ -O ₇): 159.7	
		R(O ₅ -H ₅): 1.019	A(H ₄ -O ₇ -H ₅): 104.4	A(O ₅ -H ₅ -O ₆): 163.2	
		R(O ₅ -H ₆): 1.004	A(H ₄ -O ₇ -H ₆): 107.0	A(O ₅ -H ₆ -O ₇): 159.9	
		R(O ₆ -H ₁): 0.985	A(H ₅ -O ₅ -H ₆): 108.9		
		R(O ₆ -H ₅): 1.566	A(H ₅ -O ₆ -H ₇): 123.7		
		R(O ₆ -H ₇): 0.962	A(H ₆ -O ₇ -H ₈): 122.8		
		R(O ₇ -H ₄): 0.977			
		R(O ₇ -H ₆): 1.643			
		R(O ₇ -H ₈): 0.962			
?A		?A	?A		
Frequencies	--	43.9584	73.6637	94.4810	
IR Inten	--	1.7763	5.9057	8.0971	
?A		?A	?A		
Frequencies	--	120.4786	152.7880	179.4934	
IR Inten	--	1.3678	7.9384	4.6551	
?A		?A	?A		
Frequencies	--	192.4054	242.6593	258.7404	
IR Inten	--	66.6184	50.7545	90.3418	
?A		?A	?A		
Frequencies	--	299.7225	308.9332	343.0807	
IR Inten	--	87.6468	177.1941	19.1538	
?A		?A	?A		
Frequencies	--	401.1526	417.1828	439.6802	
IR Inten	--	11.7330	36.7434	3.9215	
?A		?A	?A		
Frequencies	--	486.7745	548.2922	557.1778	
IR Inten	--	156.8392	13.9357	48.8465	
?A		?A	?A		
Frequencies	--	598.1882	682.5087	715.3022	
IR Inten	--	78.7640	17.4630	228.6230	
?A		?A	?A		
Frequencies	--	743.7355	775.0305	892.1745	
IR Inten	--	138.0392	146.6605	37.6377	
?A		?A	?A		
Frequencies	--	981.4585	1037.9211	1146.4760	
IR Inten	--	81.9469	216.9623	124.2055	
?A		?A	?A		
Frequencies	--	1216.2074	1354.2746	1450.0886	
IR Inten	--	340.2045	622.5994	343.6712	
?A		?A	?A		
Frequencies	--	1631.6162	1636.4423	1707.1463	
IR Inten	--	106.6245	25.0523	17.0096	
?A		?A	?A		
Frequencies	--	1767.4485	2165.1829	2861.5977	
IR Inten	--	99.6023	2104.4960	1555.0701	
?A		?A	?A		

Frequencies --	3134.9364	3450.9702	3605.2069
IR Inten --	817.6907	891.9703	569.2081
?A	?A	?A	
Frequencies --	3790.8878	3880.7539	3881.3321
IR Inten --	97.4067	170.1256	70.4247
C ₁	R(S-O ₁): 1.484	A(S-O ₁ -H ₁): 121.3	A(O ₁ -S-O ₂): 114.9
(Min. 3 M)	R(S-O ₂): 1.498	A(S-O ₂ -H ₂): 117.9	A(O ₁ -S-O ₃): 113.4
	R(S-O ₃): 1.504	A(S-O ₃ -H ₃): 115.2	A(O ₁ -S-O ₄): 103.0
	R(S-O ₄): 1.635	A(S-O ₄ -H ₄): 113.0	A(O ₂ -S-O ₃): 111.6
	R(O ₁ -H ₁): 1.710	A(H ₁ -O ₆ -H ₅): 109.7	A(O ₂ -S-O ₄): 106.4
	R(O ₂ -H ₂): 1.705	A(H ₁ -O ₆ -H ₇): 114.9	A(O ₃ -S-O ₄): 106.6
	R(O ₃ -H ₃): 1.682	A(H ₂ -O ₇ -H ₆): 111.2	A(O ₁ -H ₁ -O ₆): 157.0
	R(O ₄ -H ₄): 0.977	A(H ₂ -O ₇ -H ₈): 115.3	A(O ₂ -H ₂ -O ₇): 157.9
	R(O ₅ -H ₅): 1.004	A(H ₃ -O ₅ -H ₅): 108.0	A(O ₃ -H ₃ -O ₆): 149.4
	R(O ₅ -H ₅): 1.042	A(H ₃ -O ₅ -H ₆): 108.0	A(O ₅ -H ₅ -O ₆): 160.9
	R(O ₅ -H ₆): 1.043	A(H ₅ -O ₅ -H ₆): 113.8	A(O ₅ -H ₆ -O ₇): 160.6
	R(O ₆ -H ₁): 0.992	A(H ₅ -O ₆ -H ₇): 132.2	
	R(O ₆ -H ₅): 1.456	A(H ₆ -O ₇ -H ₈): 133.0	
	R(O ₆ -H ₇): 0.963		
	R(O ₇ -H ₂): 0.994		
	R(O ₇ -H ₆): 1.710		
	R(O ₇ -H ₈): 0.962		
?A	?A	?A	
Frequencies --	56.9657	79.6531	91.8812
IR Inten --	1.6690	8.7065	4.2459
?A	?A	?A	
Frequencies --	121.6719	161.3353	169.6489
IR Inten --	3.3124	2.3243	7.2167
?A	?A	?A	
Frequencies --	197.1133	233.9619	247.5226
IR Inten --	92.8858	41.9220	28.4485
?A	?A	?A	
Frequencies --	284.0773	302.2998	339.5933
IR Inten --	192.5929	93.1555	39.4620
?A	?A	?A	
Frequencies --	412.3944	427.8143	469.5829
IR Inten --	24.3521	10.4063	31.6037
?A	?A	?A	
Frequencies --	514.0032	524.7700	554.5021
IR Inten --	203.2413	43.4197	24.0644
?A	?A	?A	
Frequencies --	570.9931	717.9702	742.3420
IR Inten --	63.2197	40.1600	303.3801
?A	?A	?A	
Frequencies --	768.1315	806.9563	884.2576
IR Inten --	3.8108	76.8350	145.3628
?A	?A	?A	
Frequencies --	978.4386	993.3123	1108.8360
IR Inten --	76.3788	346.7214	221.2947
?A	?A	?A	
Frequencies --	1130.2558	1240.1761	1468.6045
IR Inten --	181.2574	328.8102	505.9659
?A	?A	?A	
Frequencies --	1643.3517	1648.9961	1727.1842
IR Inten --	107.4624	12.8757	47.6841
?A	?A	?A	
Frequencies --	1780.2848	2418.2210	2815.8258
IR Inten --	98.7245	1706.7464	1844.6295

?A	?A	?A	
Frequencies --	2971.1442	3448.9480	3476.0425
IR Inten --	735.6480	528.4489	1121.7144
?A	?A	?A	
Frequencies --	3780.0371	3882.0051	3886.0913
IR Inten --	103.1237	121.1626	104.8614
C ₁	R(S-O ₁): 1.447	A(S-O ₁ -H ₁): 120.4	A(O ₁ -S-O ₂): 115.6
(Min. 3 L)	R(S-O ₂): 1.456	A(S-O ₂ -H ₂): 118.4	A(O ₁ -S-O ₃): 112.8
	R(S-O ₃): 1.483	A(S-O ₃ -H ₃): 113.4	A(O ₁ -S-O ₄): 103.6
	R(S-O ₄): 1.596	A(S-O ₄ -H ₄): 108.9	A(O ₂ -S-O ₃): 111.5
	R(O ₁ -H ₁): 1.804	A(H ₁ -O ₆ -H ₅): 103.9	A(O ₂ -S-O ₄): 106.9
	R(O ₂ -H ₂): 1.805	A(H ₁ -O ₆ -H ₇): 107.5	A(O ₃ -S-O ₄): 105.3
	R(O ₃ -H ₃): 1.469	A(H ₂ -O ₇ -H ₆): 104.5	A(O ₁ -H ₁ -O ₆): 159.6
	R(O ₄ -H ₄): 0.968	A(H ₂ -O ₇ -H ₃): 107.7	A(O ₂ -H ₂ -O ₇): 160.0
	R(O ₅ -H ₅): 1.050	A(H ₃ -O ₅ -H ₅): 103.4	A(O ₃ -H ₃ -O ₅): 167.4
	R(O ₅ -H ₆): 1.017	A(H ₃ -O ₅ -H ₆): 103.4	A(O ₅ -H ₅ -O ₆): 162.7
	R(O ₅ -H ₆): 1.015	A(H ₅ -O ₅ -H ₆): 108.5	A(O ₅ -H ₆ -O ₇): 162.3
	R(O ₆ -H ₁): 0.983	A(H ₅ -O ₆ -H ₇): 124.0	
	R(O ₆ -H ₅): 1.581	A(H ₆ -O ₇ -H ₃): 124.9	
	R(O ₆ -H ₇): 0.962		
	R(O ₇ -H ₂): 0.984		
	R(O ₇ -H ₆): 1.589		
	R(O ₇ -H ₃): 0.962		
?A	?A	?A	
Frequencies --	52.6148	78.0268	87.3594
IR Inten --	2.1492	6.5966	5.3682
?A	?A	?A	
Frequencies --	121.8224	160.0149	166.6939
IR Inten --	2.0304	0.1484	5.4724
?A	?A	?A	
Frequencies --	193.6823	237.0276	252.5661
IR Inten --	92.3943	46.9079	28.1600
?A	?A	?A	
Frequencies --	287.2752	304.1849	340.4050
IR Inten --	205.2045	96.7423	26.8626
?A	?A	?A	
Frequencies --	430.7359	446.0508	451.9447
IR Inten --	23.1556	14.1014	26.9938
?A	?A	?A	
Frequencies --	500.7797	548.1777	580.8063
IR Inten --	183.7811	45.5309	26.5453
?A	?A	?A	
Frequencies --	595.7263	706.2065	737.8278
IR Inten --	84.6062	47.5945	267.1361
?A	?A	?A	
Frequencies --	761.1961	838.0038	896.3980
IR Inten --	0.3050	131.7075	100.1426
?A	?A	?A	
Frequencies --	974.3603	1043.0852	1147.6132
IR Inten --	66.0319	379.0275	105.0340
?A	?A	?A	
Frequencies --	1169.4619	1294.2400	1460.3436
IR Inten --	292.1882	355.1784	486.1543
?A	?A	?A	
Frequencies --	1637.4862	1642.4693	1715.7654
IR Inten --	102.1904	15.4327	36.5237
?A	?A	?A	
Frequencies --	1765.7733	2345.3662	2849.4291

