

Supporting Information

**Theoretical Study of Oxidation Reactions of Sulfurous Acid/Sulfite with Ozone**

**to Produce Sulfuric Acid/Sulfate with Atmospheric Implications**

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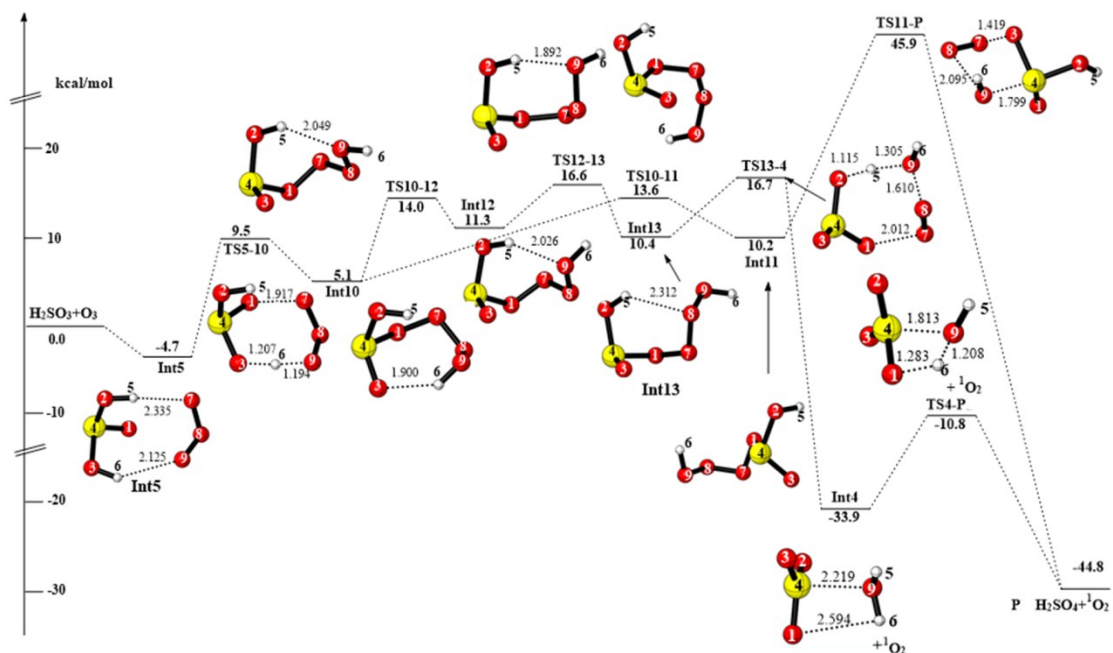
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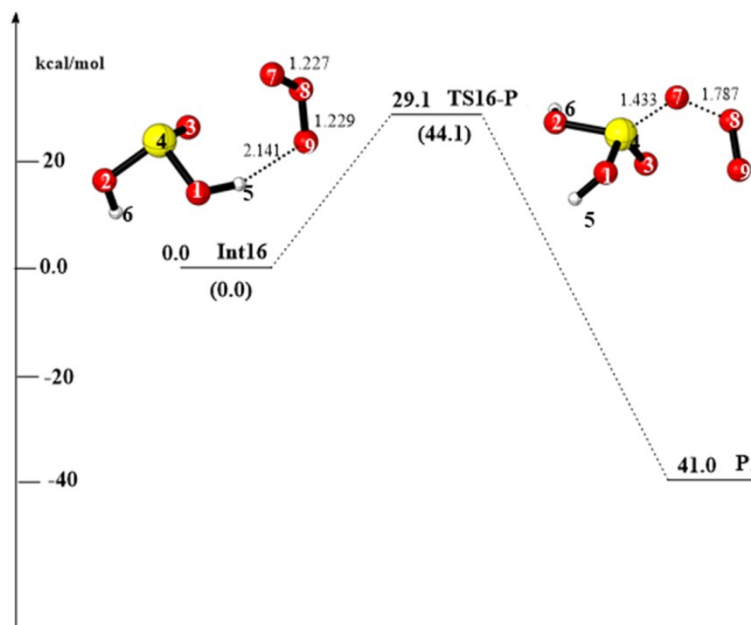
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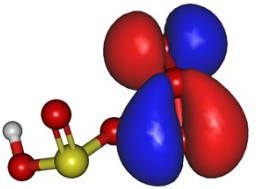
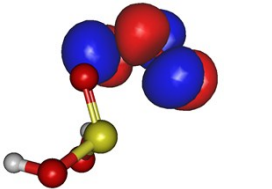
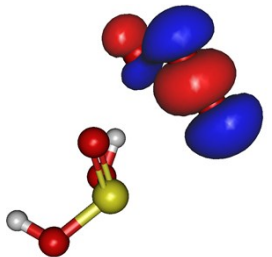
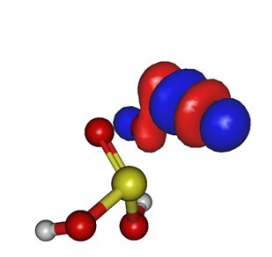
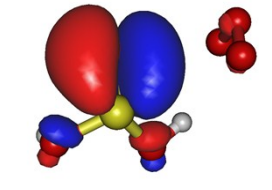
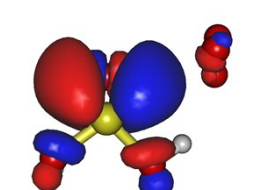
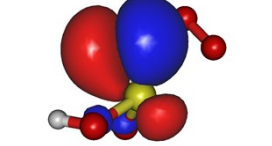
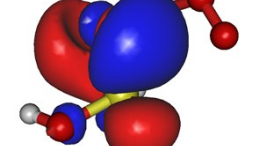
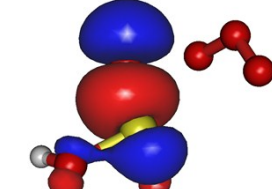
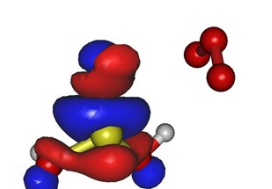
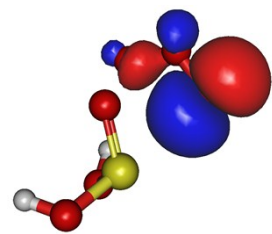
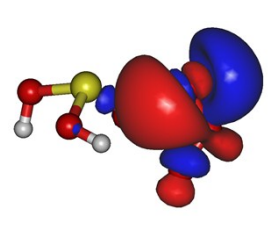


