Supplementary Information

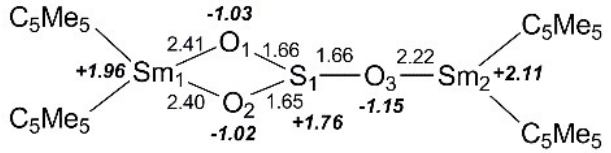
SO_2 and SO_3 reactions with $[(C_5Me_5)_2Sm\text{-}O\text{-}Sm(C_5Me_5)_2]$: A DFT investigation and Comparison with CO_2 reactivity

Elisa Louyriac[a], Peter W. Roesky[b] and Laurent Maron*[a]

[a] *LPCNO, Université de Toulouse, CNRS, INSA, UPS, 135 Avenue de Rangueil, 31077 Toulouse, France. E-mail: laurent.maron@irsamc.ups-tlse.fr*

[b] *Institute of Inorganic Chemistry Karlsruhe Institute of Technology (KIT), Engesserstraße 15, 76131 Karlsruhe, Germany. E-mail: roesky@kit.edu; Fax: +49 721 6084 4854.*

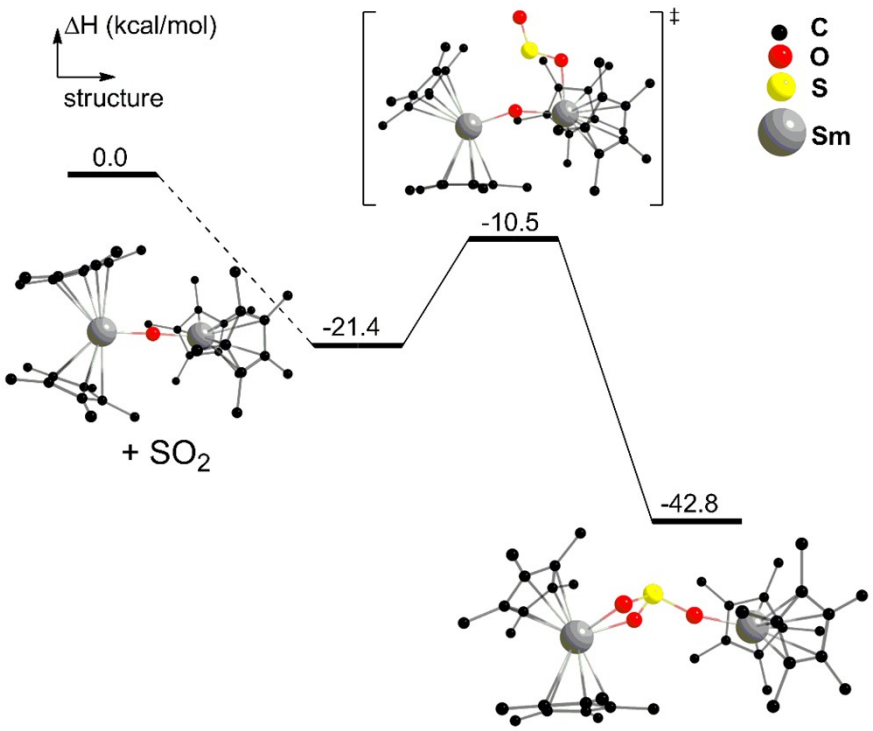
Fig. S1 Computed geometric parameters of the sulfite product obtained for the reaction of SO_2 with



O_1-S_1-O_2 = 99°
O_2-S_1-O_3 = 105°
O_1-S_1-O_3 = 105°
O_1-Sm_1-O_2 = 63°
S_1-O_3-Sm_2 = 150°
S_1-O_1-Sm_1 = 97°
S_1-O_2-Sm_1 = 98°

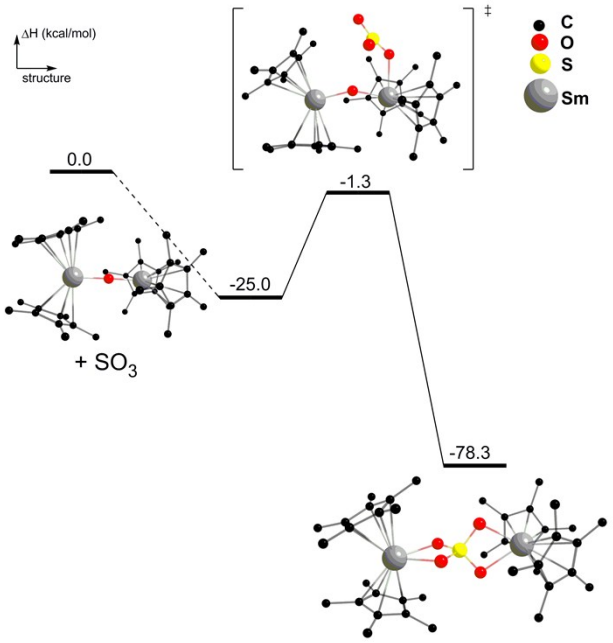
$[Cp^*_2Sm\text{-}O\text{-}SmCp^*_2]$. NPA charges are denoted in italic-bold.

Fig. S2 Computed enthalpy profile for the reaction of SO_2 with [Cp*$_2$Sm-O-SmCp*$_2$]. Hydrogen



atoms are omitted for clarity.

Fig. S3 Computed enthalpy profile for the reaction of SO_3 with [Cp*$_2$Sm-O-SmCp*$_2$]. Hydrogen atoms are omitted for clarity.



