Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supplementary Information

Kinetic study of isoprene hydroxy hydroperoxide radicals reacting with sulphur dioxide and their global-scale impact on sulphate formation

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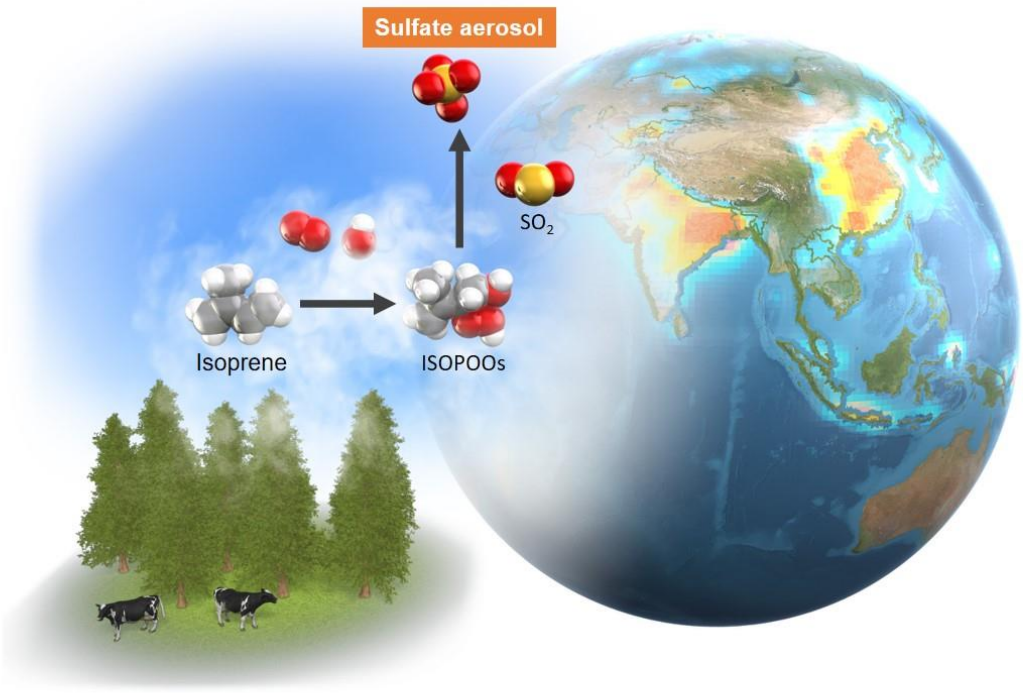

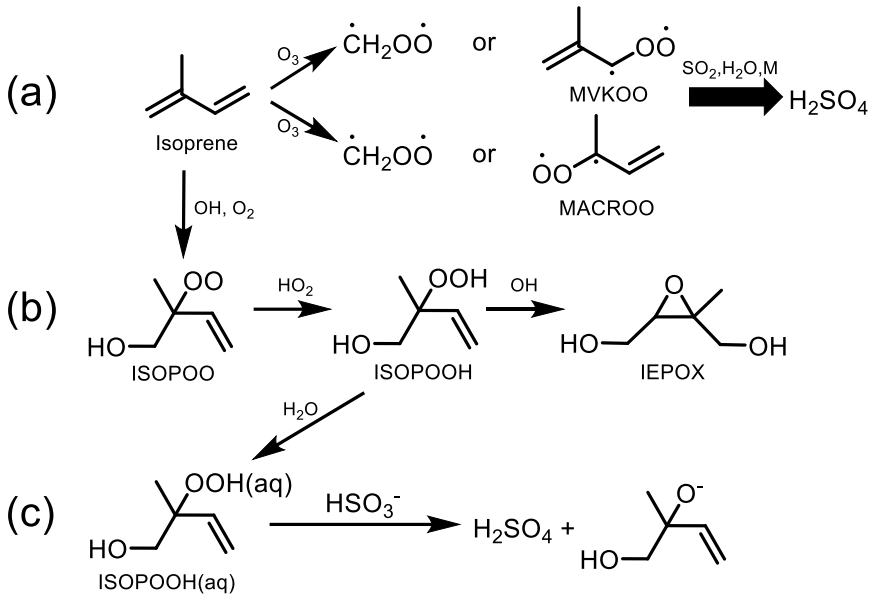

Figure S1: Chemical reactions of isoprene-derived particulate formations for the formation of (a) three Criegee intermediates (CIs), namely formaldehyde oxide (CH_2OO), methyl-vinyl-ketone oxide (MVKOO), methacrolein oxide (MACROO) and SO_4^{2-}(p) in the gaseous phase, (b) ISOPOOs, ISOPOOHs and IEPOXs in the gaseous phase, and (c) SO_4^{2-}(p) by the oxidation of HSO_3^- from ISOPOOHs in the liquid phase. Figure S1 was obtained from Hata et al. (2023)[9], which is freely licensed under CC BY 4.0 DEED.

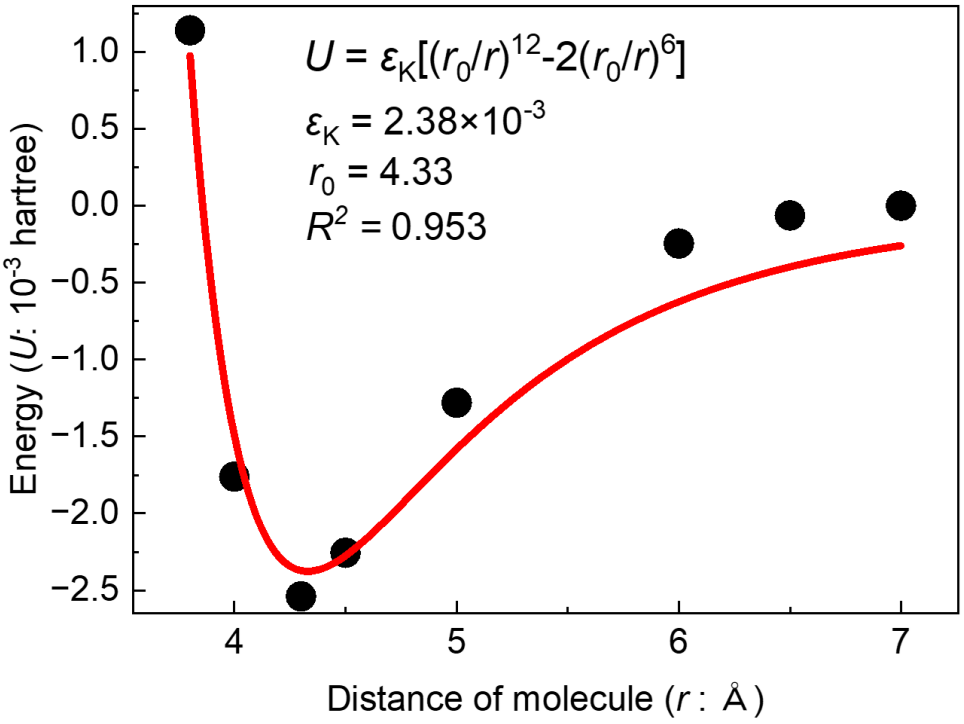

Figure S2: Lennard–Jones potential of 1,2−ISOPOOSO$_2$ calculated using G16, the theoretical level of M06-2X/aug-cc-pV(T+*d*)Z. Here, ε_K is the well-depth of the potential (Hartree), r_0 is the molecular distance (Å) when dU/dt = 0 and R^2 is the coefficient of determination. The collision diameter, σ, was determined by $\sigma = 2^{-1/16}r_0$.

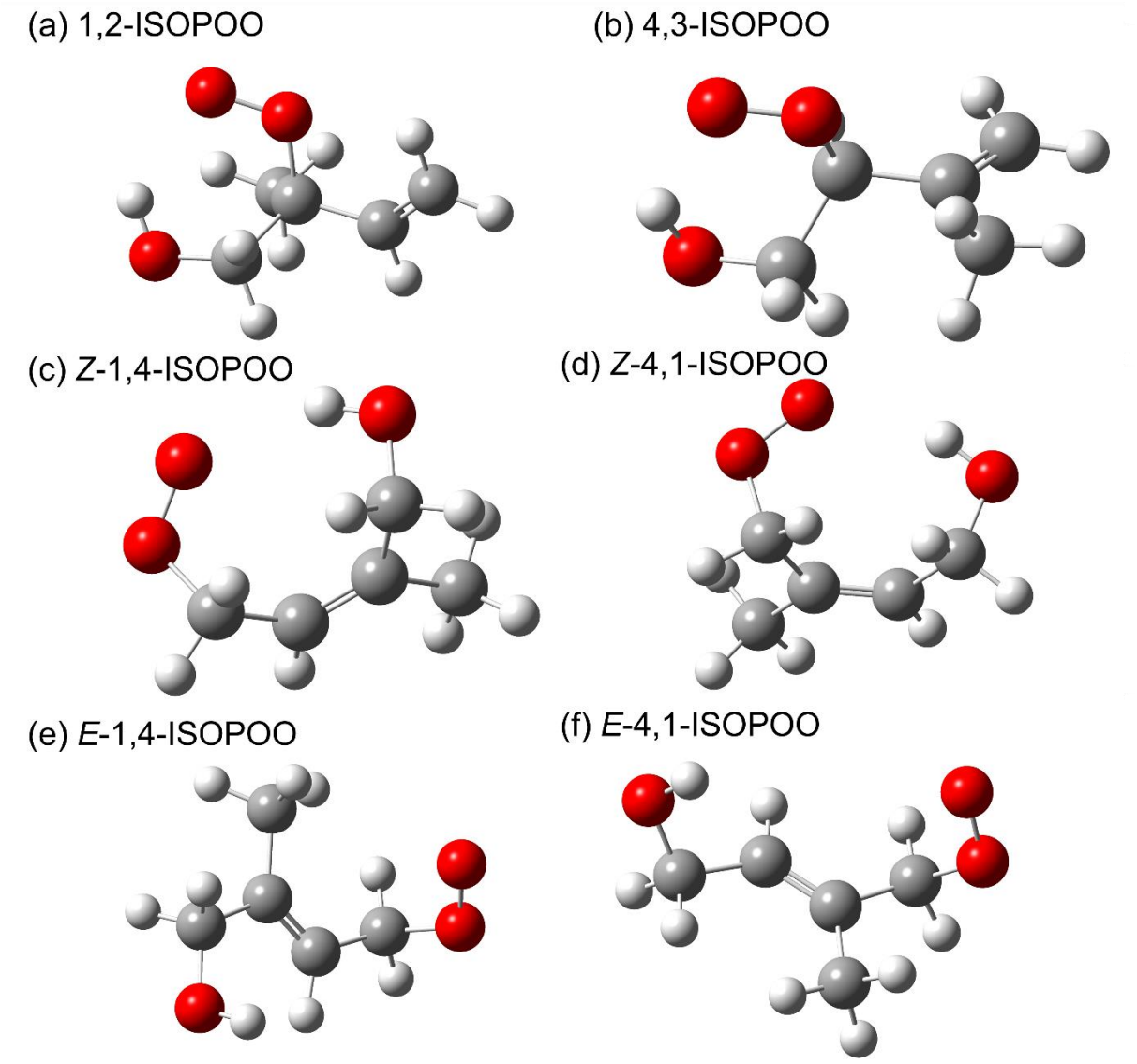

Figure S3: Optimized structures of the six ISOPOO isomers. The Cartesian coordinates of each structure are listed in Tables S1–S6.

Table S1: Optimised coordinates of 1,2−ISOPOO calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

Atom	X	Y	Z
C	-0.177385	-0.204699	0.231345
C	0.70977	-0.849466	-0.843535
C	-1.595443	-0.652673	0.032211
C	-2.567663	0.058122	-0.514975
O	2.085531	-0.804621	-0.576007
O	-0.191154	1.249124	0.034315
O	0.996754	1.754125	-0.07162
H	2.333163	0.122045	-0.494241
H	-2.413289	1.072582	-0.854726
H	-3.557483	-0.361444	-0.627507
H	0.459016	-0.381712	-1.80163
H	0.438413	-1.903509	-0.905558
H	-1.783847	-1.666775	0.368711
C	0.313031	-0.483105	1.641108
H	0.348101	-1.559875	1.803289
H	1.315825	-0.085839	1.774814
H	-0.362817	-0.033573	2.36642

Table S2: Optimised coordinates of 4,3-ISOPOO calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

Atom	X	Y	Z
C	-0.059157	-0.030873	-0.396237
C	-0.84549	-1.058865	0.411173
C	1.421519	-0.073447	-0.149096
C	1.867788	0.078588	1.275622
C	2.255937	-0.262744	-1.161613
O	-2.116257	-1.328417	-0.121666
O	-0.481667	1.322527	-0.02481
O	-1.766722	1.477915	-0.085036
H	-2.59104	-0.492345	-0.171597
H	-0.291269	-0.145063	-1.455401
H	1.897782	-0.364719	-2.177616
H	3.324526	-0.325406	-1.002667
H	1.50433	-0.748629	1.888748
H	2.952958	0.100972	1.340915
H	1.471329	0.998627	1.707129
H	-0.905856	-0.719287	1.451189
H	-0.289173	-1.996305	0.392298

Table S3: Optimised coordinates of *Z*−1,4-ISOPOO calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

Atom	X	Y	Z
C	0.999916	-0.56053	0.119155
C	1.123628	0.770557	0.820766
C	-0.131136	-1.261591	0.051455
C	-1.432245	-0.865062	0.658766
O	1.108451	1.825752	-0.121531
H	0.231579	1.826062	-0.52225
H	-1.335126	-0.204393	1.515223
H	2.088601	0.828161	1.325623
H	0.346414	0.911669	1.573172
H	-0.144344	-2.174667	-0.533381
C	2.24313	-1.00095	-0.59052
H	2.592982	-0.198603	-1.241914
H	3.039218	-1.197873	0.130716
H	2.078932	-1.89705	-1.184873
O	-2.27596	-0.158483	-0.307767
O	-1.792316	1.00004	-0.614086
H	-2.039412	-1.726329	0.927037