**Fig. S1** CCSD(T)/aug-cc-pVTZ // M06-2X /6-311++G(3df,3pd) energy profile and the optimized geometries of the stationary points for the reaction of  $\text{H}_2\text{SO}_3 + \text{O}_3$  (distances are in angstroms)

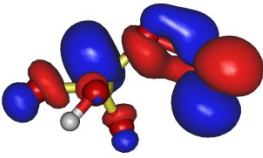
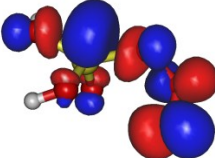
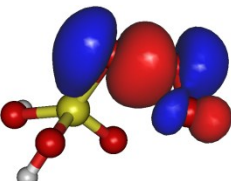
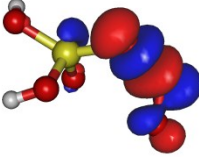
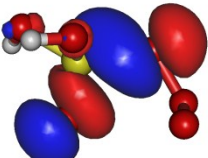
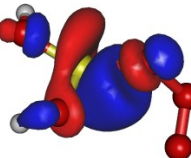
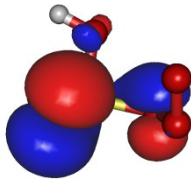
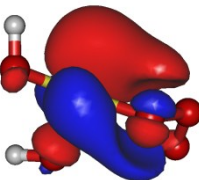
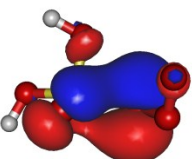
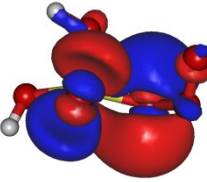
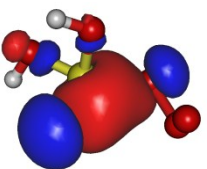
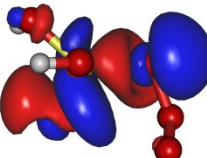


**Figure S2** CCSD(T)/aug-cc-pVTZ // M06-2X /6-311++G(3df,3pd) + ZPE energy profile and the optimized geometries of the stationary points for the reaction of H<sub>2</sub>SO<sub>3</sub> + O<sub>3</sub>. The data in brackets are calculated at CASPT2//CASSCF/ aug-cc-pVTZ level of theory. (distances are in angstroms).

**Table S1** Molecular orbitals and occupation numbers of Int16 from the CASSCF calculations

Orbital NO.	CAS(12e,12o)	Occ.	Orbital NO.	CAS(12 e,12o)	Occ.
HOMO		1.78	LOMO	0.22	
HOMO-1		1.97	LOMO -1	0.33	
HOMO-2		1.97	LOMO -2	0.029	
HOMO-3		1.97	LOMO-3	0.025	
HOMO-4		1.97	LOMO-4	0.024	
HOMO-5		1.98	LOMO-5	0.015	

**Table S2** Molecular orbitals and occupation numbers of TS16-P from the CASSCF calculations.

Orbital NO.	CAS(12e,12o)	Occ.	Orbital NO.	CAS(12 e,12o)	Occ.
HOMO		1.37	LOMO	0.63	
HOMO-1		1.94	LOMO -1	0.065	
HOMO-2		1.96	LOMO -2	0.039	
HOMO-3		1.97	LOMO-3	0.026	
HOMO-4		1.98	LOMO-4	0.017	
HOMO-5		1.98	LOMO-5	0.013	

## Rate Constant Calculations

For reaction (R1), there are two successive unimolecular reaction steps from Int1, and the total unimolecular rate constants can be calculated according to canonical unified statistical theory as expressed by eq 1:

$$\frac{1}{k_{uni}} = \frac{1}{k_{1-2}} + \frac{1}{k_{2-P}} \quad (1)$$

When applying the steady-state approximation for Int1, and assuming that Int1 is in equilibrium with the initial reactants, the total rate constants can be obtained from

$$k = \frac{k_1 k_{uni}}{k_{-1} + k_{uni}} \quad (2)$$

When  $k_{uni} \ll k_{-1}$ , the total rate constants can be obtained from eq 3:

$$k = K_{eq} k_{uni} \quad (3)$$

where  $K_{eq}$  is the equilibrium constant for the formation of Int1 and was calculated using the MultiWell software.<sup>1</sup>  $k_{uni}$  were carried out in terms of the transition state theory (TST) with Wigner Tunneling corrections and KiSTheP software<sup>2</sup> was used. With regard to reaction (2), the total rate constants were obtained according to the following eq 4.

$$\frac{1}{k} = \frac{1}{k_{R-14}} + \frac{1}{k_{14-P}} \quad (4)$$

For the  $\text{HSO}_3^- + \text{O}_3$  reaction, the energy barrier of TS1-P is merely 0.3 kcal/mol, which indicates that  $k_{-1}'$  is not much greater than  $k_{uni}'$ . Accordingly, the overall rate constants are evaluated according to eq 5, where  $k_1'$  is calculated by hard-sphere collision theory<sup>3</sup> accompanied by obtaining  $k_{-1}$  based on the data of  $K_{eq}'$  and  $k_{-1}'$ .