Computational details:

Calculations were performed with the Gaussian 09 program[1] at the DFT level of theory using the hybrid functional B3PW91[2,3]. Samarium was treated with a large-core Stuttgart Dresden relativistic effective core potential (RECP), adapted to the +3 oxidation state, used in combination with its optimized basis set augmented by a set of f polarization functions (α=1.000)[4]. Hydrogen, oxygen, carbon and sulfur atoms were described with a 6-31G+(d,p) double – ζ quality basis set. Electronic energies and enthalpies were computed at T = 298 K in the gas phase. Geometry optimizations were performed without any symmetry constraints and analytical frequency calculations allowed to verify the nature of the extrema. Intrinsic Reaction Coordinates (IRC) were carried out to verify the connections of the optimized transition states. Natural Bond Orbital (NBO) analysis[5] was used to analyze electronic density.

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[1] Gaussian 09 Revision **D.01**; Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; others. *Gaussian Inc Wallingford CT* **2009**.

[2] A. D. Becke, *J. Chem. Phys.*, 1993, **98** (7), 5648–5652.

[3] K. Burke, J. P. Perdew, Y. Wang, In *Electronic Density Functional Theory: Recent Progress and New Directions*; Dobson, J. F., Vignale, G., Das, M. P., Eds.; Plenum: New York, 1998.

[4] M. Dolg, H. Stoll, A. Savin, H. Preuss, *Theor. Chim. Acta.*, 1989, **75**, 173.

[5] A. E. Reed, L. A. Curtiss, F. Weinhold, *Chem. Rev.*, 1988, **88** (6), 899–926.

Electronic energies, Enthalpy, Gibbs free energies and optimized geometries:

SO_2
E = -160.457225
H = -160.447531
G = -160.476743

S	-0.061004	0.000000	-0.035190
O	0.013204	0.000000	1.497540
O	1.303538	0.000000	-0.737350

SO_3
E = -235.542261
H = -235.527956
G = -235.559594

S	0.000000	0.000000	-0.000024
O	0.000000	0.000000	1.522960
O	1.318920	0.000000	-0.761468
O	-1.318920	0.000000	-0.761468

Cp^*_2 Sm-O-Sm Cp^*_2 complex
E = -1704.910988
H = -1703.962765
G = -1704.118476

C	1.890814	2.027246	4.742494
C	2.599201	0.961009	5.363227
C	2.075276	0.783854	6.680888
C	1.036028	1.734364	6.870067
C	0.906965	2.491079	5.665187
Sm	0.037078	-0.033857	4.893078
C	-0.830026	-2.570213	5.639391
C	-0.925910	-1.834000	6.859670
C	-1.963080	-0.873848	6.711415
C	-2.518415	-1.024181	5.403202
C	-1.831619	-2.083463	4.747759
C	-0.202631	-2.171460	8.130843
C	-2.556448	-0.019917	7.795079
C	-3.744380	-0.309357	4.909990
C	-2.170294	-2.662470	3.406141
C	0.034935	-3.781840	5.425259
C	0.345145	2.048123	8.165044
C	2.697282	-0.087633	7.734105
C	3.820726	0.265727	4.832153
C	0.025792	3.697125	5.490345
C	2.193762	2.630268	3.402880
O	-0.004352	0.001291	2.763184
Sm	-0.030977	0.005329	0.633033
C	1.902844	-1.987591	0.752560
C	2.554758	-0.899226	0.108880
C	1.994308	-0.751964	-1.197468
C	0.987221	-1.741945	-1.355566
C	0.915551	-2.494493	-0.143466
C	-1.082486	1.765443	-1.321827
C	-2.089334	0.777503	-1.149639
C	-2.623319	0.918693	0.168314
C	-1.955200	2.001025	0.805577
C	-0.984389	2.510561	-0.106765
C	-0.395050	2.119474	-2.608260
C	-2.677141	-0.100792	-2.216708
C	-3.822059	0.176240	0.687074
C	-2.286683	2.574144	2.151349
C	-0.144337	3.743041	0.085751
H	-1.408815	3.013724	2.634487
H	-3.044600	3.366446	2.075621
H	-2.680780	1.812475	2.830939
H	-4.750748	0.573436	0.253475
H	-3.798371	-0.892972	0.443571
H	-3.916586	0.265618	1.772122
H	-1.986802	-0.258499	-3.048775
H	-2.964349	-1.088469	-1.837657
H	-3.587952	0.350208	-2.635807
H	0.624734	2.484824	-2.450407
H	-0.334303	1.266904	-3.291115
H	-0.939253	2.914956	-3.137031
H	0.845294	3.655266	-0.377811
H	-0.623456	4.623945	-0.364307
H	0.009979	3.974745	1.143902
H	-2.643848	-1.923380	2.753158
H	-1.281695	-3.031352	2.884496
H	-2.866097	-3.508292	3.497151
H	-3.853177	-0.390603	3.825651
H	-4.655685	-0.734217	5.354029
H	-3.743652	0.757874	5.162869
H	-2.888197	0.957496	7.426057
H	-3.440350	-0.504691	8.233659
H	-1.853042	0.160482	8.611465
H	-0.149073	-1.317494	8.812623
H	-0.715024	-2.980501	8.670742
H	0.822449	-2.510917	7.950877
H	1.032989	-3.672612	5.865726
H	-0.413131	-4.674310	5.884507
H	0.168905	-4.008544	4.363249
H	-0.685616	2.386304	8.018588
H	0.313083	1.183476	8.834741
H	0.869160	2.850512	8.703726
H	-0.137098	3.936913	4.435308
H	-0.959863	3.570842	5.953501
H	0.476107	4.587683	5.951064
H	3.017243	-1.059404	7.340471
H	3.593579	0.389052	8.156064
H	2.016175	-0.280316	8.566452
H	2.645725	1.901664	2.723359
H	1.291870	3.010899	2.913474
H	2.894831	3.472122	3.489993
H	3.908724	0.369043	3.747789
H	4.736849	0.689680	5.267092
H	3.833791	-0.806117	5.064573
C	2.262937	-2.571160	2.086489
H	1.389888	-2.986233	2.599603
H	2.994866	-3.384752	1.985315
H	2.702808	-1.822085	2.751730
C	0.273657	-2.090493	-2.629242
C	3.760825	-0.154854	0.607328
C	2.559139	0.133825	-2.270800