IR Inten	--	94.5044	1823.9646	1822.5314
?A		?A	?A	
Frequencies	--	2991.9401	3461.2242	3484.9556
IR Inten	--	694.8293	487.4061	1137.7813
?A		?A	?A	
Frequencies	--	3788.4683	3882.7411	3885.5141
IR Inten	--	103.3923	124.3083	101.7663
C ₁		R(S-O ₁): 1.451	A(S-O ₁ -H ₁): 110.0	A(O ₁ -S-O ₂): 120.2
(Min. 4 M)		R(S-O ₂): 1.454	A(S-O ₂ -H ₂): 136.8	A(O ₁ -S-O ₃): 106.5
		R(S-O ₃): 1.582	A(S-O ₃ -H ₃): 112.9	A(O ₁ -S-O ₄): 109.2
		R(S-O ₄): 1.603	A(S-O ₄ -H ₄): 108.7	A(O ₂ -S-O ₃): 110.2
		R(O ₁ -H ₁): 2.178	A(H ₁ -O ₇ -H ₄): 97.9	A(O ₂ -S-O ₄): 105.8
		R(O ₂ -H ₂): 1.876	A(H ₁ -O ₇ -H ₃): 106.9	A(O ₃ -S-O ₄): 103.9
		R(O ₃ -H ₃): 1.019	A(H ₂ -O ₆ -H ₅): 99.0	A(O ₁ -H ₁ -O ₇): 126.3
		R(O ₄ -H ₄): 0.996	A(H ₂ -O ₆ -H ₇): 106.7	A(O ₂ -H ₂ -O ₆): 157.5
		R(O ₅ -H ₅): 1.570	A(H ₃ -O ₅ -H ₆): 109.0	A(O ₃ -H ₃ -O ₅): 176.8
		R(O ₅ -H ₆): 0.987	A(H ₃ -O ₅ -H ₆): 118.9	A(O ₄ -H ₄ -O ₇): 161.3
		R(O ₅ -H ₆): 0.962	A(H ₄ -O ₇ -H ₃): 126.0	A(O ₅ -H ₅ -O ₆): 162.5
		R(O ₆ -H ₂): 0.974	A(H ₅ -O ₅ -H ₆): 107.0	
		R(O ₆ -H ₅): 1.735	A(H ₅ -O ₆ -H ₇): 125.2	
		R(O ₆ -H ₇): 0.962		
		R(O ₇ -H ₁): 0.969		
		R(O ₇ -H ₄): 1.717		
		R(O ₇ -H ₃): 0.962		
?A		?A	?A	
Frequencies	--	28.4596	33.8450	55.0709
IR Inten	--	3.0546	2.2001	6.2297
?A		?A	?A	
Frequencies	--	112.1325	129.3776	171.0847
IR Inten	--	2.4853	15.2854	29.4307
?A		?A	?A	
Frequencies	--	215.0598	220.0625	227.0880
IR Inten	--	91.5041	45.1577	55.3121
?A		?A	?A	
Frequencies	--	234.0143	278.5255	321.0034
IR Inten	--	111.8253	25.1105	21.8172
?A		?A	?A	
Frequencies	--	324.5810	368.8392	373.7799
IR Inten	--	172.8151	1.7171	7.2158
?A		?A	?A	
Frequencies	--	409.9694	487.4513	523.1443
IR Inten	--	23.4905	56.2081	249.8923
?A		?A	?A	
Frequencies	--	528.4485	530.3392	532.6714
IR Inten	--	12.4974	66.6204	42.8602
?A		?A	?A	
Frequencies	--	633.4645	807.7742	818.8713
IR Inten	--	189.3118	86.4239	79.1929
?A		?A	?A	
Frequencies	--	890.8751	900.8403	1053.2913
IR Inten	--	195.3927	358.9396	68.5140
?A		?A	?A	
Frequencies	--	1139.7139	1268.7928	1354.4968
IR Inten	--	285.7330	188.0505	81.0744
?A		?A	?A	
Frequencies	--	1410.6221	1617.4466	1632.3814
IR Inten	--	298.8928	61.0309	78.1872
?A		?A	?A	

Frequencies --	1662.6025	2820.1623	3247.9258
IR Inten --	20.8925	2117.8936	1094.1581
?A	?A	?A	
Frequencies --	3402.2173	3655.4677	3741.5494
IR Inten --	720.7543	517.0637	92.7026
?A	?A	?A	
Frequencies --	3877.2237	3888.8064	3891.2154
IR Inten --	86.6613	142.0614	94.9585
C ₁	R(S-O ₁): 1.431	A(S-O ₁ -H ₁): 110.0	A(O ₁ -S-O ₂): 119.9
(Min. 4 L)	R(S-O ₂): 1.434	A(S-O ₂ -H ₂): 138.4	A(O ₁ -S-O ₃): 106.7
	R(S-O ₃): 1.553	A(S-O ₃ -H ₃): 113.0	A(O ₁ -S-O ₄): 109.0
	R(S-O ₄): 1.571	A(S-O ₄ -H ₄): 109.0	A(O ₂ -S-O ₃): 110.0
	R(O ₁ -H ₁): 2.185	A(H ₁ -O ₇ -H ₄): 96.5	A(O ₂ -S-O ₄): 106.0
	R(O ₂ -H ₂): 1.896	A(H ₁ -O ₇ -H ₅): 106.8	A(O ₃ -S-O ₄): 104.0
	R(O ₃ -H ₃): 1.019	A(H ₂ -O ₆ -H ₅): 98.9	A(O ₁ -H ₁ -O ₇): 126.3
	R(O ₄ -H ₄): 0.997	A(H ₂ -O ₆ -H ₇): 106.6	A(O ₂ -H ₂ -O ₆): 156.2
	R(O ₅ -H ₃): 1.568	A(H ₃ -O ₅ -H ₅): 109.0	A(O ₃ -H ₃ -O ₆): 177.0
	R(O ₅ -H ₅): 0.987	A(H ₃ -O ₅ -H ₆): 119.0	A(O ₄ -H ₄ -O ₇): 162.3
	R(O ₅ -H ₆): 0.962	A(H ₄ -O ₇ -H ₅): 125.4	A(O ₅ -H ₅ -O ₆): 162.7
	R(O ₆ -H ₂): 0.974	A(H ₅ -O ₅ -H ₆): 107.0	
	R(O ₆ -H ₅): 1.736	A(H ₅ -O ₆ -H ₇): 125.0	
	R(O ₆ -H ₇): 0.962		
	R(O ₇ -H ₁): 0.969		
	R(O ₇ -H ₄): 1.704		
	R(O ₇ -H ₅): 0.962		
?A	?A	?A	
Frequencies --	23.9060	32.6976	53.8524
IR Inten --	2.9159	1.9352	5.9111
?A	?A	?A	
Frequencies --	111.3639	128.2237	166.6870
IR Inten --	2.0874	16.7090	31.7449
?A	?A	?A	
Frequencies --	217.7105	221.4679	226.1925
IR Inten --	61.4114	78.5991	61.0789
?A	?A	?A	
Frequencies --	231.9989	279.8485	314.4079
IR Inten --	89.9095	20.9258	92.4790
?A	?A	?A	
Frequencies --	322.0370	362.1581	390.1540
IR Inten --	113.4511	8.7672	1.7004
?A	?A	?A	
Frequencies --	427.5347	489.3957	520.2161
IR Inten --	40.8466	54.0113	281.2345
?A	?A	?A	
Frequencies --	552.9240	558.2367	561.2134
IR Inten --	7.4358	39.3060	43.8907
?A	?A	?A	
Frequencies --	611.7199	832.0232	861.8287
IR Inten --	185.7398	94.5107	90.1095
?A	?A	?A	
Frequencies --	897.1928	943.3488	1045.7085
IR Inten --	154.8764	364.9717	85.9041
?A	?A	?A	
Frequencies --	1197.5148	1311.5960	1362.4343
IR Inten --	262.4570	141.5486	80.4280
?A	?A	?A	
Frequencies --	1442.0612	1620.0686	1627.5351
IR Inten --	366.4338	54.1607	76.1405

?A	?A	?A	
Frequencies --	1662.7499	2828.2824	3235.8869
IR Inten --	21.5265	2144.0830	1131.3706
?A	?A	?A	
Frequencies --	3405.6789	3663.1675	3742.3452
IR Inten --	725.0785	487.5176	94.1010
?A	?A	?A	
Frequencies --	3877.8464	3888.6657	3890.2186
IR Inten --	86.1187	155.2219	82.9443
Min. 1 S	141 fkn.	E = -929.610191547	ZPE = 0.113984
Min. 2 S	141 fkn.	E = -929.609104113	ZPE = 0.114493
Min. 3 S	141 fkn.	E = -929.608335484	ZPE = 0.113806
Min. 1 M	232 fkn.	E = -929.768704953	ZPE = 0.114175
Min. 2 M	232 fkn.	E = -929.772077906	ZPE = 0.114243
Min. 3 M	232 fkn.	E = -929.773250982	ZPE = 0.114084
Min. 4 M	232 fkn.	E = -929.774682538	ZPE = 0.113500
Min. 1 L	249 fkn.	E = -929.839657670	ZPE = 0.114756
Min. 2 L	249 fkn.	E = -929.843861830	ZPE = 0.114518
Min. 3 L	249 fkn.	E = -929.846460571	ZPE = 0.114628
Min. 4 L	249 fkn.	E = -929.848264005	ZPE = 0.114228

HSO₂(OH)

C ₁	R(S-O ₁): 1.441	A(S-O ₃ -H ₂): 109.3	A(O ₁ -S-O ₂): 123.6
(Min. M)	R(S-O ₂): 1.451	A(H ₁ -S-O ₁): 108.2	A(O ₁ -S-O ₃): 107.3
	R(S-O ₃): 1.634	A(H ₁ -S-O ₂): 108.5	A(O ₂ -S-O ₃): 108.1
	R(S-H ₁): 1.363	A(H ₁ -S-O ₃): 98.2	
	R(O ₃ -H ₂): 0.970		

?A	?A	?A	
Frequencies --	211.9625	396.6253	444.6456
IR Inten --	120.5133	23.3887	29.3213
?A	?A	?A	
Frequencies --	555.7709	771.8631	1021.7469
IR Inten --	52.0351	223.5143	3.9973
?A	?A	?A	
Frequencies --	1078.1107	1127.1510	1154.5689
IR Inten --	33.2705	10.6871	196.4900
?A	?A	?A	
Frequencies --	1379.8949	2539.3228	3766.4506
IR Inten --	306.4114	40.3088	134.3662

C ₁	R(S-O ₁): 1.421	A(S-O ₃ -H ₂): 109.3	A(O ₁ -S-O ₂): 123.2
(Min. L)	R(S-O ₂): 1.430	A(H ₁ -S-O ₁): 107.8	A(O ₁ -S-O ₃): 107.5
	R(S-O ₃): 1.600	A(H ₁ -S-O ₂): 108.4	A(O ₂ -S-O ₃): 108.3
	R(S-H ₁): 1.351	A(H ₁ -S-O ₃): 98.9	
	R(O ₃ -H ₂): 0.969		

?A	?A	?A	
Frequencies --	249.4651	425.1180	467.4826
IR Inten --	108.0411	21.5001	28.3781
?A	?A	?A	
Frequencies --	580.3130	823.5315	1062.7465
IR Inten --	48.8796	210.9046	7.4587
?A	?A	?A	
Frequencies --	1108.1976	1158.3475	1210.2389
IR Inten --	29.6027	11.0817	176.6909
?A	?A	?A	
Frequencies --	1443.6196	2583.3354	3771.4474
IR Inten --	286.5568	26.4933	140.2774
Min. M	108 fkn.	E = -625.082127921	ZPE = 0.032915
Min. L	125 fkn.	E = -625.147673890	ZPE = 0.033908