$$k' = \frac{k_1' k_{uni}'}{k_{-1}' + k_{uni}'} \quad (5)$$

1 (a) J. R. Barker, T. L. Nguyen, J. F. Stanton, C. Aieta, M. Ceotto, F. Gabas, T. J. D. Kumar, C. G. L. Li, L. L. Lohr, A. Maranzana, N. F. Ortiz, J. M. Preses, J. M. Simmie, J. A. Sonk, and P. J. Stimac; MultiWell-2017 Software Suite; J. R. Barker, University of Michigan, Ann Arbor, Michigan, USA, 2016; <http://clasp-research.engin.umich.edu/>

[multiwell/](#). (b) John R. Barker, *Int. J. Chem. Kinetics*, 33, 232-45 (2001). (c) John R. Barker, *Int. J. Chem. Kinetics*, 41, 748-763 (2009).".

2 S. Canneaux, F. Bohr and E. Henon, *Journal of Computational Chemistry*, 2014, **35**, 82-93.

3 W. H. Miller, *Journal of Chemical Physics*, 1976, **65**, 2216-2223.

**Table S3** The electronic energies, ZPE, and T1 diagnostic values of the stationary points in H<sub>2</sub>SO<sub>3</sub>+O<sub>3</sub> reaction (Energy unit: Hartree)

Species	E <sub>elect</sub> , M062x	ZPE	E <sub>elect</sub> , CCSD(T)	T1 diagnostic value
H <sub>2</sub> SO <sub>3</sub>	-625.05417	0.03359	-624.33004	0.017
O <sub>3</sub>	-225.39663	0.008152	-225.14923	0.024
<sup>1</sup> O <sub>2</sub>	-700.28673	0.040145	-699.46154	0.015
H <sub>2</sub> SO <sub>4</sub>	-150.25992	0.004046	-150.09154	0.015
Int1	-850.45857	0.043578	-849.48564	0.021
Int2	-850.54957	0.04819	-849.54909	0.017
Int3	-850.54306	0.04805	-849.54288	0.017
Int4	-700.26348	0.03869	-699.44279	0.016
Int5	-850.46197	0.04367	-849.48864	0.020
Int6	-850.51798	0.04660	-849.5216	0.017
Int7	-850.52193	0.04686	-849.52432	0.017
Int8	-850.54428	0.04777	-849.54387	0.017
Int9	-850.54957	0.04819	-849.54909	0.016
Int10	-850.46264	0.04567	-849.47506	0.02
Int11	-850.45279	0.04505	-849.46633	0.019
Int12	-850.45244	0.04546	-849.46499	0.019
Int13	-850.45392	0.04495	-849.46594	0.02
Int14	-850.47947	0.04812	-849.48593	0.016
Int15	-850.40811	0.04587	-849.42550	0.035
Int16	-850.4605	0.04378	-849.42059	0.021
TS1-2	-850.43147	0.04156	-849.45461	0.033
TS2-P	-850.51799	0.04320	-849.52480	0.024
TS2-3	-850.53635	0.04762	-849.53549	0.017
TS3-4	-850.49779	0.04314	-849.50513	0.024
TS4-P	-700.22609	0.03572	-699.40301	0.016
TS5-6	-850.41636	0.03626	-849.44766	0.019
TS6-7	-850.5179	0.04641	-849.52163	0.017
TS7-8	-850.47437	0.04309	-849.47919	0.017
TS7-9	-850.48522	0.04350	-849.48719	0.018
TS7-P	-850.4983	0.04442	-849.50664	0.025
TS8-4	-850.50592	0.04533	-849.51464	0.024
TS8-9	-850.52944	0.04763	-849.52938	0.018
TS9-P	-850.51799	0.04320	-849.52480	0.024
TSR-14	-850.42816	0.04418	-849.45136	0.026
TSR-15	-850.3921	0.04394	-849.42069	0.035



TS15-P	-850.37447	0.04231	-849.39650	0.02
TS14-P	-850.44297	0.04470	-849.45588	0.034
TS14-2	-850.46451	0.04429	-849.47038	0.019
TS5-10	-850.43709	0.04005	-849.46244	0.033
TS10-12	-850.44704	0.04422	-849.45937	0.019
TS12-13	-850.4421	0.04416	-849.45516	0.020
TS10-11	-850.44766	0.044705		0.01891727
TS13-4	-850.40043	0.039992	-849.45088	0.041
TS11-P	-850.35849	0.042508	-849.4069	0.029
TS16-P	-850.39444	0.042045	-849.43925	0.068

**Table S4** The electronic energies, ZPE, and T1 diagnostic values of the stationary points in  $\text{HSO}_3^- + \text{O}_3$  reaction (Energy unit: Hartree)

Species	$E_{\text{elects, M062x}}$	ZPE	$E_{\text{elects, CCSD(T)}}$	T1 diagnostic value
$\text{HSO}_3^-$	-624.52347	0.02158	-623.79903	0.020
$\text{HSO}_4^-$	-699.78183	0.02786	-698.95511	0.016
Int1'	-849.93528	0.03156	-848.95745	0.022
Int2'	-850.06497	0.03648	-849.06245	0.017
Int3'	-849.93339	0.03155	-848.95907	0.028
Int4'	-849.95975	0.03325	-848.97160	0.021
Int5'	-849.94915	0.03305	-848.96074	0.021
Int6'	-849.89721	0.03232	-848.91309	0.026
TS1-2'	-849.93289	0.03103	-848.95694	0.022
TS2-P'	-850.03449	0.03275	-849.03973	0.024
TS1-P'	-849.93416	0.03124	-848.95666	0.025
TS3-4'	-849.93165	0.03071	-848.95920	0.035
TS4-5'	-849.94658	0.03271	-848.95767	0.021
TS5-2'	-849.87216	0.03090	-848.91387	0.031
TSR-6'	-849.89376	0.02983	-848.91156	0.028
TS6-P'	-849.86390	0.03105	-848.89663	0.031

**Table S5** The Cartesian coordinates of all species for the  $\text{H}_2\text{SO}_3/\text{HOSO}_2^- + \text{O}_3$  reaction. The Cartesian coordinates are obtained at the M06-2X /6-311++G(3df,3pd) level of theory.