C	0.085836	-3.732779	0.056749
H	0.198509	-1.234999	-3.306952
H	0.806880	-2.883457	-3.172787
H	-0.742470	-2.457002	-2.451557
H	2.841252	1.124251	-1.894976
H	3.468846	-0.307528	-2.702375
H	1.856335	0.285183	-3.093557
H	3.876792	-0.248253	1.689912
H	4.682424	-0.546369	0.153878
H	3.727974	0.915317	0.369267
H	-0.916689	-3.644268	-0.378232
H	0.556167	-4.605945	-0.417091
H	-0.037812	-3.978044	1.115830

SO_2 insertion - adduct

E = -1865.403137

H = -1864.444365

G = -1864.608411

C	1.268466000	-2.270000000	2.243403000
C	1.199387000	-1.867767000	3.613166000
C	-0.069258000	-2.266712000	4.123786000
C	-0.803491000	-2.868096000	3.061273000
C	0.033181000	-2.882578000	1.902795000
Sm	-0.575603000	-0.194134000	2.224257000
C	-2.935638000	1.193351000	2.686260000
C	-2.004253000	2.201832000	2.307452000
C	-1.039304000	2.312202000	3.347603000
C	-1.405970000	1.410761000	4.395334000
C	-2.581234000	0.723288000	3.988943000
C	-2.071713000	3.036640000	1.061577000
C	0.059282000	3.333626000	3.451578000
C	-0.762333000	1.386101000	5.752066000
C	-3.450670000	-0.161757000	4.835135000
C	-4.195575000	0.822994000	1.953219000
C	2.330609000	-1.301908000	4.427293000
C	-0.458907000	-2.271450000	5.572832000
C	-2.133391000	-3.558619000	3.188937000
C	-0.266061000	-3.567484000	0.600777000
C	2.477131000	-2.216161000	1.356766000
O	-0.180497000	0.272177000	0.174712000
Sm	0.562695000	0.448575000	-1.819929000
C	3.288382000	1.062955000	-1.723345000
C	2.916583000	1.553496000	-3.005828000
C	2.065011000	2.678098000	-2.813891000
C	1.901943000	2.877308000	-1.404758000
C	2.665354000	1.888415000	-0.732363000
C	3.464802000	1.064892000	-4.316058000
C	1.666611000	3.665605000	-3.870214000
C	1.210567000	4.046049000	-0.764723000
C	2.891559000	1.807926000	0.747223000
C	4.311102000	-0.004568000	-1.464167000
C	-1.274872000	0.999059000	-4.091144000
C	-0.632117000	-0.175353000	-4.501696000
C	-1.096343000	-1.240363000	-3.650489000
C	-1.997114000	-0.674895000	-2.664121000
C	-2.117182000	0.687959000	-2.937652000
C	-1.345605000	2.292229000	-4.838103000
C	0.206625000	-0.366988000	-5.730494000
C	-0.946442000	-2.677173000	-3.943028000
C	-2.779469000	-1.460358000	-1.657786000
C	-3.081366000	1.649156000	-2.316221000
S	2.094418000	-2.895287000	-2.881359000
O	1.385749000	-1.687783000	-2.085507000
H	0.211594000	-4.557150000	0.557341000
H	-1.340165000	-3.732814000	0.466764000
H	0.096996000	-2.991771000	-0.256154000
H	2.995334000	-3.185927000	1.338200000
H	3.208118000	-1.478910000	1.703508000
H	2.214479000	-1.969896000	0.323542000
H	1.974500000	-0.647524000	5.230698000
H	2.918742000	-2.097967000	4.905172000
H	3.029124000	-0.718931000	3.817277000
H	-0.004961000	-1.445404000	6.127436000
H	-0.126181000	-3.200226000	6.058262000
H	-1.541522000	-2.211039000	5.714208000
H	-2.008654000	-4.631448000	3.392697000
H	-2.730849000	-3.147507000	4.008367000
H	-2.735075000	-3.481556000	2.275813000
H	0.330435000	1.303093000	5.701725000
H	-1.124597000	0.554252000	6.360552000
H	-0.980261000	2.309800000	6.306186000
H	-2.930831000	-0.513085000	5.729689000
H	-3.808507000	-1.045592000	4.294578000
H	-4.343471000	0.381076000	5.175657000
H	-4.468618000	-0.228372000	2.101409000
H	-4.108490000	0.989969000	0.875455000
H	-5.051839000	1.419019000	2.300762000
H	0.986365000	2.917061000	3.863999000
H	-0.230217000	4.160837000	4.115254000
H	0.303509000	3.772637000	2.480607000
H	-1.630193000	4.025089000	1.224170000
H	-1.543720000	2.569617000	0.221132000
H	-3.110653000	3.198719000	0.754953000
H	-3.391355000	1.322023000	-1.321519000
H	-2.666359000	2.657631000	-2.218345000
H	-3.989726000	1.739585000	-2.929112000
H	-1.358673000	3.162830000	-4.175143000
H	-0.512357000	2.411899000	-5.533142000
H	-2.270749000	2.334010000	-5.430752000
H	1.063300000	-1.021387000	-5.546691000
H	-0.384665000	-0.811236000	-6.543957000
H	0.594478000	0.584476000	-6.103514000
H	0.722597000	4.170063000	-3.641532000
H	2.428321000	4.452716000	-3.966124000
H	1.566378000	3.203333000	-4.856111000
H	0.832041000	3.797915000	0.230529000
H	1.893946000	4.899401000	-0.647582000
H	0.359800000	4.401257000	-1.356324000
H	4.412752000	-0.679178000	-2.319074000
H	5.301646000	0.437212000	-1.285336000
H	4.070809000	-0.613238000	-0.586685000
H	3.109108000	0.785166000	1.069994000
H	3.741806000	2.431728000	1.058022000
H	3.497078000	-0.028167000	-4.371836000
H	2.864168000	1.414032000	-5.161186000
H	4.487563000	1.432996000	-4.478529000
H	-3.729924000	-1.815968000	-2.079733000
H	-2.225404000	-2.334881000	-1.307932000
H	-3.019263000	-0.852440000	-0.781081000
H	-0.007856000	-3.117032000	-3.519611000
H	-1.763207000	-3.272130000	-3.524680000
H	-0.876161000	-2.866976000	-5.019034000
H	2.016390000	2.155584000	1.305484000