Table S4: Optimised coordinates of *Z*-4,1-ISOPOO calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

Atom	X	Y	Z
C	0.999916	-0.56053	0.119155
C	1.123628	0.770557	0.820766
C	-0.131136	-1.261591	0.051455
C	-1.432245	-0.865062	0.658766
O	1.108451	1.825752	-0.121531
H	0.231579	1.826062	-0.52225
H	-1.335126	-0.204393	1.515223
H	2.088601	0.828161	1.325623
H	0.346414	0.911669	1.573172
H	-0.144344	-2.174667	-0.533381
C	2.24313	-1.00095	-0.59052
H	2.592982	-0.198603	-1.241914
H	3.039218	-1.197873	0.130716
H	2.078932	-1.89705	-1.184873
O	-2.27596	-0.158483	-0.307767
O	-1.792316	1.00004	-0.614086
H	-2.039412	-1.726329	0.927037

Table S5: Optimised coordinates of *E*−1,4-ISOPOO calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

Atom	X	Y	Z
C	0.76018	0.413879	0.235058
C	2.195876	0.194555	-0.171306
C	-0.027288	-0.613124	0.542749
C	-1.465408	-0.509935	0.917132
O	2.58483	-1.147405	-0.326967
H	2.089679	-1.529555	-1.056426
H	-1.733332	0.44842	1.353896
H	2.845191	0.61456	0.600511
H	2.386696	0.770628	-1.085182
H	0.389229	-1.611871	0.505957
C	0.362392	1.858204	0.22286
H	-0.604923	2.039957	0.679605
H	1.114966	2.462024	0.734159
H	0.306667	2.213245	-0.807954
O	-2.332226	-0.690262	-0.243998
O	-2.24998	0.318299	-1.052402
H	-1.769686	-1.313945	1.583411

Table S6: Optimised coordinates of *E*-4,1-ISOPOO calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

Atom	X	Y	Z
C	0.084581	0.163418	0.376671
C	1.288533	-0.67979	0.687322
C	-1.122352	-0.391461	0.471631
C	-2.451382	0.255862	0.236035
O	2.149006	-0.781212	-0.475108
H	-2.347492	1.289957	-0.095348
H	1.010152	-1.704038	0.924324
H	1.897475	-0.250953	1.48302
H	-1.189309	-1.443069	0.736157
C	0.385894	1.58707	0.014193
H	0.898084	2.083834	0.84057
H	1.065477	1.624665	-0.838027
H	-0.505866	2.156254	-0.228405
O	-3.231022	-0.49375	-0.682724
H	-3.027058	0.264592	1.162475
H	-2.738213	-0.578464	-1.502979
O	3.060154	0.143291	-0.49178

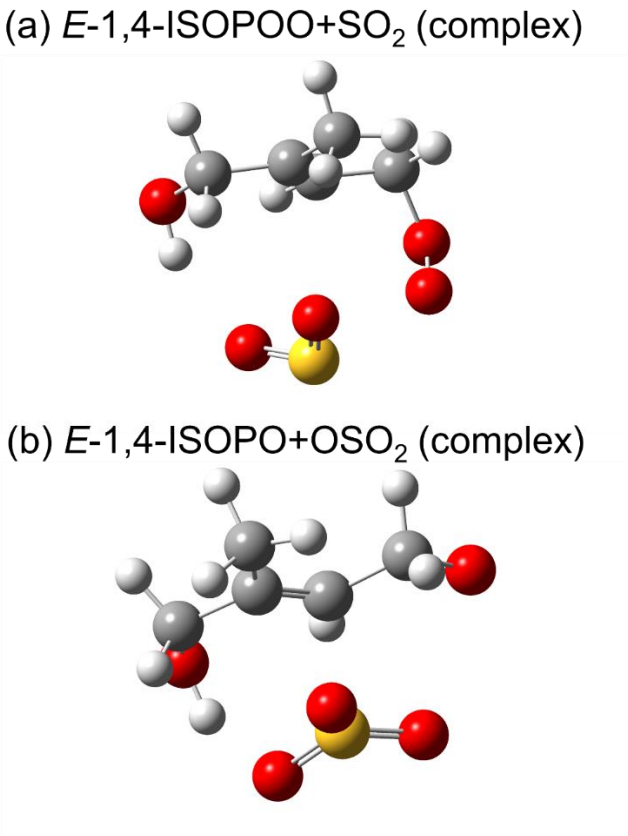

Figure S4: Optimised structures of *E*−1,4-ISOPOO+SO_2 and *E*−1,4-ISOPO+OSO_2 complexes

The Cartesian coordinates of the structures are listed in Tables S21 and S22.

Table S7: Optimised coordinates of the complex of *E*−1,4-ISOPOO+SO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	-0.469893	1.41967	0.337087
C	-1.915027	1.304439	-0.084621
C	0.504609	1.323287	-0.563386
C	1.960882	1.406373	-0.287711
O	-2.126092	1.055824	-1.448358
H	-1.87218	0.143055	-1.623022
H	2.204596	1.599102	0.753197
H	-2.422389	2.243388	0.152284
H	-2.379401	0.529676	0.537668
H	0.230928	1.178076	-1.601884
C	-0.303011	1.648744	1.80867
H	0.727386	1.574759	2.143489
H	-0.681447	2.63717	2.078357
H	-0.889002	0.914234	2.362226
O	2.634668	0.155662	-0.644964
O	2.211895	-0.840357	0.059899
H	2.463327	2.132658	-0.924609
S	-0.265204	-2.070074	0.162857
O	-0.880735	-1.633695	-1.066312
O	-0.815225	-1.543186	1.381778

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	0.389272	-1.440556	0.344754
C	1.841256	-1.402901	-0.067642
C	-0.572802	-1.304776	-0.56395
C	-2.033293	-1.306414	-0.298068
O	2.074172	-1.181315	-1.432616
H	1.865946	-0.259881	-1.62132
H	-2.294754	-1.492404	0.73969
H	2.299154	-2.36335	0.183272
H	2.340388	-0.6455	0.549261
H	-0.284599	-1.184476	-1.601645
C	0.201066	-1.64367	1.81754
H	-0.828232	-1.524338	2.142239
H	0.537721	-2.642699	2.103047
H	0.811324	-0.926062	2.367116
O	-2.630675	-0.015749	-0.649449
O	-2.161278	0.945873	0.073692
H	-2.571997	-1.997843	-0.94392
S	0.383014	2.054605	0.146424
O	0.960843	1.569993	-1.069787
O	0.887418	1.525296	1.371119

Table S8: Optimized coordinates of the complex of *E*−1,4-ISOPO+OSO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	-0.928371	0.988686	0.313395
C	-2.2514	0.503711	-0.214975
C	0.16565	1.052709	-0.470056
C	1.494536	1.630156	-0.051005
O	-2.268057	0.181079	-1.57441
H	-1.87666	-0.692676	-1.679643
H	1.887504	1.162534	0.864556
H	-2.978654	1.305496	-0.056202
H	-2.573774	-0.338966	0.408322
H	0.072551	0.814387	-1.524424
C	-0.944516	1.415928	1.745504
H	0.050558	1.472201	2.177641
H	-1.409514	2.40284	1.815823
H	-1.539875	0.727338	2.344612
O	2.450125	1.593658	-1.023154
O	1.761452	-1.27301	-0.453501
H	1.383226	2.696265	0.216185
S	0.486683	-1.347914	0.191896
O	-0.617069	-1.936018	-0.516562
O	0.421339	-1.256952	1.620829

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	-0.919498	0.989521	0.312177
C	-2.246269	0.513609	-0.215118
C	0.176074	1.041905	-0.470326
C	1.506588	1.617528	-0.053285
O	-2.267008	0.190829	-1.574344
H	-1.880262	-0.684882	-1.680431
H	1.897313	1.153887	0.865124
H	-2.967072	1.321106	-0.055953
H	-2.574392	-0.326101	0.409141
H	0.081729	0.802357	-1.524282
C	-0.93426	1.424722	1.741941
H	0.060279	1.471712	2.176344
H	-1.387473	2.4176	1.804861
H	-1.539491	0.74688	2.343331
O	2.463125	1.571536	-1.024163
O	1.746886	-1.279602	-0.43593
H	1.398536	2.685503	0.207341
S	0.475972	-1.346498	0.193894
O	-0.617257	-1.921487	-0.519537
O	0.399189	-1.257251	1.611461

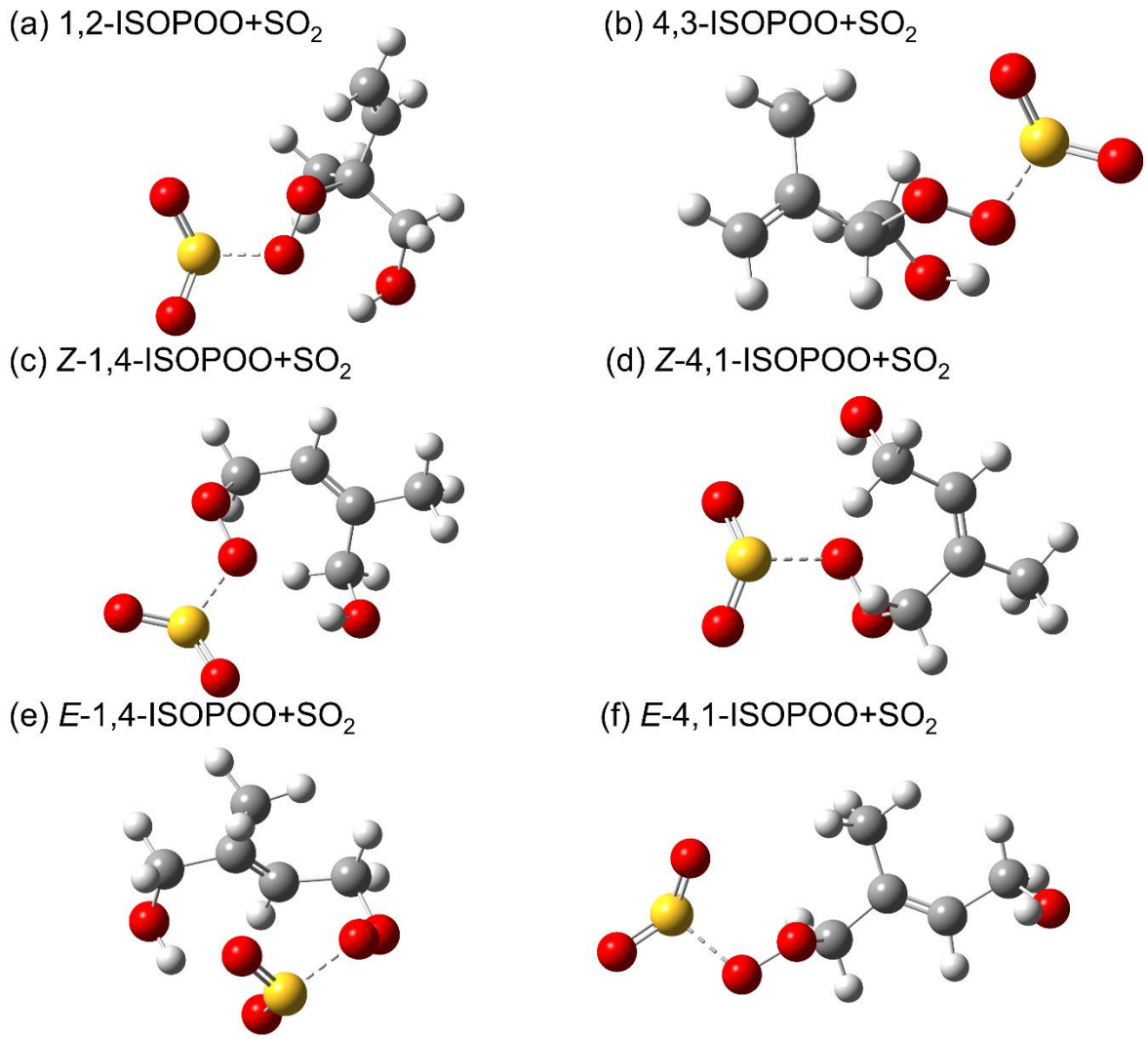

Figure S5: Transition-state optimised structures of the six isomers of ISOPOOs + SO_2 reactions. The Cartesian coordinates of each structure are listed in Tables S9–S14.