$\text{H}_2\text{SO}_3$				
S	-0.00001700	0.11143200	-0.43456400	
O	0.00094900	1.35290300	0.31108300	
O	1.23375100	-0.73921700	0.15059400	
H	1.46689900	-0.39570600	1.02675500	

H	-1.46633200	-0.39528100	1.02766100
O	-1.23473600	-0.73767600	0.15065000
O <sub>3</sub>			
O	1.05461800	-0.20990200	0.00000000
O	0.00000000	0.41968000	0.00000000
O	-1.05461800	-0.20977800	0.00000000
<sup>1</sup> O <sub>2</sub>			
O	0.00000000	0.00000000	0.59284400
O	0.00000000	0.00000000	-0.59284400
H <sub>2</sub> SO <sub>4</sub>			
S	0.00011600	0.09103200	0.12032300
O	0.00187100	1.49456500	0.19786600
O	0.00003800	-0.76026400	1.25899200
H	-1.55790300	-1.17523100	-0.51459600
H	1.55586100	-1.17755000	-0.51523800
O	1.22291500	-0.31245100	-0.78517600
O	-1.22480000	-0.30981600	-0.78359900
Int1			
S	-1.26163700	0.11324000	-0.37004300
O	-2.60205800	-0.19713800	0.04177600
O	-0.72600400	1.05951000	0.82761700
H	0.19242600	1.30896900	0.64619200
H	-0.64442100	-1.58760400	0.77550600
O	-0.34947700	-1.18907400	-0.05890500
O	1.74176600	0.66609100	-0.88887300
O	2.33727600	-0.22878600	-0.28527200
O	2.17827100	-0.30225200	0.92603000
Int2			
S	-0.71328800	-0.17682100	0.01326600
O	-1.72114800	-0.41910900	0.96918600
O	-0.15320200	-1.17790600	-0.81378600
H	1.96245900	-0.97438700	-0.56818500
H	-1.70880900	1.61014800	-0.48079500
O	-1.14948600	0.97534100	-0.95003300
O	0.46514100	0.50926600	0.85954500
O	1.56859500	0.74576000	-0.01537800
O	2.38497100	-0.35918100	0.05505600
Int3			

S	-0.81170400	-0.04065600	-0.00250200
O	-1.12852100	-0.34363600	1.34108100
O	-1.71584800	-0.20749500	-1.06563500
H	2.02604500	1.12353000	-0.18835100
H	-0.37307700	1.82801400	0.84663700
O	-0.21638300	1.42997400	-0.02092700
O	0.48828200	-0.84428700	-0.48131500
O	1.55855000	-0.56835300	0.41831800
O	2.43070600	0.24616600	-0.26880500
Int4			
S	0.40805800	-0.00010300	-0.03598900
O	0.37321800	1.22441000	-0.74908400
O	0.75782600	-0.00397400	1.33197000
H	-2.11921900	-0.77271500	-0.18076900
H	-2.12201300	0.77565200	-0.17578300
O	-1.78697000	0.00058100	0.28857800
O	0.36996300	-1.22117900	-0.75491600
Int5			
S	1.47768100	0.22536300	0.25864300
O	0.39726800	0.19811100	1.22822300
O	1.54406600	-1.24956200	-0.37056000
H	0.65375900	-1.63436000	-0.39051600
H	-0.06820800	1.03675400	-0.95899700
O	0.90380000	1.04850000	-0.99230600
O	-2.00153100	0.94676500	-0.08112500
O	-2.25256800	-0.21614900	0.21655000
O	-1.61959200	-1.10369000	-0.34938000
Int6			
S	-1.09806600	-0.12688100	-0.02752800
O	-1.07405500	-0.85179400	1.18005800
O	-1.70104200	1.15016200	-0.09302500
H	0.98849000	1.61588800	-0.59986900
H	1.65751600	-1.11835600	-0.83467400
O	-0.62402000	-0.72246000	-1.22505800
O	1.92972200	-0.93110400	0.07631400
O	2.26747400	0.40834100	0.05672000
O	1.06730200	1.13842500	0.23936400
Int7			
S	-1.02929300	0.16158100	0.07096800
O	-1.77809200	-0.14286900	-1.08767000

O	-1.20592000	-0.59995600	1.24908900
H	0.81684700	-1.86007300	-0.55403200
H	1.87359900	1.27946000	0.01007200
O	-0.30249000	1.37996900	0.13551200
O	2.45818500	0.52090600	-0.15844300
O	1.75183100	-0.51676900	0.39114000
O	0.79876600	-0.89186600	-0.60356900
Int8			
S	0.82280900	-0.04282100	-0.00769300
O	1.71964700	0.31534900	1.02217800
O	1.09271800	-1.01994500	-0.98065300
H	-2.95969000	0.27397300	0.67963400
H	0.17686800	1.95750300	-0.17401400
O	0.32971300	1.22183800	-0.78316700
O	-2.36032500	0.43663800	-0.06270000
O	-1.57283200	-0.70090700	-0.07061400
O	-0.50668500	-0.44626600	0.82713900
Int9			
S	-0.71328800	-0.17682100	0.01326600
O	-1.72114800	-0.41910900	0.96918600
O	-0.15320200	-1.17790600	-0.81378600
H	1.96245900	-0.97438700	-0.56818500
H	-1.70880900	1.61014800	-0.48079500
O	-1.14948600	0.97534100	-0.95003300
O	0.46514100	0.50926600	0.85954500
O	1.56859500	0.74576000	-0.01537800
O	2.38497100	-0.35918100	0.05505600
Int10			
H	-0.87166400	1.51370800	-0.22016300
S	1.29176500	-0.10755400	-0.21924500
O	0.92827200	1.19353100	-0.73754200
O	1.07980600	-0.09143300	1.34926000
H	0.20118400	0.26541400	1.57781300
O	0.04697200	-1.15229700	-0.62119900
O	-1.10174800	-1.04557000	0.19597500
O	-1.90376200	-0.04359200	-0.29067200
O	-1.54925900	1.13207900	0.37296300
Int11			
H	-1.82470400	-1.41574400	-0.71878600
S	0.99203000	-0.08779700	-0.43353400