O	2.725567000	-2.391089000	-4.220149000

SO_2 insertion - transition state

E = -1865.385756
H = -1864.427048
G = -1864.584730

C	-0.670568	-3.926379	-3.822073
C	-0.736689	-3.192681	-2.594139
C	-1.988864	-3.473022	-1.977530
C	-2.731119	-4.310189	-2.856400
C	-1.905133	-4.609848	-3.986318
Sm	-2.560948	-1.908418	-4.289064
C	-4.988909	-0.624846	-4.226455
C	-4.060556	0.393386	-4.586268
C	-3.279122	0.697755	-3.435032
C	-3.742930	-0.112986	-2.357784
C	-4.797982	-0.931296	-2.844062
C	-3.996360	1.085676	-5.912011
C	-2.337390	1.855878	-3.257148
C	-3.347010	0.098850	-0.925828
C	-5.725508	-1.777769	-2.021233
C	-6.101074	-1.157314	-5.083413
C	0.408257	-2.447609	-1.963906
C	-2.334366	-3.171076	-0.550222
C	-4.027623	-5.005504	-2.548770
C	-2.240596	-5.659928	-5.008521
C	0.583930	-4.118403	-4.624869
O	-2.295531	-1.790456	-6.448526
Sm	-1.939519	-0.671109	-8.335758
C	0.794916	-0.438799	-7.901295
C	0.634413	0.105003	-9.209467
C	-0.050002	1.344607	-9.088544
C	-0.340238	1.558091	-7.707034
C	0.194784	0.455578	-6.973713
C	1.258187	-0.464031	-10.451305
C	-0.190058	2.388086	-10.157365
C	-0.843976	2.855429	-7.137661
C	0.232705	0.305198	-5.481785
C	1.600598	-1.658508	-7.569310
C	-3.551163	0.340140	-10.529331
C	-2.924835	-0.827695	-11.019723
C	-3.527286	-1.951334	-10.360067
C	-4.508819	-1.464623	-9.444295
C	-4.532211	-0.053179	-9.549864
C	-3.464379	1.720054	-11.110006
C	-1.966047	-0.914776	-12.170587
C	-3.362569	-3.387833	-10.718764
C	-5.449066	-2.350141	-8.679090
C	-5.575643	0.875988	-9.002031
S	-1.509830	-3.928116	-7.952747
O	-1.026423	-2.761822	-8.921482
H	-2.419354	-6.625538	-4.516548
H	-3.150025	-5.436045	-5.582263
H	-1.426756	-5.811759	-5.720191
H	1.227311	-4.872917	-4.150421
H	1.181347	-3.202956	-4.690422
H	0.390974	-4.460375	-5.643344
H	0.065315	-1.651788	-1.293927
H	1.041205	-3.116767	-1.363764
H	1.062877	-1.986690	-2.711732
H	-1.878628	-2.243354	-0.195489
H	-1.967169	-3.975502	0.103054
H	-3.412332	-3.098524	-0.383430
H	-3.848277	-6.030814	-2.194236
H	-4.594850	-4.492103	-1.768278
H	-4.677930	-5.090648	-3.427684
H	-2.260250	0.136683	-0.786724
H	-3.735692	-0.682659	-0.269973
H	-3.743145	1.055797	-0.556940
H	-5.258941	-2.120309	-1.093895
H	-6.072418	-2.664800	-2.561022
H	-6.622041	-1.208844	-1.737246
H	-6.342195	-2.201947	-4.855037
H	-5.854127	-1.105931	-6.146142
H	-7.026667	-0.582703	-4.936274
H	-1.397018	1.579000	-2.765534
H	-2.800048	2.631182	-2.630571
H	-2.085317	2.331573	-4.207988
H	-3.000125	1.493727	-6.112346
H	-4.259318	0.399666	-6.725029
H	-4.700581	1.926805	-5.972773
H	-6.125065	0.440012	-8.163795
H	-5.156971	1.828786	-8.660761
H	-6.313855	1.117932	-9.779965
H	-3.479612	2.504163	-10.344780
H	-2.561048	1.859600	-11.706937
H	-4.320626	1.911717	-11.772755
H	-1.210993	-1.693057	-12.022019
H	-2.490856	-1.145084	-13.108071
H	-1.434988	0.028446	-12.324367
H	-1.082049	3.007343	-10.025107
H	0.674070	3.068228	-10.145187
H	-0.234427	1.953777	-11.160338
H	-1.059623	2.775157	-6.068771
H	-0.089200	3.647250	-7.244868
H	-1.752628	3.220804	-7.631465
H	1.589730	-2.386860	-8.384146
H	2.649979	-1.395007	-7.375301
H	1.227038	-2.169243	-6.678210
H	0.353433	-0.748108	-5.200706
H	1.076368	0.848242	-5.033176
H	1.096859	-1.544561	-10.534489
H	0.862175	0.000483	-11.358266
H	2.344907	-0.301890	-10.455713
H	-6.270627	-1.780344	-8.237752
H	-5.901540	-3.098582	-9.342251
H	-4.954845	-2.898314	-7.866959
H	-3.240647	-4.033351	-9.832333
H	-4.256110	-3.767591	-11.233887
H	-2.499129	-3.558784	-11.365869
H	-0.675858	0.688653	-5.003847
O	-0.409330	-5.009401	-7.887765