Table S9: Optimized coordinates of the transition state of 1,2−ISOPOO + SO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	1.415296	0.035164	0.231105
C	1.915953	1.347689	-0.392392
C	2.51641	-0.984965	0.161568
C	2.5555	-2.042933	-0.630951
O	1.138712	2.479989	-0.099257
O	0.344777	-0.524102	-0.582562
O	-0.648653	0.359521	-0.770271
H	0.283979	2.387079	-0.528381
H	1.751583	-2.280344	-1.312982
H	3.403718	-2.712453	-0.605937
H	2.020029	1.184814	-1.469601
H	2.907872	1.545567	0.01387
H	3.337399	-0.780079	0.840198
C	0.916581	0.216742	1.65485
H	1.747559	0.535764	2.283235
H	0.153837	0.990142	1.705365
H	0.526415	-0.726589	2.034755
S	-2.201412	-0.125615	0.24205
O	-3.245872	0.553705	-0.480533
O	-2.192493	-1.564644	0.310323

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	1.417872	0.035576	0.232862
C	1.908218	1.349696	-0.39558
C	2.524297	-0.978469	0.160873
C	2.570207	-2.032477	-0.636559
O	1.128855	2.47902	-0.097461
O	0.346027	-0.531393	-0.574604
O	-0.645396	0.348613	-0.772159
H	0.270763	2.381127	-0.518728
H	1.768452	-2.271047	-1.320755
H	3.421925	-2.697609	-0.61358
H	2.005044	1.186245	-1.473415
H	2.90238	1.551624	0.003089
H	3.343242	-0.772254	0.841562
C	0.922644	0.217355	1.657671
H	1.751809	0.550991	2.280862
H	0.149342	0.980219	1.706986
H	0.54624	-0.728967	2.04371
S	-2.211185	-0.126999	0.239915
O	-3.237841	0.544984	-0.491985
O	-2.196604	-1.553527	0.323214

Table S10: Optimised coordinates of the transition state of 4,3-ISOPOO + SO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	-1.320783	0.525172	-0.361992
C	-0.856764	1.233415	0.908177
C	-2.456714	-0.431345	-0.123761
C	-2.231049	-1.484087	0.921851
C	-3.582946	-0.300281	-0.810043
O	-0.190221	2.44699	0.665026
O	-0.261027	-0.312374	-0.904696
O	0.892455	0.368987	-1.039808
H	0.547524	2.287081	0.070681
H	-1.575631	1.267701	-1.119449
H	-3.701855	0.469563	-1.561081
H	-4.422741	-0.960422	-0.637204
H	-2.116105	-1.03374	1.910288
H	-3.068898	-2.175973	0.959451
H	-1.317796	-2.044006	0.715248
H	-0.249108	0.541735	1.504347
H	-1.741136	1.480254	1.49512
S	2.183523	-0.264344	0.208652
O	3.427528	0.012526	-0.460552
O	1.80613	-1.62362	0.504878

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	-1.324022	0.523625	-0.362498
C	-0.8615	1.236383	0.905832
C	-2.458476	-0.434017	-0.122596
C	-2.23162	-1.483886	0.925652
C	-3.584725	-0.306346	-0.80949
O	-0.197052	2.450073	0.65891
O	-0.261352	-0.313406	-0.901791
O	0.889225	0.367136	-1.037695
H	0.550954	2.286031	0.07862
H	-1.578593	1.263355	-1.122697
H	-3.704611	0.461538	-1.562379
H	-4.423565	-0.967349	-0.635305
H	-2.117043	-1.030911	1.912917
H	-3.068636	-2.176679	0.965043
H	-1.317822	-2.043445	0.720366
H	-0.25264	0.547685	1.504
H	-1.746802	1.483511	1.491267
S	2.19206	-0.26809	0.210087
O	3.419918	0.020176	-0.459352
O	1.817743	-1.617585	0.498101

Table S11: Optimised coordinates of the transition state of *Z*−1,4-ISOPOO + SO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	-2.327604	0.095832	0.133796
C	-1.616185	-1.003295	0.88497
C	-1.851242	1.331474	-0.012514
C	-0.556698	1.839912	0.527527
O	-1.17957	-2.024039	0.008177
H	-0.496976	-1.666458	-0.569481
H	-0.227005	1.325016	1.43084
H	-2.318663	-1.482715	1.568501
H	-0.78608	-0.622647	1.481791
H	-2.41563	2.038934	-0.60972
C	-3.617526	-0.329129	-0.498259
H	-3.45178	-1.21243	-1.11568
H	-4.337797	-0.610435	0.273079
H	-4.049118	0.459923	-1.109709
O	0.527059	1.727993	-0.429823
O	0.70216	0.4445	-0.769127
H	-0.586784	2.909627	0.722078
S	2.13741	-0.3601	0.218113
O	2.258492	-1.602024	-0.503101
O	3.227709	0.580323	0.222045

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	-2.333628	0.093357	0.135798
C	-1.619382	-1.005033	0.885227
C	-1.85655	1.328275	-0.014245
C	-0.560695	1.836483	0.522724
O	-1.177972	-2.020864	0.00492
H	-0.503793	-1.653857	-0.576646
H	-0.229841	1.323048	1.426299
H	-2.320584	-1.489453	1.566459
H	-0.790921	-0.623091	1.483428
H	-2.42173	2.035165	-0.611365
C	-3.625545	-0.331873	-0.491953
H	-3.462385	-1.217495	-1.106769
H	-4.34442	-0.609512	0.282006
H	-4.057525	0.455652	-1.10511
O	0.522397	1.720302	-0.435504
O	0.699399	0.438287	-0.769913
H	-0.589218	2.906697	0.714481
S	2.149037	-0.362769	0.218137
O	2.283535	-1.58556	-0.5098
O	3.21147	0.591572	0.236763

Table S12: Optimised coordinates of the transition state of *Z*-4,1-ISOPOO + SO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	2.185404	-0.431853	0.116257
C	1.079665	-1.201384	0.778079
C	2.242833	0.897447	0.130908
C	1.255519	1.846141	0.742827
O	0.054297	-1.583758	-0.167714
H	1.780982	2.611421	1.313557
H	0.583758	-0.658147	1.581936
H	1.425929	-2.162439	1.155727
H	3.049081	1.377648	-0.415638
C	3.177347	-1.280046	-0.624093
H	3.709317	-1.943375	0.0611
H	2.664802	-1.913858	-1.351085
H	3.906228	-0.669141	-1.151238
O	0.534298	2.543333	-0.256882
H	0.572859	1.340979	1.429465
H	0.107423	1.899404	-0.831309
O	-0.491975	-0.490092	-0.716151
S	-2.134577	-0.00474	0.180256
O	-2.820737	-1.235957	0.475024
O	-2.687352	0.917914	-0.776836

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	2.187656	-0.434885	0.117318
C	1.081806	-1.202371	0.781215
C	2.245217	0.894398	0.128403
C	1.259472	1.845934	0.738628
O	0.054678	-1.583507	-0.164027
H	1.786467	2.608522	1.311606
H	0.586412	-0.657409	1.584106
H	1.427039	-2.163544	1.159374
H	3.051347	1.372858	-0.419879
C	3.179258	-1.285249	-0.62109
H	3.711391	-1.946864	0.065637
H	2.66655	-1.920882	-1.346398
H	3.908083	-0.675795	-1.149992
O	0.544494	2.547018	-0.262611
H	0.572658	1.342657	1.422408
H	0.101425	1.905527	-0.827449
O	-0.491568	-0.49114	-0.709416
S	-2.147085	-0.00784	0.182117
O	-2.833642	-1.23151	0.449088
O	-2.671269	0.928314	-0.760551

Table S13: Optimised coordinates of the transition state of *E*−1,4-ISOPOO + SO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	-1.421445	0.689053	0.226756
C	-2.420302	-0.42574	0.034843
C	-0.646209	1.073184	-0.786282
C	0.480957	2.03538	-0.695368
O	-2.326616	-1.102677	-1.191046
H	-1.445885	-1.48938	-1.258679
H	0.442698	2.678625	0.180202
H	-3.431795	-0.01629	0.093219
H	-2.307783	-1.116138	0.879877
H	-0.781443	0.593301	-1.746144
C	-1.399479	1.233803	1.622692
H	-0.77873	2.117725	1.733189
H	-2.414409	1.487613	1.935654
H	-1.03099	0.469686	2.308648
O	1.770683	1.354024	-0.659773
O	1.877111	0.616058	0.46554
H	0.581236	2.644415	-1.591925
S	1.381249	-1.198724	0.2433
O	0.85037	-1.378496	-1.08997
O	0.5167	-1.466917	1.369913

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	-1.422101	0.683566	0.23581
C	-2.416155	-0.435357	0.043564
C	-0.656989	1.079781	-0.780007
C	0.46646	2.045954	-0.688987
O	-2.333708	-1.098312	-1.190769
H	-1.452739	-1.481577	-1.272071
H	0.428239	2.685621	0.1892
H	-3.429455	-0.033392	0.119348
H	-2.288588	-1.134306	0.879538
H	-0.796831	0.606714	-1.742591
C	-1.389957	1.215762	1.636361
H	-0.776675	2.104754	1.747935
H	-2.40363	1.456411	1.963375
H	-1.00584	0.44917	2.311005
O	1.75978	1.369682	-0.658078
O	1.870751	0.623836	0.458577
H	0.562106	2.658689	-1.583406
S	1.384008	-1.201167	0.228258
O	0.843309	-1.37199	-1.089455
O	0.551336	-1.477171	1.361611

Table S14: Optimised coordinates of the transition state of *E*-4,1-ISOPOO + SO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	1.568	0.160879	-0.449663
C	0.364371	-0.68111	-0.745482
C	2.764554	-0.420443	-0.412446
C	4.087277	0.23248	-0.158504
O	-0.476286	-0.635177	0.425085
H	3.976785	1.290324	0.085089
H	0.611193	-1.720205	-0.958165
H	-0.224577	-0.266057	-1.57028
H	2.825748	-1.493878	-0.567224
C	1.269083	1.61941	-0.255912
H	0.981475	2.071663	-1.208019
H	0.424495	1.743148	0.422843
H	2.115362	2.17429	0.137109
O	4.810774	-0.449826	0.851987
H	4.707182	0.166201	-1.053641
H	4.287771	-0.449145	1.657804
O	-1.66063	-1.205844	0.167212
S	-2.969502	0.171277	-0.162305
O	-4.207214	-0.483886	0.170989
O	-2.530783	1.309224	0.607652

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	1.571007	0.16015	-0.448675
C	0.3677	-0.682794	-0.742586
C	2.767937	-0.420398	-0.411525
C	4.09062	0.233648	-0.160301
O	-0.475302	-0.632894	0.426638
H	3.979855	1.291694	0.082297
H	0.614473	-1.722836	-0.950528
H	-0.221091	-0.271349	-1.569143
H	2.829582	-1.494062	-0.564543
C	1.271543	1.618894	-0.257353
H	0.981532	2.068948	-1.209758
H	0.428382	1.743543	0.423037
H	2.118229	2.175183	0.13277
O	4.816131	-0.447071	0.849809
H	4.709182	0.166775	-1.056326
H	4.294506	-0.445663	1.656512
O	-1.65704	-1.203881	0.170376
S	-2.977825	0.175802	-0.159848
O	-4.200491	-0.48948	0.158512
O	-2.546084	1.300568	0.611652

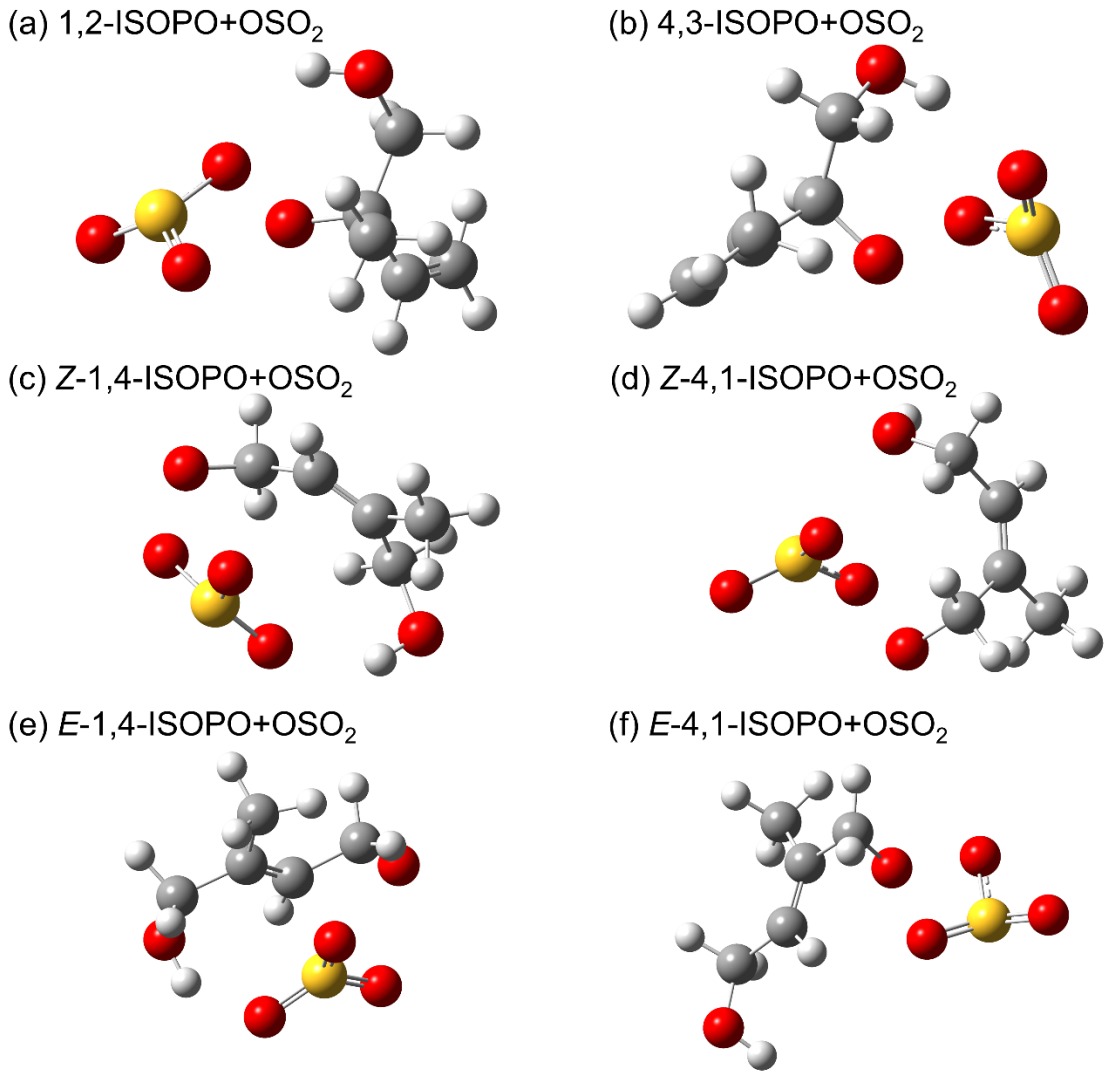

Figure S6: Transition-state optimized structures of the six isomers in the unimolecular reactions of ISOPOOSO$_2$s. The Cartesian coordinates of each structure are listed in Tables S15–S20.