O	1.53781800	1.23334500	-0.49515600
O	1.99313200	-1.03148400	0.37024300
H	2.37840800	-0.55152900	1.12140800
O	-0.07140900	-0.08224000	0.89289800
O	-1.12330500	0.79844400	0.57276800
O	-2.23894100	0.02700600	0.37839400
O	-2.15056800	-0.52356600	-0.90240700

Int12

H	2.43432800	-1.23693200	0.54818300
S	-1.35181300	0.13514300	-0.04674000
O	-1.14802700	-0.80657800	-1.10810400
O	-0.85414200	-0.52529900	1.30661700
H	-0.03655300	-1.02690900	1.12637400
O	-0.13457500	1.31268400	-0.19372300
O	1.10589300	1.00060200	0.37112500
O	1.79093800	0.16926300	-0.49117900
O	1.64381700	-1.13797700	-0.00057600

Int13

H	3.20494100	0.04197200	0.01090700
S	-1.38914600	0.01212000	-0.30120800
O	-1.52772000	-0.69692800	0.93891600
O	-0.93392800	1.50472600	0.02594200
H	-0.26369100	1.50955900	0.72858600
O	0.05546400	-0.53510500	-0.99025600
O	0.92372100	-1.06979200	-0.03623400
O	1.46779000	-0.02195900	0.68563500
O	2.42531000	0.60087600	-0.11402400

Int14

S	0.34379900	-0.10323700	-0.08031400
O	0.92440300	-0.93869700	-1.07870100
O	0.46154300	-0.55016600	1.42200400
H	-0.28065400	-1.13799400	1.62417000
H	2.24490800	0.71697800	-0.43872700
O	1.49341200	1.00097500	0.09414500
O	-1.25066600	-0.82848100	-0.20224500
O	-1.87986400	0.42164400	-0.02563100
O	-0.68195800	1.15382500	-0.19712500

Int15

S	-0.60234800	-0.16300000	-0.46060000
O	0.19556700	1.11975900	0.25145800

O	-0.84694700	-1.20219100	0.71485100
H	-1.63928900	-0.93036200	1.20008200
H	-2.27093300	1.29180000	-0.59894100
O	-2.01883300	0.63567700	0.05864500
O	1.59309900	0.98117500	0.16043600
O	1.78446400	-0.37711900	0.34408700
O	0.98612400	-0.87648000	-0.68341900
Int16			
H	-2.67441500	0.42365400	0.93707000
S	-1.09409600	-0.29905400	-0.30001300
O	-2.62046500	-0.08217000	0.11069900
O	-0.74339700	1.28645600	-0.36056700
H	0.19458600	1.38537700	-0.13444500
O	-0.36791900	-0.79937300	0.84719200
O	1.85957500	-0.44648000	-0.98787700
O	2.36133900	-0.28414000	0.11997400
O	2.00903700	0.69768600	0.77027700
TS1-2			
S	-0.87522200	-0.01963600	-0.19268700
O	-2.27162600	0.08019800	-0.46605100
O	-0.25850400	1.32662700	0.17565800
H	0.81244400	1.20489000	0.28668200
H	-1.12093300	-1.61387200	1.20833000
O	-0.65052000	-0.76863200	1.20852500
O	1.06503100	-0.62545000	-1.04466100
O	1.82498900	-0.57679600	-0.04887300
O	2.07963600	0.65444700	0.37390000
TS2-P			
S	0.68805100	-0.10368000	-0.06847900
O	1.88480600	-0.58965100	-0.63955100
O	-0.08269600	-1.06624600	0.74327400
H	-1.32649400	-0.92119000	0.59902700
H	1.75258100	1.55856200	0.65975100
O	1.03014800	1.00766200	0.98972700
O	-0.21801900	0.52917700	-1.06659900
O	-1.80733200	0.70131400	-0.09751800
O	-2.23627000	-0.45456700	0.05027600
TS2-3			
S	-0.79833400	0.05600600	-0.06921400
O	-1.79588400	-0.93366500	0.07022300

O	-1.01626900	1.27995400	-0.72723900
H	1.89719700	0.99736000	0.61711800
H	-0.22438500	-0.37194700	1.91982600
O	-0.19488800	0.40510400	1.34259600
O	0.47560400	-0.66616800	-0.79204900
O	1.62545100	-0.73932600	0.01791100
O	2.29355300	0.46391300	-0.09013400

TS3-4

S	-0.81335000	-0.13364700	-0.01621900
O	-1.00010500	-0.46440500	1.34946400
O	-1.90608200	0.25615400	-0.81996200
H	1.33079400	1.09675300	0.01795800
H	-0.09701700	1.76144700	0.96860500
O	0.13841500	1.35307200	0.12403300
O	0.18887300	-0.94011100	-0.74420500
O	1.80285800	-0.66913700	0.24024200
O	2.24851800	0.37444500	-0.24045300