SO_2 insertion - product

E = -1865.438967
H = -1864.478567
G = -1864.646604

C	1.883594	-1.938840	3.685552
C	1.300070	-1.722960	4.973626
C	0.119341	-2.517697	5.055585
C	-0.028309	-3.213595	3.814735
C	1.074992	-2.874803	2.979040

Sm	-0.430153	-0.588308	3.151701
C	-2.641387	1.004941	2.935539
C	-1.545414	1.907378	3.026857
C	-1.005317	1.812451	4.348017
C	-1.785941	0.867637	5.078288
C	-2.783573	0.349996	4.198556
C	-1.110895	2.866112	1.954311
C	0.077484	2.683241	4.924279
C	-1.718515	0.648939	6.561531
C	-3.916298	-0.562995	4.578334
C	-3.577849	0.873472	1.768319
C	1.935602	-0.945725	6.091831
C	-0.698237	-2.781831	6.287770
C	-1.088466	-4.237229	3.515971
C	1.384829	-3.458032	1.631630
C	3.195762	-1.381201	3.208587
O	-1.137176	0.901586	-0.925181
Sm	0.127691	0.716122	-2.965593
C	2.817697	0.495205	-2.403752
C	2.794720	1.044234	-3.719057
C	2.281019	2.373661	-3.631705
C	1.984208	2.640742	-2.261412
C	2.325579	1.482976	-1.504268
C	3.398580	0.408187	-4.939778
C	2.294597	3.397465	-4.730111
C	1.520728	3.957520	-1.702898
C	2.279369	1.341748	-0.011807
C	3.345396	-0.853758	-2.005551
C	-1.407250	1.709265	-5.062087
C	-0.696787	0.603687	-5.622476
C	-1.186785	-0.587349	-5.010045
C	-2.214551	-0.221187	-4.092872
C	-2.346467	1.195364	-4.119307
C	-1.334831	3.135592	-5.530715
C	0.223476	0.657960	-6.807862
C	-0.787931	-1.995737	-5.350435
C	-3.100048	-1.177016	-3.348797
C	-3.366083	1.993240	-3.357853
S	-1.153796	-0.708582	-0.531963
O	-0.044957	-1.261751	-1.616502
H	2.182372	-4.209265	1.707057
H	0.513143	-3.952378	1.195141
H	1.706314	-2.699941	0.911857
H	4.031389	-2.033382	3.497820
H	3.408211	-0.393730	3.633604
H	3.228130	-1.287620	2.118724
H	1.205926	-0.640422	6.846831
H	2.697353	-1.546931	6.606972
H	2.439166	-0.039536	5.736752
H	-0.521793	-2.033157	7.063450
H	-0.439638	-3.758536	6.719052
H	-1.775681	-2.801725	6.087606
H	-0.780329	-5.237860	3.849006
H	-2.031923	-4.012972	4.025628
H	-1.300642	-4.310899	2.444439
H	-0.695330	0.705555	6.945681
H	-2.132039	-0.318141	6.858105
H	-2.297591	1.420286	7.088151
H	-3.658196	-1.217912	5.416374
H	-4.232241	-1.200873	3.745301
H	-4.800592	0.012537	4.884997
H	-3.925926	-0.155882	1.622516
H	-3.110240	1.203741	0.836762
H	-4.475520	1.488803	1.920127
H	0.628698	2.181340	5.726586
H	-0.341244	3.603585	5.354034
H	0.806573	2.995153	4.168660
H	-0.082807	3.209421	2.109770
H	-1.167187	2.417937	0.957051
H	-1.745576	3.762978	1.956168
H	-3.452003	1.658420	-2.318677
H	-3.112311	3.057908	-3.336154
H	-4.360858	1.910810	-3.816906
H	-1.467070	3.853509	-4.713002
H	-0.377961	3.359859	-6.009109
H	-2.120953	3.350224	-6.268180
H	0.962941	-0.148585	-6.797118
H	-0.342416	0.559245	-7.745012
H	0.770343	1.603578	-6.866465
H	1.515089	4.155369	-4.603622
H	3.255355	3.931328	-4.753103
H	2.158801	2.949231	-5.718815
H	0.923470	3.830230	-0.793991
H	2.370613	4.603479	-1.440961
H	0.909278	4.517338	-2.419182
H	3.516127	-1.493402	-2.876921
H	4.305570	-0.765675	-1.478893
H	2.649967	-1.382029	-1.343755
H	1.938515	0.344513	0.284947
H	3.272396	1.506146	0.430594
H	3.192930	-0.666630	-5.000786
H	3.029544	0.862961	-5.862566
H	4.491714	0.520956	-4.941329
H	-3.564243	-0.705680	-2.476646
H	-3.917860	-1.535066	-3.990202
H	-2.552439	-2.059972	-3.002482
H	-0.766571	-2.639257	-4.463680
H	-1.491528	-2.450506	-6.061762
H	0.203817	-2.040395	-5.812377
H	1.593865	2.065423	0.438306
O	-0.387140	-0.809100	0.940082