SO(OH) ₂			
C ₁ (Min. 1 M)	R(S-O ₁): 1.460 R(S-O ₂): 1.667 R(S-O ₃): 1.686 R(O ₂ -H ₁): 0.973 R(O ₃ -H ₂): 0.970	A(S-O ₂ -H ₁): 109.7 A(S-O ₃ -H ₂): 109.5	A(O ₁ -S-O ₂): 108.6 A(O ₁ -S-O ₃): 102.5 A(O ₂ -S-O ₃): 98.3
?A	?A	?A	
Frequencies --	256.2614	284.7664	378.0248
IR Inten --	38.5146	94.8383	22.9835
?A	?A	?A	
Frequencies --	452.2474	464.8654	667.7778
IR Inten --	68.0456	29.8575	264.9789
?A	?A	?A	
Frequencies --	708.0768	1050.8815	1082.1413
IR Inten --	206.2097	106.5538	33.1566
?A	?A	?A	
Frequencies --	1228.6187	3709.8369	3763.1765
IR Inten --	179.5474	78.9419	86.1927
C ₁ (Min. 1 L)	R(S-O ₁): 1.443 R(S-O ₂): 1.632 R(S-O ₃): 1.652 R(O ₂ -H ₁): 0.974 R(O ₃ -H ₂): 0.970	A(S-O ₂ -H ₁): 109.5 A(S-O ₃ -H ₂): 109.2	A(O ₁ -S-O ₂): 107.9 A(O ₁ -S-O ₃): 102.4 A(O ₂ -S-O ₃): 99.0
?A	?A	?A	
Frequencies --	265.5489	302.6910	399.1077
IR Inten --	43.3375	86.3158	26.2229
?A	?A	?A	
Frequencies --	469.0933	494.9917	714.5446
IR Inten --	54.7390	29.1679	252.4478
?A	?A	?A	
Frequencies --	752.3702	1088.1894	1103.0416
IR Inten --	195.8006	64.0618	88.6677
?A	?A	?A	
Frequencies --	1272.7549	3699.0777	3764.3938
IR Inten --	172.3279	78.9304	89.0044
A''	A'	A'	
C _s (Min. 2 M)	R(S-O ₁): 1.474 R(S-O ₂): 1.664 R(O ₂ -H): 0.972	A(S-O ₂ -H): 109.7	A(O ₁ -S-O ₂): 106.2 A(O ₂ -S-O ₂): 100.6
A''	A'	A'	
Frequencies --	149.0812	311.8487	401.8199
IR Inten --	29.0525	28.3516	144.9124
A''	A'	A''	
Frequencies --	421.0102	459.2931	699.5228
IR Inten --	50.3859	20.5804	392.3781
A'	A''	A'	
Frequencies --	710.8243	1044.3483	1076.3314
IR Inten --	168.6613	50.0586	23.5054
A'	A''	A'	
Frequencies --	1201.9278	3714.5161	3717.3528
IR Inten --	182.2954	42.1477	103.9046
C _s (Min. 2 L)	R(S-O ₁): 1.456 R(S-O ₂): 1.631 R(O ₂ -H): 0.973	A(S-O ₂ -H): 109.3	A(O ₁ -S-O ₂): 105.8 A(O ₂ -S-O ₂): 100.8
A''	A'	A'	
Frequencies --	123.0291	335.5254	407.4685
IR Inten --	26.4816	35.7246	124.5975
A''	A'	A''	

Frequencies --	443.8200	485.4102	746.2840
IR Inten --	47.5136	16.5321	378.3241
A'	A''	A'	
Frequencies --	754.7876	1064.5427	1096.2856
IR Inten --	152.4803	51.7383	9.1835
A'	A''	A'	
Frequencies --	1241.1026	3706.5700	3709.8056
IR Inten --	191.8402	42.0141	107.9022
Min. 1 M	108 fkn.	E = -625.114711253	ZPE = 0.032001
Min. 2 M	108 fkn.	E = -625.115816123	ZPE = 0.031684
Min. 1 L	125 fkn.	E = -625.161435078	ZPE = 0.032637
Min. 2 L	125 fkn.	E = -625.162233694	ZPE = 0.032155

SO₂-H₂O

C ₁	R(S-O ₁): 1.460	A(S-O ₃ -H ₁): 116.4	A(O ₁ -S-O ₂): 117.8
(Min. M)	R(S-O ₂): 1.460	A(S-O ₃ -H ₂): 116.9	A(O ₁ -S-O ₃): 94.2
	R(S-O ₃): 2.770	A(H ₁ -O ₃ -H ₂): 105.8	A(O ₂ -S-O ₃): 94.4
	R(O ₃ -H ₁): 0.963		
	R(O ₃ -H ₂): 0.963		

?A	?A	?A	
Frequencies --	33.4202	100.4296	101.6097
IR Inten --	3.8011	24.1459	38.7280
?A	?A	?A	
Frequencies --	155.5496	223.4579	297.5786
IR Inten --	81.1247	190.3123	29.2421
?A	?A	?A	
Frequencies --	509.7901	1132.4144	1299.2770
IR Inten --	44.3609	43.0421	249.0993
?A	?A	?A	
Frequencies --	1613.2515	3806.5940	3910.8970
IR Inten --	71.9141	28.2877	83.6908

C ₁	R(S-O ₁): 1.439	A(S-O ₃ -H ₁): 116.0	A(O ₁ -S-O ₂): 118.3
(Min. L)	R(S-O ₂): 1.439	A(S-O ₃ -H ₂): 116.4	A(O ₁ -S-O ₃): 94.3
	R(S-O ₃): 2.767	A(H ₁ -O ₃ -H ₂): 105.8	A(O ₂ -S-O ₃): 94.5
	R(O ₃ -H ₁): 0.963		
	R(O ₃ -H ₂): 0.963		

?A	?A	?A	
Frequencies --	47.7417	98.6118	103.6719
IR Inten --	3.8974	16.5938	42.0883
?A	?A	?A	
Frequencies --	160.6899	221.2987	288.2393
IR Inten --	60.7909	214.7657	26.3806
?A	?A	?A	
Frequencies --	523.9686	1181.5013	1369.3684
IR Inten --	35.4213	39.9926	246.0046
?A	?A	?A	
Frequencies --	1613.0719	3806.1456	3910.7038
IR Inten --	71.3902	27.1068	82.7850
Min. M	108 fkn.	E = -625.131229092	ZPE = 0.030036
Min. L	125 fkn.	E = -625.175582114	ZPE = 0.030357

H ₂ S				
C _{2v}	R ₁ (S-H): 1.348	A ₁ (H-S-H): 92.5		
(Min. M)	Charge:	S: -0.146	H: +0.073	
	1A ₁	2A ₁	1B ₂	
	1208. (4)	2680. (2)	2695. (3)	
C _{2v}	R ₁ (S-H): 1.343	A ₁ (H-S-H): 92.5		
(Min. L)	Charge:	S: -0.354	H: +0.177	
	1A ₁	2A ₁	1B ₂	
	1213. (0)	2692. (0)	2704. (0)	
Min. M	42 fkn.	E = -399.422528079	ZPE = 0.014996	
Min. L	59 fkn.	E = -399.428078524	ZPE = 0.015057	

Table 4.

Bond lengths (Å), bond angles (deg.), vibrational frequencies (cm⁻¹), IR intensities (km/mol), absolute and zero-point energies (H) for the S₂O₆ + H₂O systems:

O ₂ SO ₂ SO ₂					
D _{2h}	R(S-O ₁): 1.695	R(O ₁ -O ₁): 2.273	A(S-O ₁ -S): 95.8		
(Min. M)	R(S-O ₂): 1.431	R(S-S): 2.515	A(O ₁ -S-O ₁): 84.2		
		A(O ₂ -S-O ₂): 124.4	A(O ₁ -S-O ₂): 110.3		
Charge:	S: +0.357	O ₁ : -0.229	O ₂ : -0.064		
1B _{2u}	1A _u	1B _{2g}	1A _g	1B _{3g}	
78.2 (1)	199.5 (0)	292.9 (0)	316.7 (0)	337.7 (0)	
1B _{1u}	1B _{1g}	1B _{3u}	2B _{2g}	2B _{2u}	
344.6 (9)	368.1 (0)	472.0 (63)	514.2 (0)	525.6 (48)	
2A _g	2B _{3u}	3A _g	2B _{1u}	3B _{3u}	
624.4 (0)	700.9 (588)	746.9 (0)	810.0 (194)	1163. (465)	
4A _g	2B _{1g}	3B _{2u}			
1215. (0)	1409. (0)	1426. (423)			
D _{2h}	R(S-O ₁): 1.654	R(O ₁ -O ₁): 2.229	A(S-O ₁ -S): 95.3		
(Min. L)	R(S-O ₂): 1.412	R(S-S): 2.444	A(O ₁ -S-O ₁): 84.7		
		A(O ₂ -S-O ₂): 123.7	A(O ₁ -S-O ₂): 110.4		
1B _{2u}	1A _u	1B _{2g}	1A _g	1B _{3g}	
91.1 (1)	215.3 (0)	339.5 (0)	342.6 (0)	363.4 (0)	
1B _{1u}	1B _{1g}	1B _{3u}	2B _{2u}	2B _{2g}	
380.6 (8)	391.8 (0)	498.8 (68)	556.3 (41)	563.5 (0)	
2A _g	2B _{3u}	3A _g	2B _{1u}	3B _{3u}	
666.2 (0)	758.0 (572)	808.7 (0)	862.5 (197)	1228. (464)	
4A _g	2B _{1g}	3B _{2u}			
1282. (0)	1476. (0)	1492. (416)			
Min. M	192 fkn.	E = -1247.70248832	ZPE = 0.026302		
Min. L	226 fkn.	E = -1247.84488261	ZPE = 0.028060		
(HO)O ₂ SOSO ₂ (OH)					
C ₁	R(S ₁ -O ₁): 1.664	A(O ₅ -S ₂ -O ₆): 124.9	A(S ₁ -O ₁ -S ₂): 122.0		
(Min. 1 M)	R(S ₁ -O ₂): 1.428	A(O ₅ -S ₂ -O ₇): 107.2	A(O ₁ -S ₁ -O ₂): 110.6		
	R(S ₁ -O ₃): 1.454	A(O ₆ -S ₂ -O ₇): 110.8	A(O ₁ -S ₁ -O ₃): 106.2		
	R(S ₁ -O ₄): 1.594	A(S ₁ -O ₃ -H ₁): 111.3	A(O ₁ -S ₁ -O ₄): 96.9		
	R(S ₂ -O ₁): 1.707	A(S ₁ -O ₄ -H ₂): 111.2	A(O ₁ -S ₂ -O ₅): 103.5		
	R(S ₂ -O ₆): 1.428	A(S ₂ -O ₇ -H ₁): 109.6	A(O ₁ -S ₂ -O ₆): 107.3		
	R(S ₂ -O ₆): 1.438	A(O ₃ -H ₁ -O ₇): 129.6	A(O ₁ -S ₂ -O ₇): 100.3		
	R(S ₂ -O ₇): 1.607		A(O ₂ -S ₁ -O ₃): 123.0		
	R(O ₃ -H ₁): 2.089		A(O ₂ -S ₁ -O ₄): 106.6		
	R(O ₄ -H ₂): 0.971		A(O ₃ -S ₁ -O ₄): 110.4		
	R(O ₇ -H ₁): 0.979				
Charge:	S ₁ : +0.511	S ₂ : +0.373	O ₁ : -0.426	O ₂ : -0.234	O ₃ : -0.109
	O ₅ : -0.284	O ₆ : -0.097	O ₇ : -0.113	H ₁ : +0.307	H ₂ : +0.329
1A	2A	3A	4A	5A	
61.1 (3)	87.7 (3)	155.6 (8)	237.7 (18)	275.2 (8)	
6A	7A	8A	9A	10A	
286.7 (5)	331.6 (59)	395.0 (28)	425.4 (1)	441.8 (33)	
11A	12A	13A	14A	15A	
469.2 (5)	496.2 (57)	516.4 (50)	529.9 (276)	585.6 (20)	
16A	17A	18A	19A	20A	
669.5 (356)	695.0 (354)	808.9 (123)	831.6 (215)	1135. (134)	
21A	22A	23A	24A	25A	
1144. (175)	1179. (137)	1208. (90)	1400. (276)	1429. (244)	
26A	27A				
3619. (177)	3744. (147)				