TS4-P

S	-0.26881700	-0.00079900	0.06361500
O	-0.66250100	1.35536700	0.14568800
O	-1.05865300	-0.94778200	-0.61640300
H	1.48670000	-0.31429900	0.36323600
H	1.59214900	0.94369400	-0.98451400
O	1.33322500	0.03379900	-0.78372800
O	0.54070800	-0.51846100	1.20487300

TS5-6

S	-1.34484600	-0.00101300	-0.23183100
O	-1.82741500	0.00116600	1.11694200
O	-0.51422300	1.21598400	-0.59089900
H	0.52001000	1.27499000	-0.09967900
H	0.52416900	-1.27421100	-0.09724400
O	-0.51277200	-1.21773500	-0.58744000
O	1.65888100	-1.08268500	0.37053400
O	2.09957500	0.00178300	-0.19312600
O	1.65512300	1.08341500	0.37226600

TS6-7

S	1.06646500	-0.13738600	0.03637000
O	1.05855600	-0.86185400	-1.17151700
O	1.71934400	1.11365000	0.12657300
H	-0.86524500	1.70916700	0.44148400

H	-1.57321400	-1.14939300	0.73402100
O	0.55344700	-0.72928100	1.22094800
O	-1.97341700	-0.89158900	-0.11101600
O	-2.20230000	0.45802100	0.03105000
O	-0.98375300	1.11585400	-0.31571500

TS7-8

S	-0.87983700	-0.06824200	-0.09110800
O	-1.56673600	-0.62881400	1.01087900
O	-1.31154900	1.13727100	-0.68493600
H	1.42535800	-0.51700800	0.90302200
H	1.46690700	-0.96417800	-0.68155700
O	-0.14940200	-0.98896600	-0.94148700
O	2.14128600	-0.54048700	-0.04872000
O	1.63806900	0.80359200	-0.07709900
O	0.64647200	0.53903500	0.89589600

TS7-9

S	-0.84997400	0.16924000	0.06212900
O	-1.58229300	0.61941900	-1.05238400
O	-0.24379400	1.08284000	0.95869000
H	1.83556900	1.21936300	0.32923500
H	-0.17504800	-1.52042600	0.03362000
O	-1.25036200	-1.14761000	0.62783300
O	0.56271300	-0.81102400	-0.63039400
O	1.72545400	-0.61530100	0.16856800
O	2.28066400	0.57082700	-0.24192700

TS7-P

S	-0.83556400	0.09830400	0.08120800
O	-1.85522600	0.27256000	-0.88038800
O	-1.06503800	-0.70471700	1.22751300
H	0.14878700	-1.80524300	-0.61099500
H	1.35207800	1.11939800	0.23059100
O	0.01031400	1.27802800	0.29544200
O	2.21236800	0.53611000	-0.11764000
O	1.83857400	-0.61771800	0.17278400
O	0.34252800	-0.87514000	-0.81257700

TS8-4

S	-0.88021400	0.12271800	0.07113400
O	-1.78789300	0.11678300	-1.01014700
O	-1.13714400	-0.61178000	1.25123800
H	2.57106200	0.62755200	-0.82748100



H	1.39781900	1.07750500	0.20593200
O	-0.06568500	1.32070300	0.22751000
O	2.28554800	0.55953700	0.09577800
O	1.46906400	-0.96032900	0.08544600
O	0.50042600	-0.88348100	-0.71440000

TS8-9

S	-0.72851900	-0.02624900	-0.13137900
O	-1.92918700	0.68326000	0.09396000
O	-0.48774700	-0.80593200	-1.27383000
H	1.95764400	-0.94830900	0.75775000
H	-0.87176000	-0.57258300	1.89643400
O	-0.43527300	-0.94844700	1.11917600
O	2.01250900	-0.56822500	-0.13209000
O	1.79021000	0.76748000	0.06823300
O	0.37078900	1.11447500	0.05553600

TS9-P

S	0.68806100	-0.10371100	0.06842200
O	1.88470900	-0.59017700	0.63935500
O	-0.08261300	-1.06586700	-0.74382100
H	-1.32676500	-0.92119700	-0.59921600
H	1.75281000	1.55877500	-0.65895800
O	1.03031100	1.00820600	-0.98909200
O	-2.23642300	-0.45450100	-0.05020400
O	-1.80715200	0.70118400	0.09740600
O	-0.21820900	0.52887800	1.06678400

TSR-14

S	0.53963900	-0.08140300	-0.11478600
O	1.28270500	-0.98140200	-0.93962200
O	0.58059700	-0.48279400	1.42848300
H	-0.09920200	-1.15675800	1.58279300
H	2.35172300	0.99345900	-0.19880900
O	1.43791000	1.21883900	0.03468100
O	-1.50480400	-0.91242800	-0.34183000
O	-1.90591000	0.19391000	0.21847000
O	-1.25134100	1.14709200	-0.34360700

TSR-15

S	-0.66958200	-0.08772800	-0.42729100
O	0.03771000	1.14553000	0.20166500
O	-0.73645500	-1.21254700	0.69302100
H	-1.45510500	-0.99479400	1.30485700

H	-2.48144500	1.15436500	-0.51312600
O	-2.20039300	0.42438200	0.05016800
O	1.72243000	0.93862000	0.24993700
O	1.82474500	-0.32739400	0.32462000
O	1.18319700	-0.81308200	-0.76379500

TS15-P

S	-0.62627600	0.09120500	-0.33786200
O	0.05603100	-0.57338500	0.88593700
O	-1.99868400	-0.66009500	-0.46144500
H	-2.40642100	-0.82770200	0.40455800
H	-0.44761100	2.00087200	0.52872800
O	-1.19439800	1.40166700	0.36655200
O	0.89814600	-1.52153200	0.23256600
O	2.16398400	0.01164500	-0.48464000
O	1.68422900	1.01264500	0.02009400