Table S15: Optimised coordinates of the transition state of 1,2−ISOPO+OSO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	1.318035	-0.097968	0.236298
C	2.02395	1.110266	-0.379111
C	2.152737	-1.369275	0.158078
C	3.284218	-1.505937	-0.516201
O	1.311416	2.313532	-0.215293
O	0.258258	-0.542676	-0.588844
O	-1.003586	0.628646	-0.552355
H	0.474509	2.247826	-0.682475
H	3.71984	-0.7066	-1.099528
H	3.825886	-2.441595	-0.488815
H	2.209878	0.903797	-1.436726
H	2.980691	1.251129	0.123739
H	1.737756	-2.20057	0.71493
C	0.874455	0.147122	1.669496
H	1.751163	0.320321	2.292762
H	0.233816	1.023745	1.722601
H	0.329625	-0.717165	2.045024
S	-2.315044	0.023237	-0.084674
O	-2.987821	-0.792427	-1.065005
O	-2.346122	-0.326815	1.315487

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	1.311781	-0.099237	0.234398
C	2.017579	1.110886	-0.377056
C	2.142808	-1.371185	0.145551
C	3.27906	-1.502928	-0.52146
O	1.309435	2.315406	-0.203561
O	0.244251	-0.534478	-0.590106
O	-1.000675	0.629064	-0.535534
H	0.471827	2.256365	-0.670266
H	3.721931	-0.697588	-1.090949
H	3.81735	-2.440709	-0.502315
H	2.199315	0.909713	-1.436447
H	2.976564	1.24631	0.122987
H	1.721912	-2.208252	0.689302
C	0.874488	0.138902	1.670571
H	1.754482	0.306248	2.290754
H	0.236637	1.017027	1.7317
H	0.329306	-0.726144	2.043763
S	-2.307764	0.021899	-0.081683
O	-2.973387	-0.769537	-1.06989
O	-2.337048	-0.349452	1.301139

Table S16: Optimised coordinates of the transition state of 4,3-ISOPO+OSO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	-1.308086	0.351989	-0.520643
C	-0.97119	1.500286	0.430262
C	-2.401098	-0.56193	0.024354
C	-2.326387	-0.921982	1.477436
C	-3.334459	-1.008019	-0.807307
O	-0.315134	2.560061	-0.220006
O	-0.294713	-0.603409	-0.66803
O	1.196559	0.208707	-1.006851
H	0.550757	2.259062	-0.50576
H	-1.593506	0.760736	-1.492742
H	-3.328991	-0.743765	-1.856226
H	-4.136281	-1.644458	-0.455289
H	-2.471524	-0.04445	2.109515
H	-3.090191	-1.654325	1.728591
H	-1.348795	-1.339706	1.71973
H	-0.390234	1.113885	1.272973
H	-1.906567	1.911082	0.810286
S	2.263837	-0.23569	-0.023009
O	2.785382	-1.560547	-0.246491
O	2.070564	0.269051	1.317935

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	-1.298154	0.347308	-0.518779
C	-0.963971	1.501357	0.425628
C	-2.400387	-0.555632	0.023475
C	-2.334988	-0.912428	1.478009
C	-3.33567	-0.994684	-0.809579
O	-0.302275	2.556524	-0.226689
O	-0.284513	-0.613471	-0.651887
O	1.18931	0.186334	-1.003845
H	0.567839	2.255825	-0.499347
H	-1.572481	0.749052	-1.496843
H	-3.32528	-0.732637	-1.859024
H	-4.144004	-1.623322	-0.458473
H	-2.473147	-0.031571	2.107068
H	-3.107667	-1.635661	1.728361
H	-1.362965	-1.339941	1.725522
H	-0.389131	1.1197	1.274685
H	-1.900837	1.916228	0.797535
S	2.258062	-0.239989	-0.025144
O	2.768795	-1.559791	-0.227934
O	2.075895	0.286232	1.296641

Table S17: Optimised coordinates of the transition state of *Z*−1,4-ISOPO+OSO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	1.513392	0.607864	0.443169
C	2.138237	0.348929	-0.90631
C	0.416053	1.341621	0.633625
C	-0.452877	1.971413	-0.404818
O	2.577631	-0.983063	-1.057008
H	1.799292	-1.549499	-1.056759
H	-0.190006	1.725674	-1.434212
H	3.034396	0.968559	-0.990195
H	1.469056	0.629749	-1.721237
H	0.066555	1.504766	1.648561
C	2.240782	-0.00832	1.599921
H	2.193493	-1.095375	1.534433
H	3.299121	0.257645	1.569947
H	1.814961	0.307446	2.549212
O	-1.815567	1.733683	-0.169687
H	-0.435276	3.069526	-0.318279
S	-1.43634	-1.062841	-0.024863
O	-2.183521	0.143014	-0.58774
O	-0.292304	-1.507639	-0.792798
O	-1.4367	-1.183755	1.410084

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	1.519173	0.604377	0.441463
C	2.137151	0.337157	-0.909714
C	0.425542	1.343155	0.633929
C	-0.443376	1.97442	-0.40293
O	2.574238	-0.996202	-1.05493
H	1.795464	-1.561915	-1.046954
H	-0.173149	1.741105	-1.433029
H	3.033569	0.955188	-1.001971
H	1.464013	0.613743	-1.722852
H	0.080233	1.509357	1.649762
C	2.248665	-0.010902	1.597306
H	2.194976	-1.097964	1.536846
H	3.308348	0.248789	1.560882
H	1.829467	0.311658	2.547253
O	-1.806618	1.719065	-0.178231
H	-0.437863	3.071188	-0.305158
S	-1.443034	-1.054889	-0.022966
O	-2.150136	0.14597	-0.625377
O	-0.291551	-1.526022	-0.740692
O	-1.492114	-1.143085	1.402026

Table S18: Optimised coordinates of the transition state of *Z*-4,1-ISOPO+OSO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	2.082052	-0.316787	0.104528
C	1.081128	-1.034123	0.971013
C	2.040003	0.997306	-0.099904
C	1.032417	1.973978	0.435172
O	0.158794	-1.78481	0.218911
H	1.540252	2.890575	0.747456
H	0.560372	-0.384234	1.671664
H	1.579144	-1.824267	1.551689
H	2.782535	1.423015	-0.771377
C	3.080159	-1.208874	-0.569899
H	3.710697	-1.710611	0.167452
H	2.561821	-1.987469	-1.13265
H	3.71919	-0.652204	-1.251591
O	0.026473	2.288343	-0.528479
H	0.49206	1.586908	1.293766
H	0.449032	2.484832	-1.368779
S	-1.909905	-0.067942	-0.157694
O	-1.768893	0.441502	1.185189
O	-3.1315	-0.720212	-0.560215
O	-0.62627	-0.625882	-0.744153

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	2.07637	-0.325034	0.104516
C	1.070211	-1.033486	0.971772
C	2.04545	0.989455	-0.099231
C	1.045723	1.974031	0.43612
O	0.139236	-1.775847	0.219486
H	1.560607	2.88731	0.746607
H	0.555779	-0.379207	1.67267
H	1.560809	-1.829187	1.550509
H	2.790895	1.409182	-0.771235
C	3.066024	-1.225464	-0.571362
H	3.692418	-1.733651	0.165084
H	2.540453	-1.998772	-1.134693
H	3.709662	-0.673849	-1.252828
O	0.041182	2.293581	-0.526517
H	0.503907	1.591816	1.296064
H	0.463661	2.481032	-1.368924
S	-1.907605	-0.063743	-0.157559
O	-1.764395	0.438431	1.175294
O	-3.119596	-0.707749	-0.55997
O	-0.631325	-0.62489	-0.737442

Table S19: Optimised coordinates of the transition state of *E*−1,4-ISOPO+OSO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	-1.520616	0.61734	0.186089
C	-2.468465	-0.515162	-0.125678
C	-0.623863	1.006169	-0.716973
C	0.487856	1.978557	-0.518834
O	-2.241388	-1.165763	-1.347469
H	-1.378212	-1.593464	-1.310562
H	0.594696	2.343645	0.503281
H	-3.491098	-0.13118	-0.156789
H	-2.422763	-1.220363	0.714117
H	-0.634162	0.534714	-1.693282
C	-1.700554	1.190427	1.558662
H	-0.962775	1.946698	1.809558
H	-2.689856	1.646953	1.636739
H	-1.646944	0.398904	2.306493
O	1.705701	1.471435	-0.999134
O	2.23013	0.213947	-0.010754
H	0.381385	2.854169	-1.179061
S	1.374903	-0.984858	0.398929
O	0.815821	-1.749335	-0.692904
O	0.640378	-0.856076	1.636142

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	-1.524056	0.615799	0.182549
C	-2.467873	-0.521836	-0.122454
C	-0.629177	1.002606	-0.723285
C	0.480932	1.977213	-0.531069
O	-2.236074	-1.18107	-1.338911
H	-1.369398	-1.601366	-1.300181
H	0.578328	2.36056	0.485027
H	-3.491554	-0.141253	-0.159238
H	-2.422091	-1.220435	0.722771
H	-0.638634	0.525144	-1.696618
C	-1.704205	1.19415	1.552761
H	-0.978114	1.964714	1.793966
H	-2.700712	1.633882	1.635242
H	-1.631762	0.407879	2.304569
O	1.704641	1.457098	-0.987877
O	2.213213	0.237891	0.03219
H	0.384291	2.839626	-1.209047
S	1.37703	-0.977428	0.400726
O	0.86105	-1.720267	-0.711918
O	0.620098	-0.885839	1.614125

Table S20: Optimized coordinates of the transition state of *E*-4,1-ISOPO+OSO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	-1.527469	0.9681	0.259614
C	-0.166291	1.274375	0.888022
C	-1.866467	-0.348449	0.23171
C	-3.185341	-0.861428	-0.225066
O	0.112089	0.917518	-0.387781
H	-3.344945	-0.527096	-1.260893
H	0.191569	0.582228	1.644886
H	-0.046112	2.332448	1.114089
H	-1.112008	-1.071034	0.535981
C	-2.375633	2.097207	-0.225114
H	-3.020828	2.458169	0.577534
H	-1.742711	2.921375	-0.547493
H	-3.003037	1.797955	-1.063168
O	-3.333706	-2.247077	-0.087073
H	-3.981322	-0.396905	0.364165
H	-2.730409	-2.704977	-0.678579
O	2.054805	0.991572	-0.469042
S	2.447635	-0.482812	-0.259796
O	3.888117	-0.586539	-0.053882
O	1.573052	-1.131222	0.734678

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	-1.527163	0.96584	0.26167
C	-0.161159	1.261244	0.886043
C	-1.876493	-0.347279	0.232542
C	-3.200415	-0.849969	-0.221784
O	0.113408	0.901419	-0.38955
H	-3.362695	-0.509248	-1.255003
H	0.192322	0.567159	1.643211
H	-0.032519	2.318593	1.11092
H	-1.128003	-1.076674	0.534906
C	-2.366085	2.103042	-0.220148
H	-2.999296	2.475477	0.586763
H	-1.726039	2.917971	-0.551976
H	-3.004763	1.807971	-1.051112
O	-3.356006	-2.235524	-0.090506
H	-3.990982	-0.384176	0.373683
H	-2.760233	-2.693548	-0.689479
O	2.051026	0.972189	-0.479752
S	2.456241	-0.482686	-0.25476
O	3.886221	-0.571961	-0.054594
O	1.592881	-1.128349	0.732441

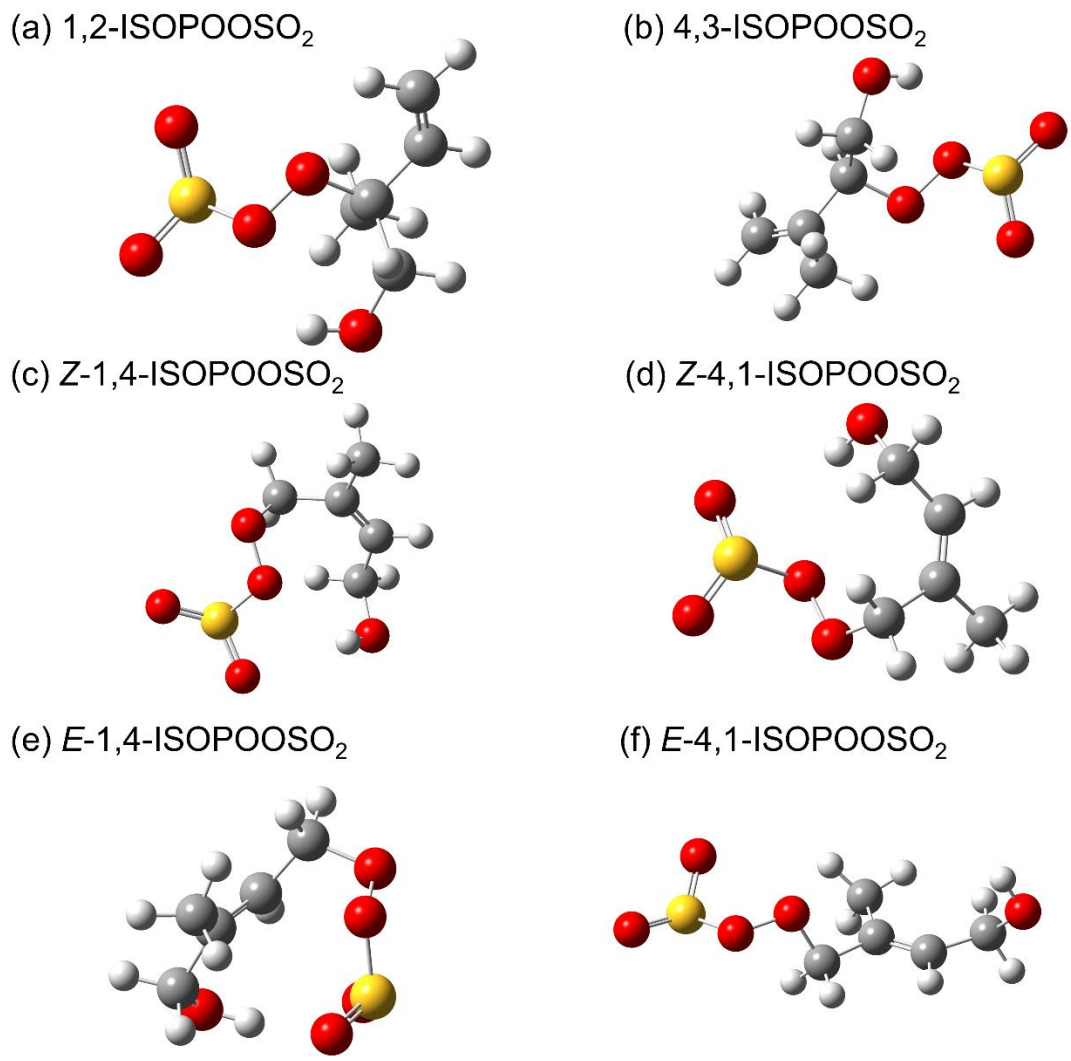

Figure S7: Optimized structures of the six isomers of $ISOPOOSO_2$. The Cartesian coordinates of each structure are listed in Tables S21–S26.