C ₁ (Min. 1 L)	R(S ₁ -O ₁): 1.631 R(S ₁ -O ₂): 1.409 R(S ₁ -O ₃): 1.432 R(S ₁ -O ₄): 1.571 R(S ₂ -O ₁): 1.666 R(S ₂ -O ₅): 1.410 R(S ₂ -O ₆): 1.418 R(S ₂ -O ₇): 1.571 R(O ₃ -H ₁): 2.112 R(O ₄ -H ₂): 0.971 R(O ₇ -H ₁): 0.977	A(O ₅ -S ₂ -O ₆): 124.5 A(O ₅ -S ₂ -O ₇): 107.3 A(O ₆ -S ₂ -O ₇): 110.7 A(S ₁ -O ₃ -H ₁): 110.5 A(S ₁ -O ₄ -H ₂): 110.9 A(S ₂ -O ₇ -H ₁): 109.5 A(O ₃ -H ₁ -O ₇): 126.9	A(S ₁ -O ₁ -S ₂): 121.8 A(O ₁ -S ₁ -O ₂): 109.9 A(O ₁ -S ₁ -O ₃): 106.7 A(O ₁ -S ₁ -O ₄): 97.5 A(O ₁ -S ₂ -O ₅): 103.6 A(O ₁ -S ₂ -O ₆): 107.3 A(O ₁ -S ₂ -O ₇): 100.6 A(O ₂ -S ₁ -O ₃): 122.8 A(O ₂ -S ₁ -O ₄): 107.0 A(O ₃ -S ₁ -O ₄): 110.0			
?A	?A	?A				
Frequencies --	61.8081	87.6197	156.1002			
IR Inten --	2.5737	3.0162	10.4889			
?A	?A	?A				
Frequencies --	251.6355	290.0063	301.8715			
IR Inten --	32.7622	7.5246	12.3198			
?A	?A	?A				
Frequencies --	337.5662	395.2388	441.3073			
IR Inten --	49.5930	30.1613	3.3401			
?A	?A	?A				
Frequencies --	462.5244	492.5916	513.5081			
IR Inten --	33.1309	2.8712	25.2271			
?A	?A	?A				
Frequencies --	546.4166	551.1549	613.0081			
IR Inten --	48.4888	324.3376	6.6136			
?A	?A	?A				
Frequencies --	709.7331	747.2929	864.1353			
IR Inten --	155.8257	533.4691	116.2713			
?A	?A	?A				
Frequencies --	886.2381	1152.2453	1196.5853			
IR Inten --	207.3915	92.2875	214.4408			
?A	?A	?A				
Frequencies --	1223.9531	1244.3935	1464.6846			
IR Inten --	86.0191	134.4908	266.2066			
?A	?A	?A				
Frequencies --	1492.5999	3646.0758	3753.0799			
IR Inten --	249.7108	170.7981	148.5950			
C ₂ (Min. 2 M)	R(S-O ₁): 1.683 R(S-O ₂): 1.426 R(S-O ₃): 1.453 R(S-O ₄): 1.594 R(O ₃ -H): 2.058 R(O ₄ -H): 0.980	A(O ₂ -S-O ₃): 123.6 A(O ₂ -S-O ₄): 107.8 A(O ₃ -S-O ₄): 110.4 A(S-O ₃ -H): 111.2 A(S-O ₄ -H): 109.9	A(S-O ₁ -S): 118.9 A(O ₁ -S-O ₂): 106.0 A(O ₁ -S-O ₃): 105.3 A(O ₁ -S-O ₄): 101.5 A(O ₃ -H-O ₄): 134.0			
Charge:	S: +0.469	O ₁ : -0.427	O ₂ : -0.229	O ₃ : -0.065	O ₄ : -0.287	H: +0.325
1A	1B	2A	2B	3A		
100.6 (0)	130.7 (6)	170.4 (9)	285.1 (5)	285.6 (4)		
4A	3B	5A	4B	6A		
288.9 (1)	379.3 (0)	423.3 (1)	455.4 (15)	464.9 (42)		
5B	6B	7A	7B	8A		
504.4 (46)	527.6 (167)	535.8 (88)	554.7 (82)	605.7 (13)		
8B	9A	9B	10A	10B		
657.4 (549)	695.0 (45)	821.6 (192)	843.2 (106)	1146. (463)		
11A	12A	11B	12B	13A		
1149. (37)	1197. (69)	1209. (133)	1393. (285)	1430. (229)		
14A	13B					
3584. (84)	3594. (304)					
C ₂	R(S-O ₁): 1.647	A(O ₂ -S-O ₃): 123.0	A(S-O ₁ -S): 119.5			

(Min. 2 L)	R(S-O ₂): 1.408	A(O ₂ -S-O ₄): 108.0	A(O ₁ -S-O ₂): 105.8	
	R(S-O ₃): 1.432	A(O ₃ -S-O ₄): 110.4	A(O ₁ -S-O ₃): 105.8	
	R(S-O ₄): 1.562	A(S-O ₃ -H): 110.6	A(O ₁ -S-O ₄): 101.7	
	R(O ₃ -H): 2.050	A(S-O ₄ -H): 109.8	A(O ₃ -H-O ₄): 132.9	
	R(O ₄ -H): 0.980			
1A	1B	2A	3A	2B
99.6 (0)	131.2 (9)	175.4 (11)	298.4 (10)	303.6 (6)
4A	3B	5A	6A	4B
305.3 (0)	384.4 (3)	439.2 (6)	471.9 (73)	475.3 (21)
5B	7A	6B	7B	8A
510.6 (6)	543.5 (54)	556.1 (257)	568.1 (65)	622.8 (4)
8B	9A	9B	10A	10B
716.0 (502)	727.7 (48)	878.7 (188)	899.4 (90)	1188. (452)
11A	12A	11B	12B	13A
1197. (83)	1220. (0)	1235. (171)	1457. (274)	1488. (252)
14A	13B			
3593. (89)	3603. (315)			
Min. 1 M	226 fkn.	E = -1324.20723038	ZPE = 0.052758	
Min. 2 M	226 fkn.	E = -1324.21364666	ZPE = 0.053383	
Min. 1 L	260 fkn.	E = -1324.35073876	ZPE = 0.054410	
Min. 2 L	260 fkn.	E = -1324.35742970	ZPE = 0.054880	

(HO)O₂SOSO₂(OH)·H₂O

C ₁	R(S ₁ -O ₁): 1.641	A(S ₁ -O ₃ -H ₁): 139.3	A(S ₁ -O ₁ -S ₂): 125.0
(Min. 1 M)	R(S ₁ -O ₂): 1.431	A(S ₁ -O ₄ -H ₂): 110.7	A(O ₁ -S ₁ -O ₂): 111.3
	R(S ₁ -O ₃): 1.456	A(S ₂ -O ₇ -H ₃): 112.6	A(O ₁ -S ₁ -O ₃): 108.0
	R(S ₁ -O ₄): 1.605	A(H ₁ -O ₈ -H ₃): 102.7	A(O ₁ -S ₁ -O ₄): 96.6
	R(S ₂ -O ₁): 1.734	A(H ₁ -O ₈ -H ₄): 107.0	A(O ₁ -S ₂ -O ₅): 101.5
	R(S ₂ -O ₆): 1.430	A(H ₃ -O ₈ -H ₄): 117.3	A(O ₁ -S ₂ -O ₆): 106.6
	R(S ₂ -O ₆): 1.444	A(O ₃ -H ₁ -O ₈): 142.6	A(O ₁ -S ₂ -O ₇): 101.0
	R(S ₂ -O ₇): 1.567	A(O ₇ -H ₃ -O ₈): 174.5	A(O ₂ -S ₁ -O ₃): 121.8
	R(O ₃ -H ₁): 1.950		A(O ₂ -S ₁ -O ₄): 106.8
	R(O ₄ -H ₂): 0.971		A(O ₃ -S ₁ -O ₄): 109.3
	R(O ₇ -H ₃): 1.029		A(O ₅ -S ₂ -O ₆): 124.3
	R(O ₈ -H ₁): 0.971		A(O ₅ -S ₂ -O ₇): 109.0
	R(O ₈ -H ₃): 1.533		A(O ₆ -S ₂ -O ₇): 111.3
	R(O ₈ -H ₄): 0.964		
?A	?A	?A	
Frequencies --	44.4384	54.1095	87.6536
IR Inten --	6.6896	1.9729	6.5156
?A	?A	?A	
Frequencies --	121.5027	159.6891	236.3519
IR Inten --	4.0243	3.9671	20.8494
?A	?A	?A	
Frequencies --	239.4175	269.1762	274.5912
IR Inten --	5.3526	21.3089	96.2511
?A	?A	?A	
Frequencies --	297.1001	329.0412	402.6567
IR Inten --	21.1091	57.7165	8.3799
?A	?A	?A	
Frequencies --	420.5371	445.5284	477.4287
IR Inten --	39.6416	8.2986	5.2277
?A	?A	?A	
Frequencies --	484.4973	513.7818	523.0818
IR Inten --	29.2161	115.9766	289.2050
?A	?A	?A	
Frequencies --	579.1713	587.6072	644.4433
IR Inten --	4.9361	274.6901	235.4580

?A	?A	?A	
Frequencies --	729.3600	818.5970	890.9465
IR Inten --	353.6181	200.4678	113.4654
?A	?A	?A	
Frequencies --	1113.1766	1139.7969	1153.3830
IR Inten --	212.3361	86.9417	202.6467
?A	?A	?A	
Frequencies --	1174.0543	1338.4930	1385.1798
IR Inten --	119.5079	144.6027	276.1863
?A	?A	?A	
Frequencies --	1433.1222	1628.1848	2677.1755
IR Inten --	230.2792	43.4339	1937.0304
?A	?A	?A	
Frequencies --	3706.0549	3746.6311	3868.7007
IR Inten --	224.0675	147.1388	152.7309
C ₁	R(S ₁ -O ₁): 1.615	A(S ₁ -O ₃ -H ₁): 137.0	A(S ₁ -O ₁ -S ₂): 123.7
(Min. 2 M)	R(S ₁ -O ₂): 1.430	A(S ₁ -O ₄ -H ₂): 108.7	A(O ₁ -S ₁ -O ₂): 107.6
	R(S ₁ -O ₃): 1.469	A(S ₂ -O ₆ -H ₁): 113.0	A(O ₁ -S ₁ -O ₃): 108.5
	R(S ₁ -O ₄): 1.600	A(S ₂ -O ₇ -H ₃): 119.8	A(O ₁ -S ₁ -O ₄): 103.0
	R(S ₂ -O ₁): 1.777	A(H ₁ -O ₈ -H ₃): 101.5	A(O ₁ -S ₂ -O ₅): 102.8
	R(S ₂ -O ₆): 1.432	A(H ₁ -O ₈ -H ₄): 108.0	A(O ₁ -S ₂ -O ₆): 102.8
	R(S ₂ -O ₆): 1.463	A(H ₃ -O ₈ -H ₄): 110.5	A(O ₁ -S ₂ -O ₇): 101.3
	R(S ₂ -O ₇): 1.516	A(O ₃ -H ₁ -O ₈): 159.8	A(O ₂ -S ₁ -O ₃): 119.8
	R(O ₃ -H ₁): 1.604	A(O ₄ -H ₂ -O ₆): 138.3	A(O ₂ -S ₁ -O ₄): 107.9
	R(O ₄ -H ₂): 0.983	A(O ₇ -H ₃ -O ₈): 173.4	A(O ₃ -S ₁ -O ₄): 108.5
	R(O ₆ -H ₂): 1.940		A(O ₅ -S ₂ -O ₆): 121.3
	R(O ₇ -H ₃): 1.218		A(O ₅ -S ₂ -O ₇): 112.6
	R(O ₈ -H ₁): 1.000		A(O ₆ -S ₂ -O ₇): 112.7
	R(O ₈ -H ₃): 1.186		
	R(O ₈ -H ₄): 0.968		
?A	?A	?A	
Frequencies --	42.7445	90.6335	91.7313
IR Inten --	4.1510	1.4561	1.1727
?A	?A	?A	
Frequencies --	160.6628	186.7725	228.5024
IR Inten --	7.6384	8.0234	31.3896
?A	?A	?A	
Frequencies --	254.6734	281.8260	289.9594
IR Inten --	85.9456	4.4305	8.2212
?A	?A	?A	
Frequencies --	293.9248	382.2621	412.9414
IR Inten --	28.9429	6.2156	60.4539
?A	?A	?A	
Frequencies --	435.9000	474.8881	500.3918
IR Inten --	12.5485	20.5006	100.8137
?A	?A	?A	
Frequencies --	518.9217	528.0204	555.2466
IR Inten --	136.9749	90.6812	94.1994
?A	?A	?A	
Frequencies --	582.3291	610.2002	652.7769
IR Inten --	137.8216	17.7722	296.8218
?A	?A	?A	
Frequencies --	708.4515	828.3006	911.7669
IR Inten --	262.9993	141.2653	91.3177
?A	?A	?A	
Frequencies --	994.0976	1142.0726	1159.9335
IR Inten --	185.7102	286.1599	255.5861
?A	?A	?A	