SO_3 insertion - adduct

E = -1940.48815

H = -1939.530588

G = -1939.693126

C	-2.176182	1.288999	-3.085559
C	-1.256907	1.748305	-4.111471
C	-0.673511	0.614890	-4.745062
C	-1.246442	-0.534686	-4.164023
C	-2.175337	-0.110433	-3.106477
C	-1.220709	3.158290	-4.601249
Sm	0.417907	0.330791	-1.834879
O	1.633511	-1.391263	-2.463237
S	0.935771	-2.929422	-2.259046
O	1.875188	-3.731868	-1.270571
C	0.201236	0.604794	-5.962184
C	-1.121696	-1.919320	-4.707003
C	-3.065362	-1.036638	-2.336416
C	-3.182125	2.194071	-2.435987
O	-0.021643	-0.052502	0.216200
Sm	-0.454856	-0.430270	2.237711
C	-2.658496	0.523328	3.722188
C	-2.797008	0.915642	2.349307
C	-1.838082	1.937400	2.090177

C	-1.077456	2.133853	3.275997
C	-1.595761	1.274692	4.286946
C	-3.823696	0.395395	1.371249
C	-1.718704	2.711650	0.816563
C	-0.067559	3.216462	3.517371
C	-1.249562	1.338394	5.743996
C	-3.599704	-0.377658	4.477452
C	1.434523	-2.445086	2.601200
C	1.443336	-1.722651	3.850719
C	0.251443	-2.057182	4.535517
C	-0.541763	-2.899534	3.670673
C	0.190655	-3.151043	2.483017
C	2.582238	-2.550935	1.645963
C	2.609387	-0.967797	4.432431
C	-0.016624	-1.821141	5.988205
C	-1.809852	-3.617087	4.038776
C	-0.187192	-4.094361	1.381901
C	3.176221	1.000767	-1.541718
C	2.979645	1.388483	-2.891282
C	2.221072	2.568648	-2.891202
C	1.866266	2.893169	-1.518323
C	2.476706	1.937511	-0.687874
C	4.164340	-0.015739	-1.064852
C	3.630298	0.733417	-4.075488
C	2.102906	3.504010	-4.044600
C	1.204139	4.164226	-1.099280
C	2.575773	1.978410	0.805782
H	-0.298381	-5.112091	1.778207
H	-1.130078	-3.834540	0.890662
H	0.566042	-4.120921	0.591118
H	3.138883	-3.481678	1.825660
H	3.298026	-1.730341	1.768355
H	2.266015	-2.613420	0.591655
H	2.286235	-0.183564	5.126923
H	3.280324	-1.632112	4.992735
H	3.219824	-0.488672	3.659420
H	0.470251	-0.911903	6.351907
H	0.376994	-2.655697	6.586368
H	-1.082464	-1.746707	6.216659
H	-1.590346	-4.628203	4.410155
H	-2.373329	-3.101439	4.822583
H	-2.473576	-3.740190	3.177573
H	-0.169867	1.362185	5.922140
H	-1.656750	0.491347	6.300173
H	-1.662726	2.249085	6.199472
H	-3.139677	-0.788721	5.380951
H	-3.944562	-1.225889	3.875428
H	-4.497655	0.169925	4.796197
H	-4.209077	-0.586095	1.673636
H	-3.387516	0.267898	0.364582
H	-4.691489	1.061963	1.282525
H	0.839974	2.848071	4.013416
H	-0.482659	3.999240	4.165483
H	0.242160	3.699621	2.587254
H	-0.705248	3.089399	0.664982
H	-1.940501	2.084830	-0.047399
H	-2.401120	3.574664	0.802075
H	-3.675714	1.738569	-1.573333
H	-2.743718	3.140333	-2.099774
H	-3.975668	2.448417	-3.152957
H	-1.132290	3.893458	-3.792422
H	-0.409986	3.337352	-5.305281
H	-2.161796	3.386847	-5.123098
H	0.935027	-0.207072	-5.924330
H	-0.393659	0.459049	-6.874226
H	0.752133	1.540933	-6.084521
H	1.198076	4.111498	-3.995514
H	2.952865	4.202602	-4.039509
H	2.125844	2.987358	-5.009945
H	1.011026	4.179276	-0.023554
H	1.843246	5.028856	-1.324776
H	0.249151	4.337425	-1.608851
H	4.324328	-0.797527	-1.810471
H	5.132011	0.466383	-0.853476
H	3.839354	-0.508394	-0.145176
H	2.755827	0.979559	1.218087
H	3.408572	2.619669	1.127178
H	3.511623	-0.354393	-4.025614
H	3.194423	1.075985	-5.019032
H	4.704063	0.954860	-4.114856
H	-3.856276	-0.495461	-1.799833
H	-3.566777	-1.731727	-3.022957
H	-2.500511	-1.660815	-1.632079
H	-1.447940	-2.668722	-3.984808
H	-1.725739	-2.020339	-5.621781
H	-0.088783	-2.157115	-4.989976
H	1.664158	2.369270	1.263592
O	-0.491004	-2.562764	-1.609970