Table S21: Optimized coordinates of 1,2-ISOPOOSO$_2$ calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	1.366383	0.06483	0.235541
C	1.817134	1.346349	-0.484355
C	2.507566	-0.915751	0.215657
C	2.585271	-2.014513	-0.516312
O	1.011807	2.474868	-0.249032
O	0.324139	-0.599053	-0.518519
O	-0.756519	0.289622	-0.695979
H	0.16056	2.34653	-0.675038
H	1.788617	-2.320339	-1.179344
H	3.459811	-2.647333	-0.459359
H	1.902381	1.113953	-1.550106
H	2.810229	1.603261	-0.115811
H	3.322853	-0.639723	0.87579
C	0.903181	0.333819	1.6583
H	1.735524	0.729949	2.239357
H	0.113811	1.082659	1.679581
H	0.561724	-0.592267	2.11963
S	-2.06738	-0.2178	0.204669
O	-3.089192	0.720689	-0.199538
O	-2.222064	-1.646162	0.055268

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	1.364084	0.065913	0.237199
C	1.808211	1.34545	-0.490422
C	2.507846	-0.911763	0.215387
C	2.589223	-2.007789	-0.5203
O	1.002802	2.473705	-0.254245
O	0.320582	-0.604816	-0.508841
O	-0.763258	0.284052	-0.686623
H	0.149264	2.343084	-0.674876
H	1.793892	-2.313724	-1.184879
H	3.465481	-2.638367	-0.464867
H	1.887251	1.109051	-1.555785
H	2.803208	1.605191	-0.129087
H	3.321834	-0.635545	0.877016
C	0.906713	0.339489	1.660851
H	1.739619	0.743335	2.235771
H	0.112822	1.083493	1.682116
H	0.572286	-0.586071	2.128224
S	-2.065152	-0.220494	0.198623
O	-3.076975	0.713556	-0.198248
O	-2.215612	-1.637789	0.059471

Table S22: Optimized coordinates of 4,3-ISOPOOSO$_2$ calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	-1.267653	0.480824	-0.388768
C	-0.841589	1.3181	0.81494
C	-2.451712	-0.403901	-0.095264
C	-2.318022	-1.333544	1.075484
C	-3.540143	-0.31747	-0.846486
O	-0.149281	2.493868	0.472844
O	-0.243799	-0.457716	-0.788709
O	0.982699	0.23406	-0.931432
H	0.600576	2.276028	-0.087006
H	-1.474517	1.144535	-1.230261
H	-3.594072	0.359907	-1.688423
H	-4.412698	-0.92253	-0.637652
H	-2.200705	-0.775297	2.006919
H	-3.197799	-1.965802	1.167597
H	-1.438153	-1.968688	0.964927
H	-0.26567	0.689714	1.506878
H	-1.740795	1.638977	1.340312
S	2.080885	-0.346216	0.183276
O	3.293082	0.340888	-0.198059
O	1.985348	-1.786283	0.240962

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	-1.264454	0.476227	-0.39052
C	-0.84501	1.325075	0.807628
C	-2.450005	-0.406123	-0.095407
C	-2.323572	-1.323863	1.085491
C	-3.533721	-0.327643	-0.854305
O	-0.15581	2.500177	0.457336
O	-0.239301	-0.466656	-0.775715
O	0.989256	0.227395	-0.918264
H	0.605621	2.278833	-0.085139
H	-1.466731	1.131955	-1.239329
H	-3.582466	0.341083	-1.703441
H	-4.407494	-0.930683	-0.644715
H	-2.209779	-0.756314	2.011706
H	-3.204859	-1.953719	1.179724
H	-1.444327	-1.961635	0.985747
H	-0.268993	0.704543	1.506406
H	-1.746989	1.647857	1.327014
S	2.081413	-0.349896	0.178877
O	3.278365	0.346376	-0.188774
O	1.992988	-1.777995	0.235752

Table S23: Optimized coordinates of *Z*-1,4-ISOPOOSO$_2$ calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	-2.232055	0.188592	0.107994
C	-1.626165	-0.964553	0.873213
C	-1.684671	1.398796	0.005761
C	-0.384151	1.829846	0.598029
O	-1.324672	-2.052596	0.021426
H	-0.518472	-1.859624	-0.468574
H	-0.10539	1.27114	1.492474
H	-2.36359	-1.340526	1.58509
H	-0.747088	-0.665218	1.446963
H	-2.187774	2.14462	-0.599834
C	-3.520966	-0.149658	-0.577368
H	-3.380228	-1.017544	-1.221634
H	-4.278911	-0.421597	0.16071
H	-3.892645	0.682185	-1.171173
O	0.704415	1.748791	-0.344605
O	0.818042	0.400689	-0.739492
H	-0.38414	2.891301	0.843259
S	1.998497	-0.357056	0.149636
O	1.893445	-1.715357	-0.342382
O	3.230062	0.394726	0.091649

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	-2.236368	0.189095	0.109214
C	-1.631085	-0.962631	0.876612
C	-1.684057	1.39642	-0.000055
C	-0.381849	1.8254	0.590245
O	-1.324544	-2.049572	0.024869
H	-0.533955	-1.841347	-0.48385
H	-0.105394	1.27099	1.487844
H	-2.369555	-1.341622	1.585613
H	-0.754159	-0.66165	1.452785
H	-2.184703	2.14122	-0.608947
C	-3.527871	-0.147653	-0.572077
H	-3.392516	-1.020404	-1.210933
H	-4.28586	-0.411044	0.169038
H	-3.896716	0.681993	-1.170709
O	0.70671	1.736963	-0.351301
O	0.822428	0.383146	-0.734022
H	-0.378288	2.888308	0.829381
S	2.000612	-0.358644	0.14441
O	1.920675	-1.703464	-0.352583
O	3.207071	0.411435	0.114986

Table S24: Optimized coordinates of *Z*-4,1-ISOPOOSO$_2$ calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	2.079468	-0.49084	0.111994
C	0.974086	-1.219836	0.819899
C	2.176496	0.836002	0.101786
C	1.248682	1.834957	0.727818
O	-0.052653	-1.647553	-0.092477
H	1.816856	2.526207	1.350555
H	0.511684	-0.645582	1.622255
H	1.32131	-2.16991	1.22811
H	2.981956	1.283908	-0.47289
C	3.024312	-1.377431	-0.645069
H	3.564993	-2.039271	0.034934
H	2.470764	-2.012711	-1.339522
H	3.748134	-0.795246	-1.210391
O	0.624134	2.638107	-0.256377
H	0.503203	1.361678	1.371858
H	0.06012	2.082427	-0.80413
O	-0.607284	-0.49388	-0.681732
S	-1.986566	-0.036177	0.13291
O	-2.842568	-1.18171	0.335134
O	-2.398159	1.121315	-0.630285

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	2.076005	-0.49497	0.111025
C	0.968828	-1.219892	0.820394
C	2.17803	0.831497	0.101255
C	1.253782	1.833459	0.727702
O	-0.060802	-1.6436	-0.090501
H	1.824028	2.52261	1.350854
H	0.510206	-0.6448	1.624115
H	1.313031	-2.1719	1.226815
H	2.984567	1.276659	-0.474051
C	3.016626	-1.3849	-0.647382
H	3.556075	-2.048505	0.031888
H	2.459782	-2.018358	-1.340855
H	3.741592	-0.805333	-1.213931
O	0.632737	2.638975	-0.256942
H	0.505975	1.362571	1.370724
H	0.069707	2.084302	-0.806616
O	-0.615161	-0.484295	-0.674823
S	-1.986198	-0.035247	0.127178
O	-2.829103	-1.173277	0.338418
O	-2.395851	1.11414	-0.626372

Table S25: Optimized coordinates of *E*-1,4-ISOPOOSO$_2$ calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	-1.486234	0.564138	0.308829
C	-2.425782	-0.598311	0.100268
C	-0.815747	1.078283	-0.720209
C	0.282408	2.078139	-0.622403
O	-2.383833	-1.175465	-1.179151
H	-1.4907	-1.500684	-1.337793
H	0.246137	2.684859	0.27997
H	-3.454153	-0.266356	0.261877
H	-2.208717	-1.342091	0.877804
H	-0.993536	0.667464	-1.705422
C	-1.377045	0.990307	1.742488
H	-0.834727	1.921418	1.87527
H	-2.374399	1.110931	2.170256
H	-0.869141	0.21587	2.32051
O	1.581609	1.439755	-0.678525
O	1.672705	0.620134	0.469839
H	0.328946	2.732185	-1.492716
S	1.53618	-0.997433	0.117232
O	0.92387	-1.195252	-1.180421
O	0.956377	-1.556674	1.320845

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	-1.499926	0.535822	0.330157
C	-2.424567	-0.637753	0.117817
C	-0.8567	1.079079	-0.70102
C	0.230276	2.090952	-0.603102
O	-2.399135	-1.189733	-1.173047
H	-1.504733	-1.499001	-1.354355
H	0.19885	2.684488	0.30822
H	-3.454789	-0.32664	0.306688
H	-2.179653	-1.39265	0.876316
H	-1.045129	0.682765	-1.690247
C	-1.367507	0.935406	1.769577
H	-0.846333	1.877606	1.908999
H	-2.356728	1.020616	2.223788
H	-0.825377	0.163251	2.319248
O	1.535612	1.468538	-0.685604
O	1.648067	0.6348	0.453951
H	0.258152	2.757804	-1.464459
S	1.565298	-0.965502	0.086235
O	0.920356	-1.173438	-1.179905
O	1.072789	-1.557823	1.297789

Table S26: Optimized coordinates of *E*-4,1-ISOPOOSO$_2$ calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
C	1.536542	0.169955	-0.466496
C	0.296887	-0.642043	-0.70403
C	2.710414	-0.453881	-0.403889
C	4.059012	0.160902	-0.194682
O	-0.488356	-0.519168	0.490513
H	3.991368	1.235005	-0.014792
H	0.511705	-1.693365	-0.890898
H	-0.283553	-0.230877	-1.537443
H	2.728761	-1.535805	-0.49781
C	1.296504	1.647689	-0.351851
H	1.017947	2.057995	-1.325412
H	0.46572	1.840474	0.327655
H	2.167363	2.19009	0.003171
O	4.761525	-0.487127	0.85266
H	4.670741	0.016677	-1.086261
H	4.240292	-0.423433	1.657129
O	-1.75537	-1.079078	0.244211
S	-2.842775	0.140031	-0.107001
O	-4.106811	-0.557991	-0.122347
O	-2.58875	1.269239	0.760259

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
C	1.53629	0.173064	-0.46881
C	0.29451	-0.635307	-0.708167
C	2.708067	-0.454447	-0.403488
C	4.058251	0.156161	-0.192238
O	-0.490208	-0.510269	0.486477
H	3.993792	1.230621	-0.013327
H	0.506772	-1.687159	-0.894924
H	-0.283965	-0.221998	-1.541689
H	2.723152	-1.536496	-0.49654
C	1.300862	1.651665	-0.355688
H	1.024124	2.061932	-1.32976
H	0.470351	1.847749	0.32319
H	2.17322	2.191609	-0.000618
O	4.756656	-0.493314	0.856956
H	4.671187	0.009207	-1.082547
H	4.233977	-0.427534	1.660317
O	-1.760605	-1.068761	0.237506
S	-2.841259	0.137494	-0.098247
O	-4.091744	-0.559607	-0.131546
O	-2.594142	1.25512	0.765381