Frequencies --	1219.6682	1361.1756	1397.8864
IR Inten --	108.5612	162.7663	398.0150
?A	?A	?A	
Frequencies --	1463.7039	1611.9189	2610.2566
IR Inten --	98.4710	54.7930	2142.5671
?A	?A	?A	
Frequencies --	3551.7287	3698.1798	3876.6721
IR Inten --	215.9269	259.7421	178.7903
Min. 1 M	260 fkn.	E = -1400.68919551	ZPE = 0.077446
Min. 2 M	260 fkn.	E = -1400.69510402	ZPE = 0.077711

Table 7.

Bond lengths (Å), bond angles (deg.), vibrational frequencies (cm⁻¹), IR intensities (km/mol), absolute and zero-point energies (H) for the ClO₃(OH) systems:

ClO ₃ (OH)									
C _s (Min. M)	R ₁ (Cl-O ₁): 1.448	R ₄ (O ₃ -H): 0.974	A ₁ (O ₁ -Cl-O ₂): 115.2						
	R ₂ (Cl-O ₂): 1.460	A ₄ (O ₂ -Cl-O ₃): 105.0	A ₂ (O ₁ -Cl-O ₃): 100.6						
	R ₃ (Cl-O ₃): 1.726	A ₅ (Cl-O ₃ -H): 105.5	A ₃ (O ₂ -Cl-O ₂): 113.7						
	Charge:	Cl: +0.329 O ₁ : -0.106	O ₂ : -0.126 O ₃ : -0.269	H: +0.297					
	1A''	1A'	2A''	2A'	3A'				
	174.5 (87)	357.5 (4)	362.5 (20)	478.7 (1)	513.8 (25)				
	3A''	4A'	5A'	6A'	4A''				
	518.8 (27)	645.1 (168)	934.8 (94)	1117. (146)	1121. (269)				
	7A'	8A'							
	1231. (156)	3712. (134)							
C _s (Min. L)	R ₁ (Cl-O ₁): 1.411	R ₄ (O ₃ -H): 0.974	A ₁ (O ₁ -Cl-O ₂): 115.1						
	R ₂ (Cl-O ₂): 1.422	A ₄ (O ₂ -Cl-O ₃): 105.1	A ₂ (O ₁ -Cl-O ₃): 100.9						
	R ₃ (Cl-O ₃): 1.662	A ₅ (Cl-O ₃ -H): 105.6	A ₃ (O ₂ -Cl-O ₂): 113.6						
	Charge:	Cl: +0.110 O ₁ : -0.057	O ₂ : -0.152 O ₃ : -0.095	H: +0.287					
	1A''	1A'	2A''	2A'	3A'				
	205.2 (89)	401.8 (5)	411.0 (15)	539.1 (3)	564.2 (21)				
	3A''	4A'	5A'	6A'	4A''				
	570.2 (24)	700.4 (191)	1041. (84)	1204. (100)	1253. (284)				
	7A'	8A'							
	1325. (231)	3715. (130)							
C _s (Min. XL)	R ₁ (Cl-O ₁): 1.411	R ₄ (O ₃ -H): 0.972	A ₁ (O ₁ -Cl-O ₂): 115.0						
	R ₂ (Cl-O ₂): 1.420	A ₄ (O ₂ -Cl-O ₃): 105.1	A ₂ (O ₁ -Cl-O ₃): 100.9						
	R ₃ (Cl-O ₃): 1.657	A ₅ (Cl-O ₃ -H): 105.9	A ₃ (O ₂ -Cl-O ₂): 113.6						
	Charge:	Cl: +1.716 O ₁ : -0.505	O ₂ : -0.695 O ₃ : -0.524	H: +0.534					
	1A''	1A'	2A''	2A'	3A'				
	192.4 (85)	404.3 (5)	413.7 (13)	545.0 (3)	567.9 (19)				
	3A''	4A'	5A'	6A'	4A''				
	574.8 (22)	705.1 (184)	1047. (81)	1207. (95)	1258. (269)				
	7A'	8A'							
	1327. (229)	3715. (123)							
Min. M	124 fkn.	E = -761.418251335	ZPE = 0.025439						
Min. L	141 fkn.	E = -761.518128107	ZPE = 0.027177						
Min. XL	220 fkn.	E = -761.537020743	ZPE = 0.027241						
ClO ₃ (OH)·H ₂ O									
C ₁ (Min. M)	R(Cl-O ₁): 1.450	R(O ₅ -H ₃): 0.963	A(O ₁ -Cl-O ₂): 114.5						
	R(Cl-O ₂): 1.462	A(Cl-O ₄ -H ₁): 104.6	A(O ₁ -Cl-O ₃): 114.6						
	R(Cl-O ₃): 1.470	A(H ₁ -O ₅ -H ₂): 110.0	A(O ₁ -Cl-O ₄): 102.3						
	R(Cl-O ₄): 1.684	A(H ₁ -O ₅ -H ₃): 122.6	A(O ₂ -Cl-O ₃): 112.8						
	R(O ₄ -H ₁): 1.002	A(H ₂ -O ₅ -H ₃): 106.7	A(O ₂ -Cl-O ₄): 106.0						
	R(O ₅ -H ₁): 1.682	A(O ₄ -H ₁ -O ₅): 169.2	A(O ₃ -Cl-O ₄): 105.0						
	R(O ₅ -H ₂): 0.965								
	Charge:	Cl: +0.293 O ₁ : -0.107 O ₂ : -0.129 O ₃ : -0.186 O ₄ : -0.330	O ₄ : -0.551	H ₁ : +0.439 H ₂ : +0.287 H ₃ : +0.285					

1A	2A	3A	4A	5A
34.9 (1)	70.7 (15)	160.3 (53)	223.0 (16)	301.1 (107)
6A	7A	8A	9A	10A
359.3 (6)	371.4 (16)	403.2 (42)	498.6 (6)	523.9 (13)
11A	12A	13A	14A	15A
524.2 (20)	670.5 (153)	851.8 (86)	926.7 (117)	1095. (286)
16A	17A	18A	19A	20A
1137. (235)	1403. (96)	1623. (74)	3173. (1283)	3798. (31)
21A				
3900. (114)				

C ₁	R(Cl-O ₁): 1.414	R(O ₅ -H ₃): 0.964	A(O ₁ -Cl-O ₂): 114.4
(Min. L)	R(Cl-O ₂): 1.426	A(Cl-O ₄ -H ₁): 103.2	A(O ₁ -Cl-O ₃): 114.5
	R(Cl-O ₃): 1.428	A(H ₁ -O ₅ -H ₂): 113.5	A(O ₁ -Cl-O ₄): 102.3
	R(Cl-O ₄): 1.622	A(H ₁ -O ₅ -H ₃): 118.9	A(O ₂ -Cl-O ₃): 112.8
	R(O ₄ -H ₁): 1.003	A(H ₂ -O ₅ -H ₃): 106.5	A(O ₂ -Cl-O ₄): 105.9
	R(O ₅ -H ₁): 1.665	A(O ₄ -H ₁ -O ₅): 175.4	A(O ₃ -Cl-O ₄): 105.5
	R(O ₅ -H ₂): 0.964		

1A	2A	3A	4A	5A
19.8 (1)	58.0 (17)	106.4 (53)	224.8 (14)	315.9 (96)
6A	7A	8A	9A	10A
346.7 (199)	410.2 (1)	432.3 (3)	560.1 (11)	577.2 (19)
11A	12A	13A	14A	15A
577.8 (10)	737.6 (187)	900.4 (89)	1035. (115)	1228. (301)
16A	17A	18A	19A	20A
1261. (228)	1421. (121)	1629. (68)	3157. (1400)	3804. (34)
21A				
3902. (113)				

Min. M	158 fkn.	E = -837.895912848	ZPE = 0.050229
Min. L	175 fkn.	E = -837.995920159	ZPE = 0.051718

		ClO ₂ (OH) ₃			
C ₁	R(Cl-O ₁): 1.472	A(O ₃ -Cl-O ₅): 80.6	A(O ₁ -Cl-O ₂): 121.7		
(Min. 1 M)	R(Cl-O ₂): 1.490	A(O ₄ -Cl-O ₅): 161.3	A(O ₁ -Cl-O ₃): 117.5		
	R(Cl-O ₃): 1.731	A(Cl-O ₃ -H ₁): 99.2	A(O ₁ -Cl-O ₄): 96.8		
	R(Cl-O ₄): 1.780	A(Cl-O ₄ -H ₂): 102.5	A(O ₁ -Cl-O ₅): 93.5		
	R(Cl-O ₅): 1.887	A(Cl-O ₅ -H ₁): 69.9	A(O ₂ -Cl-O ₃): 120.7		
	R(O ₃ -H ₁): 0.982	A(Cl-O ₅ -H ₃): 104.6	A(O ₂ -Cl-O ₄): 95.3		
	R(O ₅ -H ₁): 1.816	A(H ₁ -O ₅ -H ₃): 139.5	A(O ₂ -Cl-O ₅): 92.4		
	R(O ₄ -H ₂): 0.972	A(O ₃ -H ₁ -O ₅): 110.2	A(O ₃ -Cl-O ₄): 80.7		
	R(O ₅ -H ₃): 0.969				