SO_3 insertion - transition state

E = -1940.455904

H = -1939.492779

G = -1939.652257

C	-4.606077	-0.075843	-9.457975
C	-3.652414	0.466439	-10.382434
C	-2.980973	-0.617475	-11.010610
C	-3.510917	-1.825518	-10.477813
C	-4.520227	-1.490654	-9.514999
C	-3.620891	1.906515	-10.802277
Sm	-2.029737	-0.737102	-8.294246
O	-0.948897	-2.873197	-8.870694
S	-1.443341	-4.166151	-8.154136
O	-0.357193	-5.102016	-7.617623
C	-2.066001	-0.543951	-12.197867
C	-3.265970	-3.194072	-11.042320
C	-5.439679	-2.476315	-8.853252
C	-5.713670	0.736357	-8.847446
O	-2.295477	-1.813935	-6.419816
Sm	-2.575603	-1.926290	-4.275529
C	-4.834497	-0.904655	-2.901839
C	-4.973652	-0.613580	-4.295157
C	-4.021276	0.389140	-4.632198
C	-3.276260	0.698348	-3.458772
C	-3.791195	-0.088166	-2.387997
C	-6.027539	-1.180688	-5.202865
C	-3.884097	1.056706	-5.964417
C	-2.317509	1.841020	-3.272766
C	-3.454654	0.150668	-0.945372
C	-5.783728	-1.745518	-2.097613
C	-0.638527	-3.875311	-3.712116
C	-0.720090	-3.090865	-2.515822
C	-1.963045	-3.379141	-1.884352
C	-2.684441	-4.271999	-2.724240
C	-1.854377	-4.598776	-3.841827
C	0.611066	-4.072651	-4.519898

C	0.402847	-2.285635	-1.920931
C	-2.320713	-3.028904	-0.471331
C	-3.964814	-4.982401	-2.385066
C	-2.163705	-5.697076	-4.819571
C	0.755711	-0.600755	-7.931349
C	0.586081	-0.057649	-9.242184
C	-0.045837	1.205077	-9.112552
C	-0.299063	1.436442	-7.722441
C	0.205587	0.322751	-6.994278
C	1.589352	-1.799131	-7.591595
C	1.191078	-0.634096	-10.490232
C	-0.167353	2.256180	-10.174550
C	-0.747363	2.753579	-7.153976
C	0.284719	0.185398	-5.503270
H	-2.316470	-6.646329	-4.288338
H	-3.070463	-5.516586	-5.409098
H	-1.344929	-5.852564	-5.524022
H	1.225924	-4.875387	-4.088179
H	1.240230	-3.176507	-4.535674
H	0.407665	-4.355928	-5.555921
H	0.034612	-1.467792	-1.292389
H	1.052461	-2.905985	-1.287160
H	1.046068	-1.842376	-2.689079
H	-1.874067	-2.086116	-0.146121
H	-1.954286	-3.807226	0.213417
H	-3.400953	-2.957423	-0.316101
H	-3.761861	-5.972247	-1.951058
H	-4.562804	-4.430121	-1.655373
H	-4.593747	-5.152987	-3.266655
H	-2.374834	0.203891	-0.765256
H	-3.859697	-0.623673	-0.290991
H	-3.876333	1.108998	-0.609485
H	-5.337805	-2.082051	-1.157770
H	-6.116525	-2.637735	-2.638196
H	-6.687665	-1.176817	-1.838199
H	-6.363761	-2.169867	-4.873172
H	-5.667261	-1.288693	-6.229634
H	-6.920204	-0.540070	-5.234528
H	-1.399481	1.554848	-2.745346
H	-2.781912	2.640528	-2.678625
H	-2.024925	2.289738	-4.225544
H	-2.847252	1.348446	-6.171207
H	-4.231649	0.395948	-6.765962
H	-4.487029	1.972358	-6.035028
H	-6.194012	0.235004	-8.003257
H	-5.370404	1.714027	-8.494283
H	-6.497688	0.928732	-9.594080
H	-3.566968	2.599233	-9.953602
H	-2.775549	2.122477	-11.458790
H	-4.533459	2.165122	-11.358356
H	-1.292244	-1.317850	-12.172000
H	-2.626393	-0.685400	-13.133027
H	-1.561350	0.422774	-12.271919
H	-1.029833	2.909838	-10.017504
H	0.723828	2.900816	-10.177379
H	-0.250910	1.829676	-11.177641
H	-0.924178	2.693438	-6.076900
H	0.024519	3.521659	-7.302503
H	-1.663359	3.137267	-7.619278
H	1.646535	-2.504981	-8.423320
H	2.617670	-1.496348	-7.347349
H	1.199561	-2.344057	-6.728564
H	0.356754	-0.869221	-5.213179
H	1.170775	0.688349	-5.091078
H	1.015638	-1.711961	-10.577302
H	0.793167	-0.161518	-11.391660
H	2.279837	-0.486392	-10.502811
H	-6.292139	-1.973263	-8.388786
H	-5.847745	-3.180451	-9.589209
H	-4.942256	-3.077207	-8.082505
H	-3.631927	-3.978673	-10.375541
H	-3.792474	-3.313045	-12.000263
H	-2.205589	-3.383936	-11.244308
H	-0.585863	0.621913	-5.000982
O	-2.927065	-4.452733	-7.922826