TS14-P

S	0.39086400	0.11225400	0.05562200
O	0.68008500	1.39310400	0.57760000
O	0.25637400	-0.04488600	-1.48997400
H	1.00922100	-0.55968100	-1.81925500
H	2.37535000	-0.15644200	0.72041400
O	1.78064900	-0.67807000	0.16561500
O	-1.62219700	0.70569600	-0.10938600
O	-1.87081600	-0.55313200	0.09200400
O	-0.42889600	-0.95770600	0.79025100

TS14-2

S	0.45779500	-0.09943300	-0.06024800
O	0.82417000	-0.85690300	-1.19294200
O	0.21399600	-0.75919000	1.29006500
H	-0.78489300	-1.01647500	1.08950300
H	2.38785900	0.64045600	-0.36183000
O	1.71664000	0.75058700	0.32519300
O	-1.57786200	-0.71538800	-0.16375400
O	-1.81510500	0.65475000	-0.03822800
O	-0.47779900	1.17201200	-0.19079700

TS5-10

H	-0.68736700	1.23190100	0.00381400
S	1.28015700	0.07523400	-0.37721700
O	0.46204500	1.34465400	-0.34847100
O	1.63480200	-0.19868300	1.15904300

H	0.82774600	-0.34109800	1.67762000
O	0.37259900	-1.06091400	-0.74782800
O	-1.22845200	-1.08414000	0.30629400
O	-2.00884500	-0.25132900	-0.15486600
O	-1.81001100	0.98859400	0.33008200

TS10-12

H	-2.27066100	1.69367800	-0.17964100
S	1.34385600	-0.16198200	-0.09853400
O	1.18099600	0.94917100	-0.98837000
O	0.91635300	0.28244300	1.36275700
H	0.10622800	0.82284100	1.32516100
O	0.06025500	-1.23969600	-0.39799000
O	-1.13622400	-1.00523100	0.30547400
O	-1.88870700	-0.12667900	-0.39087300
O	-1.54982900	1.14939000	0.16287900

TS12-13

H	2.65875300	0.92718400	-0.33037100
S	-1.32121400	-0.10802300	-0.10765000
O	-1.21045700	-0.04965000	1.32157000
O	-0.84703900	1.28220000	-0.71648700
H	0.00844800	1.57467500	-0.35445100
O	-0.15374500	-1.11534400	-0.71365200
O	1.24017500	-1.08952700	-0.30714200
O	1.49905400	-0.18053300	0.66174100
O	1.78104000	1.05616800	0.05487300

TS10-11

H	-1.98311300	0.83957000	-1.19252600
S	1.09716600	0.36389500	-0.38383800
O	0.78342500	1.17268900	0.75511800
O	2.34574200	-0.55808700	-0.02162400
H	2.30285100	-0.84613700	0.90463100
O	-0.05044400	-0.90004800	-0.41245100
O	-0.96817900	-0.80711800	0.64411000
O	-2.18052500	-0.49486900	0.08101100
O	-2.16431800	0.86046300	-0.24250200

TS13-4

H	2.13052600	1.63529400	0.61651100
S	-1.23846400	-0.00842400	-0.19467600
O	-1.76680200	-0.13328000	1.12978200
O	-0.58170000	1.34355800	-0.45380800

H	0.52524400	1.30914400	-0.32323500
O	-0.42442600	-1.07235500	-0.78638300
O	1.48160200	-1.23346000	-0.13435700
O	1.64872600	-0.32825300	0.68954700
O	1.78755800	1.07258400	-0.09208900
TS11-P			
H	-0.92708800	1.05123600	-1.41770200
S	0.74121400	0.25085300	-0.14672900
O	0.95665800	0.65779500	1.20257100
O	2.08349400	-0.61310600	-0.49566100
H	2.63263400	-0.71144200	0.29791400
O	-0.32679400	-1.08862000	-0.22861700
O	-1.44926100	-0.73626200	0.56242400
O	-2.26830500	-0.04058300	-0.10016500
O	-0.69141400	1.27659400	-0.50712100
TS16-P			
S	-0.95430700	0.00000000	-0.28104400
O	-2.39429300	-0.00005500	-0.46103700
O	-0.63875700	1.23877400	0.66245700
H	-1.46575500	1.53799600	1.07041900
H	-1.46570600	-1.53812800	1.07032900
O	-0.63868400	-1.23876500	0.66246200
O	1.04349500	0.00006600	-0.86058700
O	1.85619100	0.00008900	0.32839100
O	3.04709600	-0.00009300	-0.03719200
HSO <sub>3</sub> <sup>-</sup>			
S	-0.17756600	0.03959900	-0.37844700
O	-0.04678400	1.37215800	0.25545200
O	1.33951900	-0.62505000	0.06826800
H	1.59376100	-0.06984600	0.81608300
O	-1.13682200	-0.81757600	0.33116400
HSO <sub>4</sub> <sup>-</sup>			
S	0.14184500	0.03027000	-0.00560800
O	0.90207800	-1.19098500	-0.06654100
O	0.15954600	0.83554400	-1.20926100
H	-1.95961600	0.24728100	0.04603000
O	0.30191600	0.79992400	1.21025700
O	-1.40227700	-0.53593400	0.07100700

Int1'