Charge:	Cl: +0.261	O ₁ : -0.045	O ₂ : -0.139	O ₃ : -0.167	O ₄ : -0.307	O ₅ :
-0.495	H ₁ : +0.334	H ₂ : +0.264	H ₃ : +0.294			
1A	2A	3A	4A	5A		
111.7 (48)	199.0 (47)	222.9 (29)	295.7 (24)	373.2 (35)		
6A	7A	8A	9A	10A		
421.4 (6)	457.5 (5)	464.0 (6)	485.1 (1)	522.1 (9)		
11A	12A	13A	14A	15A		
570.8 (71)	609.9 (213)	632.9 (353)	879.8 (90)	1038. (194)		
16A	17A	18A	19A	20A		
1099. (156)	1202. (6)	1302. (201)	3555. (144)	3744. (104)		
21A						
3785. (105)						

C ₁ (Min. 1 L)	R(Cl-O ₁): 1.433 R(Cl-O ₂): 1.446 R(Cl-O ₃): 1.663 R(Cl-O ₄): 1.730 R(Cl-O ₅): 1.852 R(O ₃ -H ₁): 0.982 R(O ₅ -H ₁): 1.786 R(O ₄ -H ₂): 0.970 R(O ₅ -H ₃): 0.967	A(O ₃ -Cl-O ₅): 81.5 A(O ₄ -Cl-O ₅): 162.6 A(Cl-O ₃ -H ₁): 100.0 A(Cl-O ₄ -H ₂): 102.8 A(Cl-O ₅ -H ₁): 69.5 A(Cl-O ₅ -H ₃): 103.9 A(H ₁ -O ₅ -H ₃): 135.0 A(O ₃ -H ₁ -O ₅): 108.8	A(O ₁ -Cl-O ₂): 121.9 A(O ₁ -Cl-O ₃): 117.9 A(O ₁ -Cl-O ₄): 96.4 A(O ₁ -Cl-O ₅): 92.7 A(O ₂ -Cl-O ₃): 120.0 A(O ₂ -Cl-O ₄): 95.5 A(O ₂ -Cl-O ₅): 92.3 A(O ₃ -Cl-O ₄): 81.0
?A	?A	?A	
Frequencies --	94.5580	208.7943	237.3504
IR Inten --	59.7384	41.0968	24.8029
?A	?A	?A	
Frequencies --	312.0177	381.3677	466.8995
IR Inten --	23.3035	60.5267	5.7834
?A	?A	?A	
Frequencies --	512.3541	520.8880	529.1828
IR Inten --	3.0342	8.0227	3.2524
?A	?A	?A	
Frequencies --	576.2558	627.3538	638.8898
IR Inten --	44.7643	160.3374	173.7569
?A	?A	?A	
Frequencies --	661.5955	985.0670	1108.6607
IR Inten --	294.4774	94.5995	135.5162
?A	?A	?A	
Frequencies --	1209.9114	1252.9538	1359.7864
IR Inten --	237.7029	9.2312	232.2299
?A	?A	?A	
Frequencies --	3549.7144	3758.3737	3799.0206
IR Inten --	146.6740	99.4137	89.5324
C ₁ (Min. 2 M)	R(Cl-O ₁): 1.472 R(Cl-O ₂): 1.477 R(Cl-O ₃): 1.757 R(Cl-O ₄): 1.772 R(Cl-O ₅): 1.891 R(O ₃ -H ₁): 0.982 R(O ₅ -H ₁): 1.848 R(O ₄ -H ₂): 0.972 R(O ₅ -H ₃): 0.969	A(O ₃ -Cl-O ₅): 80.3 A(O ₄ -Cl-O ₅): 164.0 A(Cl-O ₃ -H ₁): 100.3 A(Cl-O ₄ -H ₂): 105.0 A(Cl-O ₅ -H ₁): 70.6 A(Cl-O ₅ -H ₃): 104.6 A(H ₁ -O ₅ -H ₃): 137.7 A(O ₃ -H ₁ -O ₅): 108.8	A(O ₁ -Cl-O ₂): 124.5 A(O ₁ -Cl-O ₃): 114.3 A(O ₁ -Cl-O ₄): 97.0 A(O ₁ -Cl-O ₅): 93.0 A(O ₂ -Cl-O ₃): 121.0 A(O ₂ -Cl-O ₄): 91.8 A(O ₂ -Cl-O ₅): 92.5 A(O ₃ -Cl-O ₄): 84.2
?A	?A	?A	
Frequencies --	161.5013	192.8259	242.9419
IR Inten --	8.8009	39.7809	91.5175
?A	?A	?A	
Frequencies --	321.0740	364.6402	415.0226
IR Inten --	22.2370	26.6530	8.6295
?A	?A	?A	
Frequencies --	449.7141	459.6178	482.8230
IR Inten --	3.8168	7.4438	1.2007
?A	?A	?A	
Frequencies --	519.0620	569.2850	617.9884
IR Inten --	21.0885	98.1026	241.9184
?A	?A	?A	
Frequencies --	637.9006	901.5935	1040.5929
IR Inten --	244.8707	98.4095	173.4856
?A	?A	?A	
Frequencies --	1100.9804	1207.8733	1242.6595
IR Inten --	96.5349	174.1248	108.2197
?A	?A	?A	

Frequencies --	3569.0587	3734.1360	3783.7164
IR Inten --	131.2196	92.5963	104.9742
C ₁	R(Cl-O ₁): 1.434	A(O ₃ -Cl-O ₅): 81.7	A(O ₁ -Cl-O ₂): 125.4
(Min. 2 L)	R(Cl-O ₂): 1.436	A(O ₄ -Cl-O ₅): 166.3	A(O ₁ -Cl-O ₃): 114.8
	R(Cl-O ₃): 1.683	A(Cl-O ₃ -H ₁): 100.4	A(O ₁ -Cl-O ₄): 96.4
	R(Cl-O ₄): 1.720	A(Cl-O ₄ -H ₂): 105.0	A(O ₁ -Cl-O ₅): 92.0
	R(Cl-O ₅): 1.854	A(Cl-O ₅ -H ₁): 69.7	A(O ₂ -Cl-O ₃): 119.6
	R(O ₃ -H ₁): 0.982	A(Cl-O ₅ -H ₃): 103.8	A(O ₂ -Cl-O ₄): 91.7
	R(O ₅ -H ₁): 1.814	A(H ₁ -O ₅ -H ₃): 130.2	A(O ₂ -Cl-O ₅): 92.2
	R(O ₄ -H ₂): 0.971	A(O ₃ -H ₁ -O ₅): 108.2	A(O ₃ -Cl-O ₄): 85.0
	R(O ₅ -H ₃): 0.967		

?A	?A	?A	
Frequencies --	179.3089	213.1881	267.4845
IR Inten --	17.5549	46.5842	66.4214
?A	?A	?A	
Frequencies --	328.9354	372.1543	462.7364
IR Inten --	27.4991	56.9781	10.1805
?A	?A	?A	
Frequencies --	503.3187	514.8520	531.2036
IR Inten --	5.0125	3.7357	3.4076
?A	?A	?A	
Frequencies --	572.7504	625.9461	651.4044
IR Inten --	71.6673	157.3567	197.4889
?A	?A	?A	
Frequencies --	670.8517	1002.2545	1109.4496
IR Inten --	217.2065	104.9537	124.6953
?A	?A	?A	
Frequencies --	1195.2839	1284.0758	1315.6492
IR Inten --	117.3578	209.6067	151.7095
?A	?A	?A	
Frequencies --	3547.7960	3743.6481	3796.9350
IR Inten --	125.4826	82.2496	90.2243
Min. 1 M	158 fkn.	E = -837.799572898	ZPE = 0.050054
Min. 2 M	158 fkn.	E = -837.800872514	ZPE = 0.050154
Min. 1 L	175 fkn.	E = -837.885058258	ZPE = 0.051922
Min. 2 L	175 fkn.	E = -837.886441081	ZPE = 0.052145

ClO₂(OH)·H₂O₂

C ₁	R(Cl-O ₁): 1.484	R(O ₅ -H ₂): 1.789	A(O ₁ -Cl-O ₂): 112.5			
(Min. M)	R(Cl-O ₂): 1.503	R(O ₅ -H ₃): 0.968	A(O ₁ -Cl-O ₃): 106.4			
	R(Cl-O ₃): 1.737	A(Cl-O ₂ -H ₁): 121.4	A(O ₂ -Cl-O ₃): 104.0			
	R(O ₄ -O ₅): 1.448	A(Cl-O ₃ -H ₂): 103.9	A(O ₄ -O ₅ -H ₂): 115.4			
	R(O ₂ -H ₁): 1.923	A(H ₂ -O ₅ -H ₃): 122.5	A(O ₄ -O ₅ -H ₃): 102.3			
	R(O ₃ -H ₂): 0.994	A(O ₂ -H ₁ -O ₄): 157.8	A(O ₅ -O ₄ -H ₁): 100.9			
	R(O ₄ -H ₁): 0.978	A(O ₃ -H ₂ -O ₅): 165.5				
Charge:	Cl: +0.669	O ₁ : -0.293	O ₂ : -0.404	O ₃ : -0.374	O ₄ : -0.333	O ₅ :
-0.295	H ₁ : +0.383	H ₂ : +0.366	H ₃ : +0.281			
1A	2A	3A	4A	5A		
50.6 (4)	74.7 (6)	157.6 (6)	174.7 (2)	229.7 (17)		
6A	7A	8A	9A	10A		
328.5 (70)	348.5 (66)	387.8 (12)	483.8 (16)	582.9 (77)		
11A	12A	13A	14A	15A		
593.6 (147)	737.2 (101)	924.4 (85)	943.0 (8)	1047. (260)		
16A	17A	18A	19A	20A		
1282. (46)	1352. (65)	1509. (34)	3332. (631)	3595. (338)		
21A						
3766. (59)						
C ₁	R(Cl-O ₁): 1.446	R(O ₅ -H ₂): 1.752	A(O ₁ -Cl-O ₂): 112.0			

(Min. L)	R(Cl-O ₂): 1.465	R(O ₅ -H ₃): 0.968	A(O ₁ -Cl-O ₃): 105.9
	R(Cl-O ₃): 1.667	A(Cl-O ₂ -H ₁): 122.7	A(O ₂ -Cl-O ₃): 104.0
	R(O ₄ -O ₅): 1.448	A(Cl-O ₃ -H ₂): 105.4	A(O ₄ -O ₅ -H ₂): 113.5
	R(O ₂ -H ₁): 1.964	A(H ₂ -O ₅ -H ₃): 121.2	A(O ₄ -O ₅ -H ₃): 102.2
	R(O ₃ -H ₂): 0.997	A(O ₂ -H ₁ -O ₄): 158.0	A(O ₅ -O ₄ -H ₁): 101.0
	R(O ₄ -H ₁): 0.977	A(O ₃ -H ₂ -O ₅): 171.5	
?A	?A	?A	
Frequencies --	40.5997	62.3105	152.1086
IR Inten --	3.4603	5.9646	8.7861
?A	?A	?A	
Frequencies --	159.8035	227.4139	330.8710
IR Inten --	2.6685	17.1332	125.0028
?A	?A	?A	
Frequencies --	395.3336	436.2290	514.4044
IR Inten --	11.5175	0.9249	55.5103
?A	?A	?A	
Frequencies --	539.0006	661.8102	749.6007
IR Inten --	49.4035	149.5459	117.5645
?A	?A	?A	
Frequencies --	943.2705	1019.5833	1156.7900
IR Inten --	2.4919	92.8255	278.4795
?A	?A	?A	
Frequencies --	1321.3403	1347.7682	1496.4306
IR Inten --	62.9522	50.4824	26.0464
?A	?A	?A	
Frequencies --	3259.6824	3611.6980	3765.6227
IR Inten --	816.8934	319.5220	58.9070
Min. M	158 fkn.	E = -837.902252500	ZPE = 0.049892
Min. L	175 fkn.	E = -837.966503203	ZPE = 0.050556