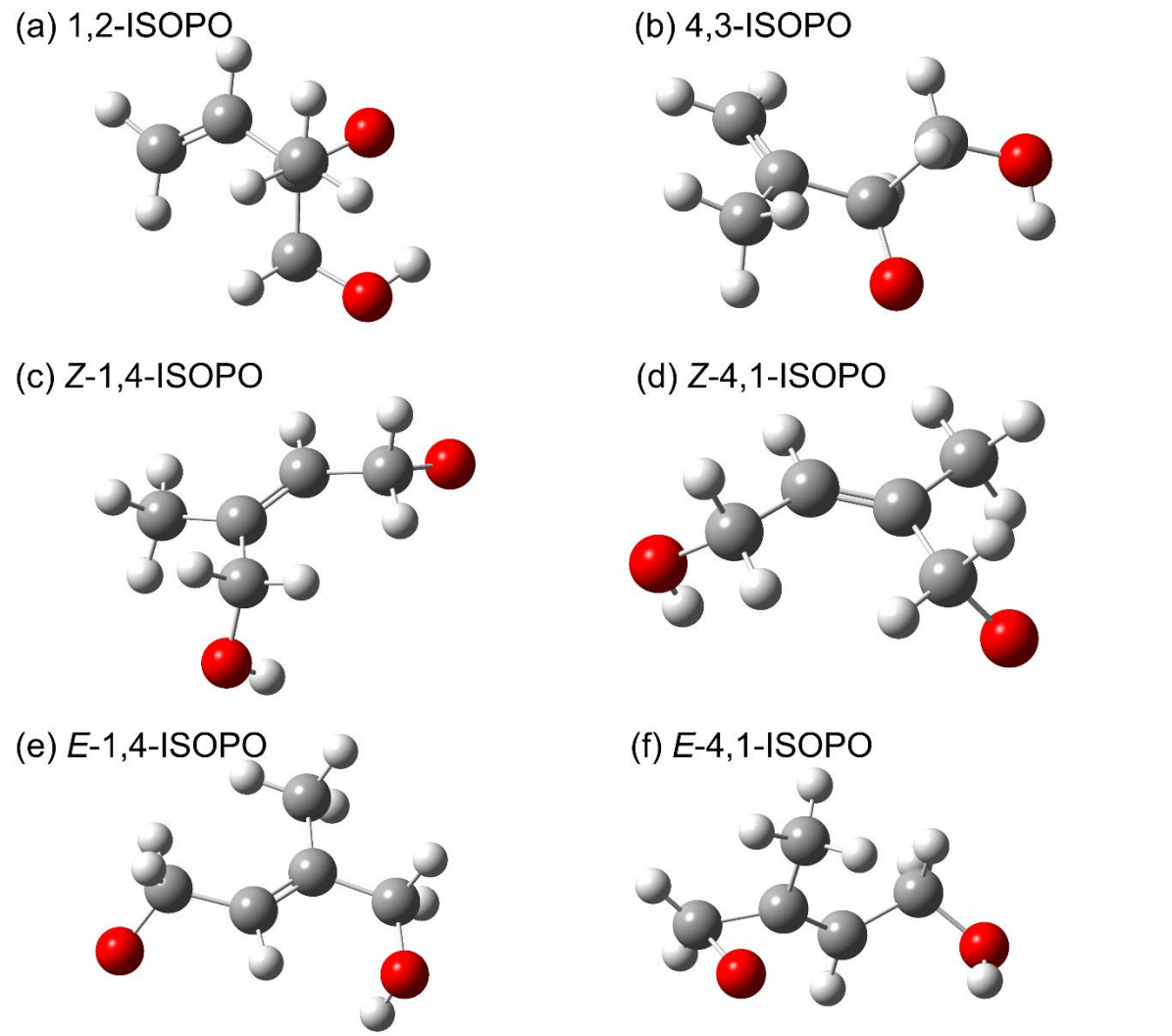

Figure S8: Optimized structures of the six isomers of ISOPO. The Cartesian coordinates of each structure are listed in Tables S27–S32.

Table S27: Optimized coordinates of 1,2-ISOPO calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

Atom	X	Y	Z
C	0.043547	0.322076	0.108387
C	-0.656089	-1.025719	-0.129551
C	1.547014	0.232441	0.190259
C	2.274331	-0.830498	-0.112064
O	-2.052935	-0.883911	-0.096412
O	-0.4589	0.904811	1.252472
H	-2.27073	-0.399121	0.707227
H	1.832657	-1.761217	-0.44356
H	3.352683	-0.803287	-0.0387
H	-0.310666	-1.736363	0.628208
H	-0.393651	-1.415105	-1.112902
H	2.021622	1.14769	0.528799
C	-0.348617	1.326777	-1.007268
H	0.037749	0.937671	-1.947974
H	-1.430627	1.412845	-1.061791
H	0.09452	2.299224	-0.806374

Table S28: Optimized coordinates of 4,3-ISOPO calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

Atom	X	Y	Z
C	0.237036	0.001477	0.515454
C	1.218191	-0.443121	-0.635849
C	-1.198827	-0.182985	0.083276
C	-1.829267	0.975538	-0.62515
C	-1.817367	-1.331773	0.320606
O	2.549378	-0.383417	-0.227322
O	0.602291	1.274685	0.79441
H	2.72516	0.502189	0.105367
H	0.504631	-0.658985	1.353015
H	-1.323932	-2.135354	0.854903
H	-2.833866	-1.506849	-0.005836
H	-1.224188	1.289279	-1.478355
H	-2.826525	0.720894	-0.976244
H	-1.891607	1.836391	0.040656
H	1.018167	0.184798	-1.508177
H	0.980205	-1.477324	-0.872061

Table S29: Optimized coordinates of *Z*-1,4-ISOPO calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

Atom	X	Y	Z
C	-0.527821	0.494496	0.16981
C	-1.165833	-0.818178	0.543947
C	0.786674	0.691759	0.102181
C	1.885463	-0.297713	0.360984
O	-2.021906	-1.300749	-0.480776
H	-1.501791	-1.417316	-1.280255
H	1.542892	-1.332433	0.468788
H	-1.810234	-0.670367	1.412345
H	-0.426027	-1.57294	0.812951
H	1.153677	1.673643	-0.18142
C	-1.504147	1.595218	-0.131407
H	-2.198021	1.287578	-0.913471
H	-2.105304	1.818725	0.752926
H	-0.995602	2.504213	-0.444737
O	2.910647	-0.226399	-0.547079
H	2.384467	-0.067413	1.322625

Table S30: Optimized coordinates of *Z*-4,1-ISOPO calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

Atom	X	Y	Z
C	0.589808	0.447975	0.156673
C	1.207863	-0.90806	0.398287
C	-0.719133	0.683579	0.215575
C	-1.833049	-0.285381	0.46863
O	2.148652	-1.272498	-0.529021
H	-2.338124	-0.036149	1.402712
H	0.478245	-1.712127	0.535874
H	1.778337	-0.88024	1.347833
H	-1.06219	1.700129	0.043014
C	1.5834	1.533419	-0.134953
H	2.295285	1.632848	0.688214
H	2.163417	1.289835	-1.024648
H	1.088281	2.490173	-0.283201
O	-2.833789	-0.188362	-0.533658
H	-1.478032	-1.313775	0.556734
H	-2.417464	-0.313006	-1.390363

Table S31: Optimized coordinates of *E*-1,4-ISOPO calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

Atom	X	Y	Z
C	0.52614	0.471163	0.040702
C	1.933928	-0.069635	-0.021445
C	-0.509933	-0.335438	0.240635
C	-1.956996	0.050009	0.306271
O	2.04874	-1.469671	0.034826
H	1.600064	-1.846821	-0.726705
H	-2.151081	1.097695	0.05252
H	2.500789	0.316729	0.829007
H	2.416738	0.328405	-0.923029
H	-0.327953	-1.395279	0.379333
C	0.465964	1.960981	-0.132569
H	-0.545133	2.355853	-0.120311
H	1.026602	2.454027	0.6648
H	0.934852	2.252274	-1.07452
O	-2.783541	-0.775748	-0.413006
H	-2.331091	-0.06201	1.342782

Table S32: Optimized coordinates of *E*-4,1-ISOPO calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

Atom	X	Y	Z
C	-0.810338	0.079924	-0.046424
C	-1.99651	-0.654119	-0.544943
C	0.50778	-0.530097	-0.21844
C	1.772644	0.20704	-0.465138
O	-1.683049	-0.659768	0.829286
H	1.638131	1.279249	-0.297487
H	-1.858583	-1.600198	-1.056353
H	-2.880377	-0.087922	-0.820501
H	0.551926	-1.612092	-0.210978
C	-0.907946	1.574776	0.107844
H	-0.558929	2.084137	-0.790284
H	-1.943485	1.853896	0.289322
H	-0.30745	1.915063	0.95182
O	2.846671	-0.294483	0.321105
H	2.105118	0.083435	-1.500156
H	2.550895	-0.346704	1.234091

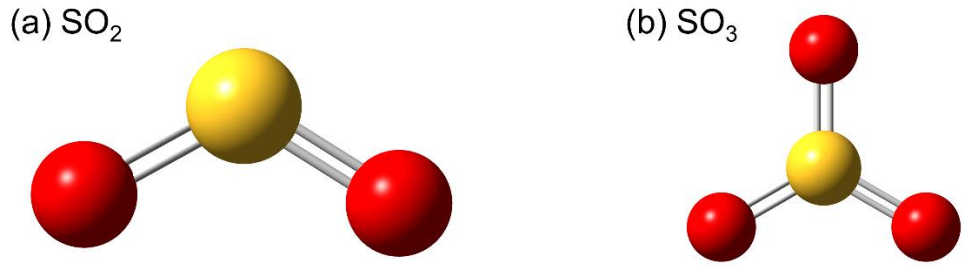

Figure S9: Optimized structures of SO_2 and SO_3. The Cartesian coordinates of each structure are listed in Tables S33–S34.

Table S33: Optimized coordinates of SO_2 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
S	0	0	0.370193
O	0	1.230522	-0.370193
O	0	-1.230522	-0.370193

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
S	0	0	0.362373
O	0	1.226801	-0.362373
O	0	-1.226801	-0.362373

Table S34: Optimized coordinates of SO_3 calculated by G16 at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

M06-2X/aug-cc-pVTZ			
Atom	X	Y	Z
S	0	0	0
O	0	1.4263524	0
O	-1.235257	-0.713176	0
O	1.2352574	-0.713176	0

M06-2X/aug-cc-pV(T+*d*)Z			
Atom	X	Y	Z
S	0	0	0
O	0	1.415585	0
O	1.225933	-0.707792	0
O	-1.225933	-0.707792	0

Table S35: Vibrational frequencies of ISOPOOs calculated by G16 at the M06-2X/aug-cc-pVTZ level of theory.