SO_3 insertion - product

E = -1940.582164
H = -1939.615577
G = -1939.778730

C	-1.780195	1.806723	-4.115870
C	-0.871526	1.334848	-5.108770
C	-0.583074	-0.033744	-4.825071
C	-1.344741	-0.415775	-3.677681
C	-2.086183	0.718646	-3.242889
C	-0.506071	2.069343	-6.365415
Sm	0.540351	1.344014	-2.730159
O	-0.404293	1.737700	-0.495964
S	-0.003873	0.353166	0.161018
O	0.809274	-0.382999	-0.989998
C	0.230277	-0.962486	-5.683633
C	-1.440257	-1.801326	-3.105965
C	-3.114529	0.737677	-2.149634
C	-2.437131	3.158783	-4.096315
O	0.835354	0.533776	1.495032
Sm	-0.586320	-0.836505	2.968495
C	-2.627883	-0.266733	4.730720
C	-2.897370	0.515481	3.567236
C	-1.898217	1.525666	3.469838
C	-0.996531	1.357238	4.560600
C	-1.453508	0.260095	5.350869
C	-4.095403	0.374854	2.671942
C	-1.875447	2.649530	2.476987
C	0.152895	2.264642	4.899463
C	-0.917607	-0.104874	6.706066
C	-3.548506	-1.310003	5.297985
C	1.375516	-2.694883	2.466913
C	1.288063	-2.616442	3.890648
C	0.041066	-3.184573	4.288575
C	-0.656343	-3.580743	3.107735
C	0.176008	-3.290474	1.984448
C	2.578183	-2.340411	1.640622
C	2.391211	-2.167308	4.808291
C	-0.348367	-3.544902	5.692369
C	-1.951658	-4.343294	3.064209
C	-0.108482	-3.670404	0.559972
C	2.967748	2.218039	-1.786573
C	3.242098	1.669949	-3.074802
C	2.660104	2.526538	-4.055817
C	1.996469	3.590050	-3.370359
C	2.192965	3.398763	-1.968759
C	3.520129	1.713860	-0.485007
C	4.121405	0.482724	-3.353670
C	2.929858	2.451424	-5.531384
C	1.380913	4.808924	-3.998980

C	1.758057	4.340736	-0.882942
H	0.271610	-4.678725	0.344387
H	-1.181312	-3.678132	0.344401
H	0.359026	-2.983037	-0.149906
H	3.267244	-3.193732	1.573292
H	3.139356	-1.503980	2.068542
H	2.304008	-2.055268	0.621518
H	2.009353	-1.811791	5.770808
H	3.087795	-2.988748	5.026393
H	2.986367	-1.358483	4.370295
H	0.119684	-2.890067	6.432101
H	-0.028660	-4.570144	5.925855
H	-1.430167	-3.507556	5.851414
H	-1.772737	-5.427507	3.050873
H	-2.580704	-4.135529	3.935535
H	-2.540216	-4.111915	2.169309
H	0.176904	-0.071571	6.748858
H	-1.227314	-1.105555	7.016714
H	-1.283385	0.596607	7.468627
H	-3.048435	-1.939493	6.038656
H	-3.958180	-1.971578	4.526428
H	-4.406365	-0.843648	5.801752
H	-4.458676	-0.657670	2.627323
H	-3.876964	0.691466	1.647735
H	-4.932212	0.989533	3.031838
H	0.930059	1.747875	5.473034
H	-0.179305	3.115146	5.510828
H	0.625704	2.679848	4.003709
H	-0.860929	3.009625	2.285761
H	-2.295574	2.358975	1.511083
H	-2.461312	3.502329	2.847445
H	-2.700859	3.470545	-3.080629
H	-1.795021	3.935574	-4.524347
H	-3.369236	3.158286	-4.678555
H	-0.383674	3.144373	-6.201026
H	0.416587	1.693940	-6.814388
H	-1.298453	1.953010	-7.118182
H	0.707427	-1.755834	-5.097776
H	-0.397141	-1.460965	-6.435589
H	1.019898	-0.435376	-6.228835
H	2.199610	3.016837	-6.114565
H	3.918791	2.871629	-5.761771
H	2.930742	1.422934	-5.909012
H	0.502585	5.163559	-3.448071
H	2.095664	5.642915	-4.023868
H	1.067720	4.625268	-5.030766
H	3.639371	0.626643	-0.483685
H	4.508872	2.152520	-0.291079
H	2.879469	1.963771	0.364976
H	1.544141	3.812999	0.050406
H	2.537452	5.085855	-0.671788
H	4.049741	-0.275792	-2.566841
H	3.872579	-0.001843	-4.304006
H	5.178550	0.776527	-3.415845
H	-3.172121	1.713081	-1.657090
H	-4.111632	0.516215	-2.554928
H	-2.901875	0.000208	-1.371383
H	-1.656704	-1.785805	-2.034633
H	-2.239131	-2.373440	-3.597846
H	-0.512461	-2.366750	-3.239708
H	0.853629	4.893819	-1.157224
O	-1.260363	-0.500651	0.628368