		C1O(OH) ₅	
C ₁	R(Cl-O ₁): 1.509	A(Cl-O ₂ -H ₁): 103.3	A(O ₁ -Cl-O ₂): 93.6
(Min. M)	R(Cl-O ₂): 1.776	A(Cl-O ₃ -H ₂): 101.6	A(O ₁ -Cl-O ₃): 96.7
	R(Cl-O ₃): 1.782	A(Cl-O ₄ -H ₃): 101.5	A(O ₁ -Cl-O ₄): 97.5
	R(Cl-O ₄): 1.810	A(Cl-O ₅ -H ₄): 101.0	A(O ₁ -Cl-O ₅): 96.0
	R(Cl-O ₅): 1.812	A(Cl-O ₆ -H ₁): 70.0	A(O ₁ -Cl-O ₆): 176.9
	R(Cl-O ₆): 1.848	A(Cl-O ₆ -H ₅): 103.3	A(O ₂ -Cl-O ₃): 92.7
	R(O ₂ -H ₁): 0.974	A(H ₁ -O ₆ -H ₅): 141.9	A(O ₂ -Cl-O ₄): 168.9
	R(O ₃ -H ₂): 0.973	A(O ₂ -H ₁ -O ₅): 102.9	A(O ₂ -Cl-O ₅): 91.0
	R(O ₄ -H ₃): 0.973		A(O ₂ -Cl-O ₆): 102.9
	R(O ₅ -H ₄): 0.973		A(O ₃ -Cl-O ₄): 86.7
	R(O ₆ -H ₁): 1.998		A(O ₃ -Cl-O ₅): 166.3
	R(O ₆ -H ₅): 0.972		A(O ₃ -Cl-O ₆): 83.5
			A(O ₄ -Cl-O ₅): 87.0
			A(O ₄ -Cl-O ₆): 85.6
			A(O ₅ -Cl-O ₆): 83.9

?A	?A	?A	
Frequencies --	122.5035	207.3758	250.5562
IR Inten --	24.7955	17.5410	30.3171
?A	?A	?A	
Frequencies --	268.3958	302.2386	317.1876
IR Inten --	27.0644	21.2243	19.3712
?A	?A	?A	
Frequencies --	354.8942	394.8844	399.7852
IR Inten --	10.1546	23.0249	13.8614
?A	?A	?A	
Frequencies --	417.4566	431.4627	448.0872
IR Inten --	5.7364	2.7594	7.4563

?A	?A	?A	
Frequencies --	453.4544	461.1157	466.3613
IR Inten --	7.3330	4.1739	3.7850
?A	?A	?A	
Frequencies --	474.0410	501.0591	625.3671
IR Inten --	2.6604	126.4433	328.5871
?A	?A	?A	
Frequencies --	659.0555	861.6599	1133.4132
IR Inten --	430.3825	186.6343	104.8118
?A	?A	?A	
Frequencies --	1169.3014	1177.5789	1180.3910
IR Inten --	91.2591	119.5801	97.4462
?A	?A	?A	
Frequencies --	1254.9837	3698.3625	3716.0772
IR Inten --	134.9425	97.4546	110.9854
?A	?A	?A	
Frequencies --	3722.1077	3730.9953	3748.3497
IR Inten --	99.8188	131.4030	89.9070
Min. S	119 fkn.	E = -914.075631489	ZPE = 0.073014
Min. M	192 fkn.	E = -914.207579847	ZPE = 0.075062

ClO₃(OH)·2 H₂O

C ₁	R(Cl-O ₁): 1.489	A(Cl-O ₃ -H ₁): 124.5	A(O ₁ -Cl-O ₂): 113.9
(Min. S)	R(Cl-O ₂): 1.506	A(Cl-O ₄ -H ₂): 117.0	A(O ₁ -Cl-O ₃): 110.0
	R(Cl-O ₃): 1.547	A(H ₁ -O ₅ -H ₃): 108.0	A(O ₁ -Cl-O ₄): 108.0
	R(Cl-O ₄): 1.581	A(H ₁ -O ₅ -H ₄): 115.0	A(O ₂ -Cl-O ₃): 109.7
	R(O ₃ -H ₁): 1.665	A(H ₂ -O ₅ -H ₃): 109.5	A(O ₂ -Cl-O ₄): 108.3
	R(O ₄ -H ₂): 1.442	A(H ₂ -O ₅ -H ₅): 117.6	A(O ₃ -Cl-O ₄): 106.6
	R(O ₅ -H ₁): 0.998	A(H ₃ -O ₅ -H ₄): 126.9	A(O ₃ -H ₁ -O ₅): 160.2
	R(O ₅ -H ₃): 1.326	A(H ₃ -O ₅ -H ₅): 120.7	A(O ₄ -H ₂ -O ₅): 167.0
	R(O ₅ -H ₄): 0.963		A(O ₅ -H ₃ -O ₅): 162.2
	R(O ₅ -H ₂): 1.054		
	R(O ₅ -H ₅): 1.097		
	R(O ₅ -H ₅): 0.963		

Charge: Cl: +0.800 O₁: -0.457 O₂: -0.494 O₃: -0.290 O₄: -0.327 O₅:
-0.783 O₆: -0.823 H₁: +0.493 H₂: +0.511 H₃: +0.451 H₄: +0.482
H₅: +0.437

1A	2A	3A	4A	5A
34.9 (1)	70.7 (15)	160.3 (53)	223.0 (16)	301.1 (107)
6A	7A	8A	9A	10A
359.3 (6)	371.4 (16)	403.2 (42)	498.6 (6)	523.9 (13)
11A	12A	13A	14A	15A
524.2 (20)	670.5 (153)	851.8 (86)	926.7 (117)	1095. (286)
16A	17A	18A	19A	20A
1137. (235)	1403. (96)	1623. (74)	3173. (1283)	3798. (31)
21A				
3900. (114)				

?A	?A	?A	
Frequencies --	38.6113	52.0905	112.8610
IR Inten --	3.9437	2.5059	9.4768
?A	?A	?A	
Frequencies --	167.5570	253.3307	276.6159
IR Inten --	8.6121	207.6472	60.7194
?A	?A	?A	
Frequencies --	355.6208	380.7875	406.7984
IR Inten --	139.1254	3.5704	71.1507
?A	?A	?A	
Frequencies --	477.2032	503.3692	522.3244

IR Inten	--	43.5947	49.1617	32.1654	
?A		?A	?A		
Frequencies	--	556.3348	585.2002	631.2959	
IR Inten	--	51.6728	54.9935	106.1094	
?A		?A	?A		
Frequencies	--	709.3319	785.5238	825.0927	
IR Inten	--	186.4427	242.8270	256.8872	
?A		?A	?A		
Frequencies	--	945.8489	1017.7230	1104.0144	
IR Inten	--	311.2372	196.0081	94.0256	
?A		?A	?A		
Frequencies	--	1356.7953	1419.2775	1664.1086	
IR Inten	--	448.9449	305.9375	37.4521	
?A		?A	?A		
Frequencies	--	1794.9043	1962.1984	2343.0528	
IR Inten	--	998.4723	1034.7736	2013.7084	
?A		?A	?A		
Frequencies	--	3201.1306	3843.2732	3847.4953	
IR Inten	--	1212.9541	122.6824	123.4713	
C ₁		R(Cl-O ₁): 1.450	A(Cl-O ₃ -H ₁): 128.0	A(O ₁ -Cl-O ₂): 114.9	
(Min. M)		R(Cl-O ₂): 1.464	A(Cl-O ₄ -H ₂): 107.3	A(O ₁ -Cl-O ₃): 113.2	
		R(Cl-O ₃): 1.479	A(H ₁ -O ₅ -H ₃): 103.0	A(O ₁ -Cl-O ₄): 102.9	
		R(Cl-O ₄): 1.657	A(H ₁ -O ₅ -H ₄): 106.8	A(O ₂ -Cl-O ₃): 112.0	
		R(O ₃ -H ₁): 2.021	A(H ₂ -O ₆ -H ₃): 110.3	A(O ₂ -Cl-O ₄): 106.6	
		R(O ₄ -H ₂): 1.031	A(H ₂ -O ₆ -H ₅): 118.0	A(O ₃ -Cl-O ₄): 106.0	
		R(O ₅ -H ₁): 1.536	A(H ₃ -O ₅ -H ₄): 107.4	A(O ₃ -H ₁ -O ₆): 152.2	
		R(O ₅ -H ₃): 0.985	A(H ₃ -O ₆ -H ₅): 126.2	A(O ₄ -H ₂ -O ₆): 176.5	
		R(O ₅ -H ₄): 0.963		A(O ₅ -H ₃ -O ₆): 162.0	
		R(O ₆ -H ₂): 0.969			
		R(O ₆ -H ₃): 1.746			
		R(O ₆ -H ₅): 0.962			
?A		?A	?A		
Frequencies	--	37.5382	57.1842	104.0092	
IR Inten	--	0.5189	1.6362	2.3222	
?A		?A	?A		
Frequencies	--	137.7783	203.8007	227.5489	
IR Inten	--	9.1812	115.7518	46.2364	
?A		?A	?A		
Frequencies	--	278.8295	316.2930	355.1085	
IR Inten	--	10.7577	156.7961	12.4725	
?A		?A	?A		
Frequencies	--	362.7856	399.5133	475.6796	
IR Inten	--	12.3584	25.9876	135.2475	
?A		?A	?A		
Frequencies	--	512.9034	527.7710	530.3844	
IR Inten	--	9.8993	33.0984	0.8475	
?A		?A	?A		
Frequencies	--	541.2648	694.5311	872.7087	
IR Inten	--	115.6265	129.2729	178.8706	
?A		?A	?A		
Frequencies	--	921.0442	1061.2451	1109.4832	
IR Inten	--	165.7662	104.3898	264.5511	
?A		?A	?A		
Frequencies	--	1140.6268	1451.4032	1626.5486	
IR Inten	--	251.2104	90.5622	78.9297	
?A		?A	?A		
Frequencies	--	1657.8345	2655.2735	3436.4610	
IR Inten	--	19.6313	2196.5387	674.9752	