1,2-ISOPOO		4,3-ISOPOO		*E*-1,4-ISOPOO		*Z*-1,4-ISOPOO		*E*-4,1-ISOPOO		*Z*-4,1-ISOPOO	
Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity
68.0794	1.066505178	51.6663	74.55850574	54.9071	372.5281	62.5199	118.4697225	41.486	505.0454399	34.7671	208.2531282
92.565	28.40611271	73.2788	12.30374694	75.7794	219.8029	99.762	131.6402767	63.2509	75.2014361	95.5791	108.4635456
162.0164	131.5579929	143.6606	79.41550204	119.9619	72.77974	127.6349	95.15986906	90.9529	84.66288434	129.1149	64.87352561
224.5161	3.48980607	190.0684	11.46853836	146.9799	55.75335	159.5643	41.69052951	133.3771	9.81967043	146.9822	7.070502561
245.9977	75.36788131	207.5666	23.02344953	152.3166	30.2433	205.0727	15.14071835	187.9693	84.1709318	200.5371	8.088722641
262.5079	7.39498039	226.4178	106.646322	236.3628	86.16024	240.6813	32.96025375	236.9746	78.35208228	227.6645	86.99013457
320.9483	52.6784724	312.545	53.43874046	319.1585	979.9857	313.6211	11.53743622	295.2537	146.4553274	314.2169	23.87415464
324.0103	31.31700528	360.0373	29.49853736	329.7215	263.1633	388.5626	37.63803287	345.5986	973.6420049	386.6105	31.88232377
392.7227	81.05109264	417.2427	54.41355973	384.1586	354.0094	394.1968	31.51366158	350.4417	224.8641325	438.6272	18.52508147
447.2126	43.90443642	489.2456	953.6168429	435.2436	85.77812	488.2901	341.3802202	442.6079	77.79366338	478.4865	26.31325686
488.2658	685.5928314	535.8875	38.15811011	470.0076	74.84752	516.4122	442.9092147	503.1562	44.38670238	502.6372	734.4170389
516.2753	294.6291225	550.7283	43.21902775	574.7555	58.69685	567.7482	39.96366479	544.5858	10.83523971	537.7509	42.11209003
602.6739	57.60682481	558.3402	40.68063534	616.2259	10.87036	649.533	46.49515456	611.9552	67.63566676	655.1876	53.52664584
687.7454	109.404481	741.1967	2.86826678	804.9285	5.158427	791.8073	19.8767701	824.3061	11.11679972	796.8912	37.0453856
778.7684	17.99194925	856.411	75.02011095	857.513	45.52171	878.7629	32.65923591	883.6667	64.86299432	900.5033	15.62482411
872.8685	27.94278611	884.4988	0.909737192	922.2159	154.9613	919.0381	160.2434128	938.6359	72.91571081	930.549	117.8651589
939.1561	12.0477617	976.5118	157.3376442	973.1189	52.52652	958.8486	91.22475583	978.7234	152.9112873	964.6506	79.46614954
982.347	35.95646508	993.0029	3.383545493	987.1298	57.48867	995.3155	54.95125959	995.6205	11.13730589	993.7919	50.48286752
995.4191	164.7412367	1024.788	113.9926818	1031.7231	22.64359	1057.6803	88.16894648	1054.6201	125.6999376	1063.9538	22.35846869
1040.5328	34.12293756	1055.7271	81.89523432	1066.1052	66.15647	1071.3416	1.264209675	1071.3006	66.19498787	1077.485	8.730144846
1047.2176	22.35388803	1076.6906	3.418084172	1127.5333	122.4919	1102.4308	273.6829643	1089.2137	310.5105403	1090.5031	322.673836
1124.4941	448.215495	1107.0528	5.230654147	1140.122	209.0315	1123.5434	14.17095682	1139.3669	46.66196932	1133.1268	77.30960176
1164.3874	18.31839825	1131.3566	376.8393792	1219.9033	47.19275	1199.6425	52.79246325	1197.4632	6.79700935	1189.3171	38.20246762
1213.892	86.81194962	1232.2502	75.93953089	1226.5315	4.725355	1243.1467	16.18676256	1238.4382	11.79419424	1239.5725	5.895080126
1223.7355	21.54707622	1280.7493	47.88245108	1253.874	11.4581	1273.0391	36.60355549	1252.0509	17.04601481	1275.6705	18.66275565
1280.3172	132.3441359	1299.9689	54.87639462	1296.6055	31.87289	1299.9756	17.14797937	1317.2772	82.09372808	1301.3128	36.66205736
1313.5598	4.223375303	1316.3932	16.26678827	1352.7524	5.058585	1359.6648	2.704656706	1348.2354	4.379877598	1352.7196	3.064775415
1331.2706	10.23996912	1345.9411	48.57644744	1381.7674	33.17416	1386.6385	44.21186031	1373.0948	65.7417759	1378.2533	18.13915966
1379.5987	10.04695228	1393.7552	18.76262053	1390.8621	68.69615	1400.4987	11.010804	1392.2429	65.5032449	1399.6829	6.297550356
1407.8314	45.26496367	1417	14.35028755	1418.1423	63.54517	1412.6079	23.13052439	1423.2866	81.52904911	1417.325	11.04108812
1438.7268	80.55759584	1437.6452	132.1912531	1432.69	8.549405	1428.9275	123.1253597	1433.1705	35.16543028	1434.5479	178.6600796
1456.6476	30.75153577	1460.6996	4.545461699	1478.9303	9.696662	1479.7495	27.93886678	1473.9947	15.46127104	1481.5115	21.05760747
1488.2851	20.0704912	1484.8553	24.97391201	1483.2861	16.75197	1489.0624	14.73228881	1485.5026	14.09915831	1489.0721	33.28078692
1489.3819	1.690706484	1498.7478	35.11207225	1492.6951	13.17518	1495.9625	27.82407759	1492.4762	28.40202211	1498.1183	12.36988346
1499.2508	21.58916762	1499.9618	9.192603584	1506.8527	41.91659	1527.024	15.66865411	1513.8684	11.15863462	1531.308	13.03001818
1736.1037	11.90198708	1753.4796	25.52015466	1764.8913	51.73539	1758.2354	48.97067092	1765.7682	9.251827242	1767.3055	8.126625286
3042.8959	35.44562533	3036.789	34.43757834	3017.5448	46.3969	3056.2916	14.6429287	3065.0414	3.310178928	3051.7227	17.6970428
3078.3333	7.809974464	3060.2444	14.80430571	3059.9798	19.91479	3071.5251	38.34063363	3073.6624	38.29619147	3058.2417	44.82760365
3116.0331	14.3089305	3106.339	8.263033379	3082.2545	14.77858	3110.3292	16.46125631	3088.9602	12.61177255	3104.8327	8.809526653
3153.7076	9.065904922	3114.6078	16.90193263	3110.9016	11.25877	3114.706	10.84296322	3108.1283	15.95295191	3109.2078	21.41954079
3173.0965	4.110475633	3117.0454	3.996250561	3111.9927	21.43101	3119.7585	39.02699929	3117.5777	6.490750947	3116.673	29.08751198
3174.1766	4.62060636	3156.7505	14.29510145	3164.3087	5.647901	3153.097	13.53316832	3156.1147	1.814376715	3153.0718	8.726623896
3184.7225	3.738585239	3166.9265	3.049371141	3180.9769	13.62801	3167.5833	1.449117579	3161.9169	15.91006429	3165.6117	17.70042807
3268.177	2.855536076	3252.0947	7.905695506	3198.1201	3.687497	3182.3528	16.33929673	3177.0357	16.14915535	3179.4859	7.298515389
3848.1863	72.28483732	3850.3186	81.74458852	3869.1813	41.01009	3824.9097	89.44815601	3872.0786	38.8187687	3824.7013	86.95479406

Table S36: Vibrational frequencies of ISOPOOs calculated by G16 at the M06-2X/aug-cc-pV(T+*d*)Z level of theory.

1,2-ISOPOO		4,3-ISOPOO		*E*-1,4-ISOPOO		*Z*-1,4-ISOPOO		*E*-4,1-ISOPOO		*Z*-4,1-ISOPOO	
Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity
68.0795	1.066503611	51.5564	75.32099652	54.9071	372.5281	62.5184	118.4661838	41.4842	505.0673539	34.7665	208.2567222
92.562	28.40703338	73.1481	11.69853682	75.7794	219.8029	99.7615	131.6409365	63.2506	75.20179279	95.5785	108.4642265
162.0151	131.5590485	143.7296	79.60497859	119.9619	72.77974	127.6346	95.16009272	90.9517	84.65961508	129.1148	64.87357585
224.5147	3.489827831	190.1612	11.38531923	146.9799	55.75335	159.5635	41.69323872	133.3764	9.819721967	146.981	7.070560287
245.9973	75.36800386	207.7383	23.15613144	152.3166	30.2433	205.0746	15.14057808	187.9688	84.17540044	200.5373	8.088714574
262.5075	7.394991658	226.3432	106.1297953	236.3628	86.16024	240.6816	32.96021267	236.9744	78.35383188	227.6645	86.99013457
320.9483	52.68717342	312.6458	53.03870775	319.1585	979.9857	313.6208	11.53617521	295.2531	146.470488	314.217	23.87287742
324.0103	31.31208025	360.0511	29.63812385	329.7215	263.1633	388.5624	37.63599883	345.5971	973.7616657	386.6116	31.88223306
392.7224	81.05623371	417.2896	54.4265646	384.1586	354.0094	394.1965	31.51267353	350.4412	224.7369534	438.6273	18.52598677
447.2124	43.90713223	489.6855	952.2656645	435.2436	85.77812	488.2914	341.3392777	442.6078	77.79187828	478.4866	26.31575262
488.2633	685.6396458	535.9854	38.42355813	470.0076	74.84752	516.4137	442.9473267	503.156	44.38672002	502.6361	734.416265
516.274	294.5835006	550.7875	43.32158003	574.7555	58.69685	567.7479	39.9636859	544.5856	10.83524369	537.7513	42.11205871
602.6736	57.60552959	558.3667	40.48436711	616.2259	10.87036	649.5328	46.49578307	611.9548	67.63636288	655.1873	53.52667035
687.7451	109.4033685	741.2913	2.857675541	804.9285	5.158427	791.8072	19.87677261	824.3059	11.11680241	796.8915	37.04537166
778.7687	17.99143005	856.5033	74.97429854	857.513	45.52171	878.7628	32.65923963	883.6658	64.861706	900.5035	15.62570668
872.868	27.94280212	884.5026	0.910184317	922.2159	154.9613	919.0381	160.2429788	938.636	72.91740312	930.5483	117.8656763
939.1561	12.04818649	976.5776	157.3911788	973.1189	52.52652	958.8482	91.22437783	978.7234	152.9125101	964.6508	79.46447883
982.3468	35.95687851	993.0416	3.336812352	987.1298	57.48867	995.3151	54.95088086	995.6199	11.13530913	993.7925	50.48323847
995.4176	164.7418857	1024.8489	114.0579224	1031.7231	22.64359	1057.68	88.17198896	1054.6198	125.6992168	1063.9544	22.35770617
1040.53	34.12724679	1055.7588	81.86027852	1066.1052	66.15647	1071.3421	1.264581459	1071.3007	66.19088542	1077.4853	8.730512666
1047.2171	22.35008918	1076.7259	3.422047742	1127.5333	122.4919	1102.4292	273.6808284	1089.2142	310.5144267	1090.5029	322.6749927
1124.4948	448.2166351	1107.0432	5.286195733	1140.122	209.0315	1123.5433	14.16989286	1139.3665	46.66338627	1133.1271	77.30852508
1164.3881	18.31838724	1131.3255	376.663197	1219.9033	47.19275	1199.6422	52.7921439	1197.4628	6.796345312	1189.3169	38.20280948
1213.892	86.81260691	1232.1984	76.12662044	1226.5315	4.725355	1243.1472	16.1880397	1238.4386	11.7938683	1239.5727	5.895401011
1223.7354	21.54675197	1280.76	47.71384822	1253.874	11.4581	1273.0396	36.60197424	1252.0503	17.04602298	1275.6711	18.66274688
1280.3169	132.3426089	1300.1662	55.43510283	1296.6055	31.87289	1299.9756	17.14797937	1317.2779	82.09368446	1301.3131	36.66143577
1313.5614	4.223977576	1316.3911	15.94799969	1352.7524	5.058585	1359.6648	2.704363296	1348.2356	4.379876948	1352.7195	3.064775642
1331.2703	10.2402711	1345.9521	48.53218329	1381.7674	33.17416	1386.6386	44.21185712	1373.0948	65.74206644	1378.2534	18.13886889
1379.5992	10.04665947	1393.692	18.78980606	1390.8621	68.69615	1400.4989	11.01051758	1392.2426	65.50411865	1399.6833	6.297833578
1407.8323	45.26606822	1417.0147	14.33324656	1418.1423	63.54517	1412.6083	23.13023543	1423.2866	81.52764763	1417.3257	11.04108267
1438.7263	80.5562374	1437.6171	132.1341743	1432.69	8.549405	1428.927	123.1267987	1433.1702	35.165716	1434.5479	178.6592453
1456.6466	30.75155688	1460.7301	4.544001241	1478.9303	9.696662	1479.7492	27.93860285	1473.9946	15.46100143	1481.5113	21.05734104
1488.2847	20.07049659	1484.8792	24.97942074	1483.2861	16.75197	1489.0622	14.73121914	1485.5026	14.09969542	1489.072	33.2818608
1489.3816	1.690438969	1498.7633	34.67065006	1492.6951	13.17518	1495.9626	27.82514244	1492.4759	28.40176052	1498.1182	12.36908541
1499.2506	21.58890441	1499.9776	9.627889491	1506.8527	41.91659	1527.0236	15.66865822	1513.8684	11.15837109	1531.3079	13.03001903
1736.1027	11.90199394	1753.5617	25.53056246	1764.8913	51.73539	1758.2351	48.97067927	1765.7681	9.251827765	1767.3036	8.126408289
3042.8952	35.44563348	3036.6486	34.43549207	3017.5448	46.3969	3056.2891	14.64241855	3065.04	3.309789966	3051.7233	17.6969086
3078.3348	7.809970658	3060.1108	14.80195359	3059.9798	19.91479	3071.5266	38.34087467	3073.6615	38.29840917	3058.2423	44.82733396
3116.0389	14.30890386	3106.1505	8.263663265	3082.2545	14.77858	3110.3322	16.45610992	3088.9606	12.61164176	3104.8334	8.808625238
3153.7089	9.065774687	3114.4671	16.90205574	3110.9016	11.25877	3114.7014	10.84759021	3108.1283	15.95179672	3109.2072	21.42031478
3173.0962	4.110853199	3116.9046	4.002190736	3111.9927	21.43101	3119.7612	39.02645401	3117.5764	6.490881619	3116.6725	29.08751665
3174.1776	4.62085627	3156.6351	14.29069517	3164.3087	5.647901	3153.1021	13.53327295	3156.1181	1.812225926	3153.0719	8.725990999
3184.7239	3.738082528	3166.815	3.049730456	3180.9769	13.62801	3167.585	1.450124357	3161.9199	15.91181558	3165.6107	17.70106377
3268.18	2.855411387	3251.9719	7.907711506	3198.1201	3.687497	3182.3543	16.33878759	3177.04	16.14875679	3179.4846	7.298643846
3848.1885	72.284796	3850.2354	81.64191166	3869.1813	41.01009	3824.9069	89.44811719	3872.0803	38.81875165	3824.6995	86.95441776

Table S37: Vibrational frequencies of transition state of ISOPOO-SO_2s calculated by G16 at the M06-2X/aug-cc-pVTZ level of theory.