S	-0.80413400	-0.15460000	-0.08149800
O	-1.88113600	-1.08472100	-0.46884000
O	-1.63195500	1.31501400	-0.20333200
H	-2.55485700	1.03908600	-0.26379300
O	-0.43621300	-0.23195900	1.33329800
O	2.02557800	-0.98142600	-0.41773000
O	2.08062600	0.05552500	0.26662500
O	1.77072400	1.10688000	-0.31405100
Int2'			
S	0.77900500	0.07450300	-0.05299400
O	1.70339700	0.22459100	1.03343200
O	0.15725000	1.30344100	-0.52259800
H	-1.65337900	1.08701000	-0.27634400
O	1.16452200	-0.82674600	-1.10123800
O	-0.48317200	-0.68810100	0.76213800
O	-1.58656500	-0.74455900	-0.10279800
O	-2.30676900	0.44649200	0.07159400
Int3'			
H	-0.20899000	1.28762400	0.14847200
S	1.48117300	-0.00279800	-0.26861500
O	0.70363900	1.45635800	-0.15352100
O	1.76107100	-0.39539600	1.11617500
O	0.43125200	-0.86651200	-0.88139000
O	-1.48714900	-1.06580600	0.36905200
O	-2.22035100	-0.24504900	-0.16866300
O	-2.12468500	0.96104800	0.23701700
Int4'			
H	-0.89896700	1.30676700	0.08618600
S	1.31797400	0.03303200	-0.29314500
O	0.61693300	1.33232900	-0.46046900
O	1.66290800	-0.21864600	1.09959400
O	0.02183500	-1.11285100	-0.62830300
O	-1.03086700	-1.07402700	0.30549100
O	-1.99308000	-0.20042800	-0.17470100
O	-1.80130700	1.04421200	0.43390600
Int5'			
H	-1.12807200	1.11588300	-0.82019300
S	1.07424500	0.33490700	-0.14953100
O	1.42546900	0.56626700	1.24144600
O	2.07580500	-0.38618600	-0.92243700

O	-0.09711700	-1.06982800	-0.04068700
O	-1.21573500	-0.71165200	0.70883100
O	-2.18851100	-0.29391700	-0.18275500
O	-2.00739300	1.08601600	-0.40281300
Int6'			
S	-0.70788100	-0.30267600	-0.32219900
O	0.13625200	1.06866400	0.32866700
O	-0.99719800	-1.21845900	0.75726600
H	-1.98535000	1.47530500	-0.62588800
O	-2.12026100	0.68711600	-0.09114400
O	1.51030200	1.07781700	0.03447500
O	1.94008900	-0.22438700	0.29504500
O	1.19474600	-0.96981300	-0.60167600
TS1-2'			
S	-1.20713600	-0.25869500	-0.24704100
O	-2.62779300	-0.08647200	0.08032700
O	-0.61174300	1.32255700	-0.41099400
H	-0.37631900	1.57229400	0.49367700
O	-0.43524800	-0.67950100	0.94989900
O	1.93796800	-0.63976000	-0.97163300
O	1.99015500	-0.38215200	0.22892500
O	2.20797100	0.78618000	0.55584900
TS2-P'			
S	-0.74902500	-0.01654700	0.01668000
O	-1.85026300	0.36433300	-0.81323300
O	-0.01232800	1.26901800	0.47710700
H	1.02455000	1.12287700	0.38646900
O	-1.04685300	-0.82539700	1.15854900
O	0.30345500	-0.69711700	-0.88994900
O	1.73264800	-0.70085800	0.01704200
O	2.24332400	0.48275500	-0.03118400
TS1-P'			
S	-0.81083900	-0.09652700	0.01221100
O	-1.87118500	-1.05530500	-0.31852200
O	-1.51379900	1.33968800	-0.49593500
H	-2.37376900	1.06228100	-0.83340600
O	-0.55702300	0.10773200	1.42761300
O	1.36925200	-0.93882200	-0.55888600
O	2.07768400	-0.27573400	0.22418600
O	2.41347000	0.88271000	-0.19870300

## TS3-4'

H	-0.45420100	1.26480500	-0.03959100
S	1.34070700	0.00410200	-0.27969300
O	0.51667000	1.35831200	-0.39633300
O	1.74034500	-0.16026300	1.11574300
O	0.32164800	-1.05853300	-0.68886300
O	-1.27965100	-1.08149600	0.34410700
O	-2.05568900	-0.23114800	-0.14354200
O	-1.86796100	1.00682300	0.33322300

## TS4-5'

H	-1.15002200	1.26375700	-0.50051800
S	1.07036200	0.27389700	-0.29713000
O	0.89335300	1.13402500	0.86886500
O	2.32928200	-0.45421700	-0.34826600
O	0.04429100	-1.17511300	0.13960100
O	-1.18188100	-0.81153900	0.68325000
O	-2.01251000	-0.40190800	-0.35984000
O	-2.06950800	1.00298900	-0.32678500

## TS5-2'

H	-0.90690700	1.00527400	-1.30580700
S	0.96415300	0.18982000	-0.08632000
O	1.15119000	0.43222900	1.32022100
O	2.04942300	-0.51965600	-0.73643200
O	-0.38934900	-1.09143600	-0.19834000
O	-1.48093400	-0.71581800	0.53504500
O	-2.30914300	0.00541600	-0.15897500
O	-0.83612900	1.38396500	-0.42565400

## TSR-6'

S	-0.88640400	-0.34521800	-0.23893100
O	0.03857200	0.30617900	0.92346500
O	-1.92657500	-0.96691000	0.56346600
H	-1.85236700	1.54417600	-0.01227400
O	-1.52999000	1.05975600	-0.78586900
O	1.22671100	0.95403200	0.27530600
O	2.22479600	0.03283900	0.24758700
O	1.97084000	-0.88848300	-0.74455700

## TS6-P'

S	-0.62647500	-0.30003500	-0.24721900
O	0.24522900	1.06997600	0.31551200

O	-0.96117700	-1.11344000	0.89672900
H	-1.97940500	1.43318200	-0.77758700
O	-2.10352000	0.75199000	-0.10871400
O	1.64188200	0.93108800	0.08621700
O	1.97812100	-0.35042900	0.25873300
O	0.69984000	-0.86826300	-0.85684100