?A	?A	?A	
Frequencies --	3734.8614	3872.0505	3891.4802
IR Inten --	245.5474	99.8402	157.0249
C ₁	R(Cl-O ₁): 1.413	A(Cl-O ₃ -H ₁): 128.6	A(O ₁ -Cl-O ₂): 114.7
(Min. L)	R(Cl-O ₂): 1.425	A(Cl-O ₄ -H ₂): 107.8	A(O ₁ -Cl-O ₃): 113.2
	R(Cl-O ₃): 1.438	A(H ₁ -O ₅ -H ₃): 103.7	A(O ₁ -Cl-O ₄): 103.0
	R(Cl-O ₄): 1.597	A(H ₁ -O ₅ -H ₄): 106.7	A(O ₂ -Cl-O ₃): 112.0
	R(O ₃ -H ₁): 2.076	A(H ₂ -O ₆ -H ₃): 109.8	A(O ₂ -Cl-O ₄): 106.2
	R(O ₄ -H ₂): 1.033	A(H ₂ -O ₆ -H ₅): 117.6	A(O ₃ -Cl-O ₄): 106.0
	R(O ₅ -H ₁): 1.526	A(H ₃ -O ₆ -H ₄): 107.4	A(O ₃ -H ₁ -O ₅): 148.7
	R(O ₅ -H ₃): 0.985	A(H ₃ -O ₆ -H ₅): 126.0	A(O ₄ -H ₂ -O ₆): 176.7
	R(O ₅ -H ₄): 0.963		A(O ₅ -H ₃ -O ₆): 163.0
	R(O ₆ -H ₂): 0.969		
	R(O ₆ -H ₃): 1.747		
	R(O ₆ -H ₅): 0.962		
?A	?A	?A	
Frequencies --	32.8424	53.8630	105.4165
IR Inten --	0.4991	1.6235	2.4360
?A	?A	?A	
Frequencies --	127.5154	190.9113	227.7169
IR Inten --	8.5646	109.1169	42.9277
?A	?A	?A	
Frequencies --	283.3558	303.3888	350.1802
IR Inten --	7.3354	155.4228	34.8022
?A	?A	?A	
Frequencies --	406.5217	439.2117	463.2926
IR Inten --	17.9345	22.9887	169.1022
?A	?A	?A	
Frequencies --	518.6119	571.7285	583.5877
IR Inten --	68.7103	17.3113	13.6044
?A	?A	?A	
Frequencies --	584.4015	768.0187	872.8952
IR Inten --	23.5917	147.1748	200.0881
?A	?A	?A	
Frequencies --	1025.6316	1101.8817	1204.8536
IR Inten --	144.2879	39.4607	364.3241
?A	?A	?A	
Frequencies --	1266.2896	1467.4089	1622.2491
IR Inten --	254.9360	108.6283	78.1782
?A	?A	?A	
Frequencies --	1659.6442	2629.5196	3438.9554
IR Inten --	19.5475	2231.5577	691.5269
?A	?A	?A	
Frequencies --	3747.1439	3871.8378	3892.1429
IR Inten --	197.6240	99.3779	155.6075
Min. S	119 fkn.	E = -914.232114215	ZPE = 0.073220
Min. M	192 fkn.	E = -914.374226006	ZPE = 0.075621
Min. L	209 fkn.	E = -914.473700570	ZPE = 0.077027

ClO₃(OH)·3 H₂O

C ₁	R(Cl-O ₁): 1.451	A(Cl-O ₃ -H ₁): 133.3	A(O ₁ -Cl-O ₂): 114.8
(Min. 1 M)	R(Cl-O ₂): 1.467	A(Cl-O ₄ -H ₂): 109.0	A(O ₁ -Cl-O ₃): 112.6
	R(Cl-O ₃): 1.480	A(H ₁ -O ₇ -H ₅): 110.8	A(O ₁ -Cl-O ₄): 103.4
	R(Cl-O ₄): 1.642	A(H ₁ -O ₇ -H ₇): 106.3	A(O ₂ -Cl-O ₃): 112.0
	R(O ₃ -H ₁): 1.920	A(H ₂ -O ₆ -H ₃): 118.5	A(O ₂ -Cl-O ₄): 106.7
	R(O ₄ -H ₂): 1.051	A(H ₂ -O ₆ -H ₄): 116.2	A(O ₃ -Cl-O ₄): 106.4
	R(O ₅ -H ₂): 1.461	A(H ₃ -O ₆ -H ₄): 107.5	A(O ₃ -H ₁ -O ₇): 172.2
	R(O ₅ -H ₃): 0.995	A(H ₃ -O ₆ -H ₅): 110.4	A(O ₄ -H ₂ -O ₆): 175.0

	R(O ₅ -H ₄): 0.963	A(H ₃ -O ₆ -H ₆): 121.3	A(O ₅ -H ₅ -O ₆): 174.5
	R(O ₆ -H ₃): 1.658	A(H ₅ -O ₆ -H ₆): 107.0	A(O ₆ -H ₅ -O ₇): 168.4
	R(O ₆ -H ₅): 0.983	A(H ₅ -O ₇ -H ₇): 124.7	
	R(O ₆ -H ₆): 0.962		
	R(O ₇ -H ₁): 0.971		
	R(O ₇ -H ₅): 1.749		
	R(O ₇ -H ₇): 0.962		
?A	?A	?A	
Frequencies --	30.1280	39.1191	58.6081
IR Inten --	0.8390	0.2139	1.5019
?A	?A	?A	
Frequencies --	71.8500	99.3617	145.9743
IR Inten --	0.8203	4.5469	4.5849
?A	?A	?A	
Frequencies --	194.4840	206.1658	255.0821
IR Inten --	93.7620	53.0446	114.2286
?A	?A	?A	
Frequencies --	268.1894	328.8107	340.5526
IR Inten --	75.4872	46.7147	127.2930
?A	?A	?A	
Frequencies --	350.6363	364.9543	405.7182
IR Inten --	17.9019	4.5784	51.8889
?A	?A	?A	
Frequencies --	453.9509	516.6066	527.5119
IR Inten --	31.2946	26.2832	49.8691
?A	?A	?A	
Frequencies --	534.9144	554.7959	598.3744
IR Inten --	8.5005	30.7022	137.6781
?A	?A	?A	
Frequencies --	711.5171	829.5227	917.3710
IR Inten --	105.9163	173.2966	151.3876
?A	?A	?A	
Frequencies --	982.5544	1062.3133	1132.5293
IR Inten --	155.7476	251.5155	254.3433
?A	?A	?A	
Frequencies --	1198.0213	1424.7343	1632.9234
IR Inten --	138.2814	115.5663	75.1906
?A	?A	?A	
Frequencies --	1650.4381	1682.0849	2352.9211
IR Inten --	32.9986	16.9998	2908.5185
?A	?A	?A	
Frequencies --	3240.8491	3470.3737	3711.7799
IR Inten --	1113.6909	767.4102	441.8686
?A	?A	?A	
Frequencies --	3872.3087	3883.1359	3888.3668
IR Inten --	92.5767	85.5886	144.5905
C ₁	R(Cl-O ₁): 1.414	A(Cl-O ₃ -H ₁): 129.5	A(O ₁ -Cl-O ₂): 114.6
(Min. 1 L)	R(Cl-O ₂): 1.429	A(Cl-O ₄ -H ₂): 109.5	A(O ₁ -Cl-O ₃): 112.7
	R(Cl-O ₃): 1.440	A(H ₁ -O ₇ -H ₅): 109.4	A(O ₁ -Cl-O ₄): 103.7
	R(Cl-O ₄): 1.582	A(H ₁ -O ₇ -H ₇): 106.4	A(O ₂ -Cl-O ₃): 111.8
	R(O ₃ -H ₁): 1.957	A(H ₂ -O ₅ -H ₃): 117.9	A(O ₂ -Cl-O ₄): 106.7
	R(O ₄ -H ₂): 1.053	A(H ₂ -O ₅ -H ₄): 115.7	A(O ₃ -Cl-O ₄): 106.3
	R(O ₅ -H ₂): 1.452	A(H ₃ -O ₅ -H ₄): 107.3	A(O ₃ -H ₁ -O ₇): 165.2
	R(O ₅ -H ₃): 0.995	A(H ₃ -O ₆ -H ₅): 111.7	A(O ₄ -H ₂ -O ₅): 174.6
	R(O ₅ -H ₄): 0.963	A(H ₃ -O ₆ -H ₆): 121.4	A(O ₅ -H ₅ -O ₆): 175.2
	R(O ₆ -H ₃): 1.658	A(H ₅ -O ₆ -H ₆): 106.9	A(O ₆ -H ₅ -O ₇): 169.5
	R(O ₆ -H ₅): 0.983	A(H ₅ -O ₇ -H ₇): 124.0	
	R(O ₆ -H ₆): 0.962		

	R(O ₇ -H ₁): 0.970		
	R(O ₇ -H ₅): 1.750		
	R(O ₇ -H ₇): 0.962		
?A	?A	?A	
Frequencies --	22.4656	36.2160	52.9158
IR Inten --	2.2108	0.0727	0.9557
?A	?A	?A	
Frequencies --	63.5424	113.3083	140.0714
IR Inten --	1.6897	2.8993	4.3605
?A	?A	?A	
Frequencies --	188.3715	203.6891	254.0108
IR Inten --	88.3925	44.9410	135.4250
?A	?A	?A	
Frequencies --	266.9650	333.9272	341.2018
IR Inten --	61.9606	48.9619	8.6866
?A	?A	?A	
Frequencies --	350.3322	410.5169	445.8484
IR Inten --	154.1975	0.5629	44.7800
?A	?A	?A	
Frequencies --	455.8830	532.8467	560.7667
IR Inten --	42.7555	115.4559	63.7826
?A	?A	?A	
Frequencies --	576.8857	587.0017	596.2371
IR Inten --	30.9020	13.8693	36.4642
?A	?A	?A	
Frequencies --	791.0430	835.2983	980.9993
IR Inten --	127.7349	183.9783	81.9313
?A	?A	?A	
Frequencies --	1023.6678	1176.2534	1213.9474
IR Inten --	234.2418	97.8360	291.3302
?A	?A	?A	
Frequencies --	1260.0421	1444.0104	1625.9326
IR Inten --	288.4372	124.0188	62.4245
?A	?A	?A	
Frequencies --	1648.8292	1686.3226	2313.8945
IR Inten --	39.2161	17.3029	2889.6971
?A	?A	?A	
Frequencies --	3238.1535	3466.9969	3717.6426
IR Inten --	1139.3876	760.3099	382.8565
?A	?A	?A	
Frequencies --	3871.2967	3884.0052	3888.9794
IR Inten --	91.9294	86.4772	136.7649
C ₁	R(Cl-O ₁): 1.458	A(Cl-O ₂ -H ₁): 125.0	A(O ₁ -Cl-O ₂): 111.3
(Min. 2 M)	R(Cl-O ₂): 1.502	A(Cl-O ₃ -H ₂): 125.0	A(O ₁ -Cl-O ₃): 111.3
	R(Cl-O ₃): 1.502	A(Cl-O ₄ -H ₃): 115.8	A(O ₁ -Cl-O ₄): 109.3
	R(Cl-O ₄): 1.536	A(H ₁ -O ₆ -H ₄): 103.8	A(O ₂ -Cl-O ₃): 109.2
	R(O ₂ -H ₁): 1.832	A(H ₁ -O ₆ -H ₆): 107.6	A(O ₂ -Cl-O ₄): 107.8
	R(O ₃ -H ₂): 1.833	A(H ₂ -O ₇ -H ₅): 103.8	A(O ₃ -Cl-O ₄): 107.8
	R(O ₄ -H ₃): 1.545	A(H ₂ -O ₇ -H ₇): 107.6	A(O ₂ -H ₁ -O ₆): 159.3
	R(O ₅ -H ₃): 1.027	A(H ₃ -O ₅ -H ₄): 104.0	A(O ₃ -H ₂ -O ₇): 159.3
	R(O ₅ -H ₄): 1.022	A(H ₃ -O ₅ -H ₅): 104.0	A(O ₄ -H ₃ -O ₅): 167.6
	R(O ₅ -H ₅): 1.022	A(H ₄ -O ₅ -H ₅): 108.5	A(O ₅ -H ₄ -O ₆): 163.5
	R(O ₆ -H ₁): 0.980	A(H ₄ -O ₆ -H ₆): 124.0	A(O ₅ -H ₅ -O ₇): 163.5
	R(O ₆ -H ₄): 1.554	A(H ₅ -O ₇ -H ₇): 124.0	
	R(O ₆ -H ₆): 0.962		
	R(O ₇ -H ₂): 0.980		
	R(O ₇ -H ₅): 1.554		
	R(O ₇ -H ₇): 0.962		