1,2-ISOPOO-SO_2		4,3-ISOPOO-SO_2		*E*-1,4-ISOPOO-SO_2		*Z*-1,4-ISOPOO-SO_2		*E*-4,1-ISOPOO-SO_2		*Z*-4,1-ISOPOO-SO_2	
Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity
-480.83	289.4514	-496.84	279.8728	-555.18	155.661	-471.79	197.6941	-451.44	212.4531	-458.39	183.3175
29.8298	83.14532316	31.6804	180.9813619	43.5119	39.92890602	25.9695	315.5939856	26.0816	292.0280009	20.8076	434.3978969
41.6762	122.3635238	39.0027	172.9437479	65.8359	266.5560918	37.2953	107.4064004	34.6416	150.9198561	33.0571	29.0602289
70.2201	10.30583391	57.6337	4.243178216	85.1274	88.8304208	56.3753	20.95351278	52.488	171.0512658	49.4288	23.09112491
79.8791	15.66710144	77.8144	62.94698825	95.5501	48.52822334	97.1551	32.67725984	63.1874	104.2122218	91.3417	59.73939348
151.1412	96.68022207	164.8337	59.33015382	118.3358	33.93838854	115.835	94.71094952	82.5064	14.32203452	108.7967	45.758456
174.7116	14.34671987	185.2547	8.374830151	158.2315	69.56608067	132.5698	15.20890462	126.4895	15.69713758	146.9027	12.48123447
207.8727	36.533017	197.3424	19.75469608	167.0259	49.47996475	178.3492	11.81054821	158.6217	91.67316645	149.664	14.42872575
234.2637	10.18194754	206.1445	8.122215664	210.4512	15.38501527	220.3676	111.6489473	212.2745	72.76873442	205.6064	2.46419114
247.7416	53.83896468	223.3368	21.66745042	258.8883	41.3889792	245.208	57.13990813	230.67	63.13303097	233.5933	104.6410012
277.0314	11.94235477	277.4031	72.10316583	292.7637	50.62993132	277.1372	66.58419603	258.7859	129.2308366	286.1174	114.0862016
317.8015	93.04491148	309.1905	80.09490354	332.0931	45.80514401	322.3138	19.42999658	288.1383	391.1415805	318.8641	76.5202273
352.0457	198.035403	353.6711	48.18349567	380.3685	8.466110043	367.1103	430.9036856	328.3767	1054.880505	378.4624	36.13372248
373.4855	49.40101829	389.5142	551.1824992	410.66	32.22332626	378.9891	40.71197131	364.8274	60.29901827	404.1948	606.3804134
404.7085	877.1245768	424.9726	24.22048909	437.7347	20.84219712	412.6396	91.26006756	408.1468	29.21084795	416.2178	184.4245805
432.4327	437.7220714	432.6663	117.7779911	445.9549	740.4372607	436.0397	418.7195851	418.4856	43.21852898	461.3028	210.4214905
485.5874	164.2990837	523.8276	443.3344123	478.2622	142.888937	501.3242	19.52506073	471.6283	82.88922221	489.5786	9.648798898
506.3771	76.57011391	535.8443	102.3681997	515.5608	332.4273428	521.7314	515.6870884	524.3224	450.9576461	515.1992	12.33834565
529.9269	419.0212969	551.5477	96.19004885	580.0616	87.1171232	577.9406	52.6923788	532.8164	75.58357594	522.7435	490.3742016
607.5517	44.73391927	562.093	20.99694046	606.3489	7.630102338	657.4251	40.26079153	620.3566	39.37651214	674.1911	31.79488736
686.6763	114.6600634	743.8202	0.10136806	812.3557	7.91784365	792.1771	16.36898781	836.3712	13.19303469	798.6431	47.5484931
783.3449	26.72483318	861.2456	69.79871446	870.243	26.2928731	886.2841	31.09922271	896.3696	44.92630392	910.9603	1.818298557
876.1314	23.19787188	884.1191	11.27484665	913.7294	119.879783	931.0714	110.6126646	958.513	100.8402764	937.9731	71.47138098
938.3515	16.59911478	979.521	157.827278	973.4639	49.89697922	955.2224	102.0095731	989.4514	122.3452446	966.4533	96.71649931
976.0301	73.03641986	993.1564	8.064303076	982.0894	851.4825126	1000.4627	98.80795856	1022.9475	61.64851785	1000.9204	64.9845202
999.7583	125.6341491	1023.0605	1382.166073	1004.6329	285.7599214	1040.3545	1408.724577	1053.2697	484.2111778	1043.1467	1331.31257
1040.3667	23.51956183	1032.9068	589.0998408	1029.6523	10.10936962	1053.8508	55.15195282	1063.1234	1399.043855	1065.1343	70.12850869
1044.4976	369.5981795	1058.8403	82.70186799	1071.2901	35.49602207	1071.5803	8.082438382	1075.878	219.8462847	1080.5504	18.31455962
1048.3129	1499.78718	1080.3143	17.98436275	1134.3576	183.6974452	1106.1554	324.0197884	1091.1699	144.5150811	1088.0911	331.5113326
1123.6601	454.8589325	1107.5413	53.55066506	1146.5817	98.69897456	1123.1869	17.60263991	1138.2066	92.89718175	1134.9295	87.0308588
1161.5627	43.44894135	1131.0505	312.9738278	1167.7385	201.3111942	1184.8161	319.279782	1186.6503	271.3966208	1183.4818	196.5992461
1186.0415	330.7676627	1182.6046	292.7165942	1226.9928	26.46413342	1200.5315	67.04936033	1197.0174	4.882191558	1190.2346	150.1782455
1216.2732	38.36177282	1224.0316	138.1426816	1242.0447	24.0884122	1255.8441	67.60707888	1244.1746	32.08481121	1250.9527	42.84411253
1228.9427	35.82639404	1290.1619	8.537166746	1288.5707	45.06208242	1292.327	29.96693191	1250.3886	15.59561036	1290.4865	55.38194735
1279.2522	133.0568163	1314.9783	17.58245943	1342.346	370.7584347	1356.3979	7.477337586	1346.2648	8.184656991	1340.7032	7.710674123
1333.4939	20.95078947	1351.2812	112.7589501	1349.1199	79.45085161	1375.8541	382.5994241	1374.6814	649.1148195	1372.1177	22.76698005
1372.9036	526.0199474	1371.8026	522.4265645	1378.999	9.305514843	1381.0374	146.4176076	1386.4598	193.3211856	1376.8304	486.7273189
1383.8015	6.930265937	1386.5313	31.65320439	1401.9635	52.00864088	1395.1047	48.36388133	1395.2519	76.79961956	1395.4877	14.77047739
1407.1782	51.40029212	1416.5347	7.679789107	1417.6878	88.01541287	1414.0654	23.3131971	1422.1078	64.73667173	1417.2753	17.72671057
1432.9634	62.52656212	1431.8531	110.0654485	1435.3883	8.433833825	1421.5007	72.55535782	1430.2371	62.63710256	1424.161	135.572635
1456.1194	31.89612368	1460.9832	9.784102793	1481.6341	5.891064846	1478.2262	25.15013823	1482.7971	20.2914041	1482.5324	19.52434344
1483.4196	10.19146597	1484.2839	26.25161083	1484.8806	19.93193352	1489.5819	12.13492162	1496.8389	19.99231029	1487.9109	36.74299514
1491.4049	5.904363645	1499.4381	44.56310254	1489.4928	22.51563029	1495.7046	34.47055998	1498.434	24.65707939	1497.2082	15.71103061
1500.9655	25.84184251	1506.3895	9.679599785	1505.0484	41.87009618	1521.3726	20.53892258	1515.347	13.20569894	1523.9953	17.83637852
1737.7923	19.35043077	1755.4256	23.77422548	1754.6319	71.25080634	1757.098	55.42319381	1772.6848	7.510762696	1769.3608	6.925796016
3051.2187	28.34975607	3026.8721	25.55312389	3020.3196	33.37187262	3058.7516	14.38569101	3039.0019	12.55773299	3052.2005	15.51540988
3074.6549	3.564910437	3058.3763	10.95657927	3062.8387	17.47078167	3068.6596	15.0690885	3059.5337	4.553691474	3061.3721	26.61312241
3119.3937	15.85876272	3098.5003	16.63341004	3080.643	18.18798461	3087.0451	25.26684822	3072.259	36.98763391	3093.0768	25.64591312
3149.3877	5.928890403	3115.1358	6.753505631	3107.4426	26.04575787	3112.7356	45.12259702	3107.4993	14.0078911	3105.4334	11.39973397
3166.2852	4.039940499	3118.5165	11.47727631	3116.8003	4.016148294	3119.3929	7.775467555	3116.2307	5.274294464	3111.9834	25.23589341
3174.3827	3.877442939	3157.568	13.41558388	3159.0094	6.106449752	3150.349	4.75483489	3129.7168	12.19540396	3145.5873	11.711039
3185.4054	5.148610815	3165.3726	3.239538709	3174.7584	16.00994753	3155.7485	9.30769236	3163.1523	10.47989334	3155.1161	7.418235919
3268.7322	3.403043161	3250.6187	6.713552892	3210.7067	0.65431597	3177.8862	17.51430769	3175.5254	15.04966301	3165.2241	19.7547526
3878.0752	60.55341358	3877.3823	62.27918744	3818.43	75.74791031	3847.2969	68.17485697	3874.1376	40.46242127	3851.3782	52.19102698

Table S38: Vibrational frequencies of transition state of ISOPOO-SO_2s calculated by G16 at the M06-2X/aug-cc-pV(T+*d*)Z level of theory.

1,2-ISOPOO-SO_2		4,3-ISOPOO-SO_2		*E*-1,4-ISOPOO-SO_2		*Z*-1,4-ISOPOO-SO_2		*E*-4,1-ISOPOO-SO_2		*Z*-4,1-ISOPOO-SO_2	
Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity
-482.7462	279.9917	-501.86	277.7081	-561.34	159.6331	-470.04	183.4368	-449.33	201.5693	-457.36	1741.9175
29.5059	88.29001994	33.5408	119.5958081	42.1653	40.46610047	18.5062	438.3633379	27.0198	273.3244679	27.9231	302.614775
40.4358	117.1291922	40.9454	184.5072181	63.3336	269.3272835	35.37	90.25489952	34.0985	174.9094273	35.192	18.20576329
70.0032	9.72228692	57.6641	3.908861022	84.7078	86.69429174	55.6168	23.29075629	48.6389	155.5358834	49.1006	20.58861399
79.141	11.07479824	78.054	53.63049539	94.6095	55.43271887	98.0927	36.80198122	62.9856	111.658993	90.9989	62.70005632
152.0613	95.07991252	164.5988	62.04212578	118.3607	28.68668505	115.4624	99.43917418	82.0596	13.48117585	109.8636	42.11134679
174.147	15.66234847	185.2948	8.16848272	157.906	75.17164016	130.796	12.79818303	126.1416	16.55006482	147.017	13.05494662
207.8288	35.15673155	197.2695	20.04309718	166.6581	42.70231098	178.42	11.86623247	158.5711	95.1390587	149.9858	13.28595106
234.2641	9.752787083	206.1348	8.265812603	208.3352	16.2287232	219.8946	110.8930944	211.6596	73.25155126	205.6219	2.337894875
247.0593	54.15397051	222.6731	20.36146324	257.9735	41.17078958	244.2909	57.0082118	230.5438	61.15510083	234.4461	103.6971301
276.4576	9.778047973	276.6298	76.40762232	290.8591	54.43844894	277.0893	63.50887909	257.9519	142.3413311	286.1675	113.6703102
317.8387	101.4348351	308.6804	78.09479547	331.6651	44.13096254	321.1659	18.2237433	287.6237	406.8988747	318.2918	87.31026768
351.1438	214.2031228	353.4332	43.61737781	380.5795	9.926859785	364.2108	456.559958	327.5085	1039.825584	376.0758	49.12652789
372.5569	60.12950826	391.617	546.6693916	406.7373	22.99553592	378.5343	47.37731046	364.1561	56.12998518	398.8726	598.1376636
403.5305	892.8852099	423.0874	11.87142732	437.3731	39.04997388	411.5116	74.20651657	408.0967	29.15382519	414.4557	178.3773702
431.5338	378.0506167	433.9038	122.1458382	443.3944	738.9124898	433.5337	408.5662768	415.3505	35.92998631	460.5354	180.8049965
483.172	160.9565781	529.7835	396.1140166	477.4863	130.625391	501.7923	28.13689314	471.8217	84.96230841	490.2474	9.153081058
508.9805	53.27264459	536.2824	189.5386744	521.6301	353.3403311	527.2544	547.8348384	528.9786	339.9662173	515.3527	24.99059695
534.4994	487.074994	551.6331	103.1409968	579.3645	83.87474862	578.4305	54.1209364	533.7786	222.1835154	528.8211	529.9206581
607.4804	44.86131814	562.0032	22.49737575	606.8176	7.764241387	657.814	37.80931863	620.4543	41.10249998	674.5726	32.85029026
686.9365	113.9191489	743.7886	0.151254008	811.486	8.051200039	792.2119	15.97245719	836.488	14.44549805	798.7582	46.46632569
783.2913	26.55604238	860.8092	73.1106727	868.2538	24.07687855	886.2074	32.67884303	896.2895	45.35316527	910.9737	2.330646092
875.6936	24.85088832	884.1157	11.14719185	913.5934	118.3937337	931.2369	115.4660302	957.9375	100.9212646	938.1737	70.68388104
938.4006	17.3409437	979.5385	157.9226112	973.1025	42.32661459	955.2329	102.9740265	989.3725	124.0824172	966.9184	99.82256876
976.5029	73.51336552	993.1673	5.606308167	985.3057	806.4451553	1000.2859	100.7365956	1022.507	95.56306819	1000.6039	68.3916244
999.8167	129.0782722	1030.7309	499.4462012	1003.0001	381.8226809	1047.1314	1362.008235	1053.6514	250.3796471	1048.8638	1256.367699
1040.3859	24.596249	1032.4861	1473.131384	1029.4707	11.03616144	1053.9163	66.10661218	1068.7809	1290.626715	1064.9481	97.35690404
1045.543	3.498162708	1058.6574	86.2075374	1071.4499	36.61853485	1071.4399	8.386582107	1076.7022	559.1428962	1080.7544	29.49613508
1053.8867	1848.165135	1080.0928	12.85953019	1134.5058	187.4831369	1105.8907	343.0896183	1091.5046	110.9135521	1088.6929	341.780027
1124.2395	468.6777542	1107.3416	53.05486649	1146.6637	102.4295508	1123.3179	18.81944171	1138.0499	91.44608953	1134.6955	92.13269788
1161.6882	31.67305322	1131.1226	322.7926198	1188.3539	209.5377652	1196.8114	110.5103886	1197.0241	5.543717648	1186.368	29.23697846
1206.5989	379.7664454	1205.538	310.9288951	1226.7799	25.9728074	1209.2663	288.3547385	1208.5697	292.1803464	1210.7129	333.3630422
1216.5327	34.37184209	1224.3568	145.0401093	1241.749	23.97752652	1255.5051	70.26966887	1243.922	30.83927	1251.303	48.48701906
1228.7107	17.71462737	1289.8928	8.800599778	1288.0709	46.23636713	1292.1174	29.19775965	1250.4681	15.67852435	1289.9934	53.67220459
1279.3888	130.5876466	1315.1404	19.59206862	1348.4133	11.70949368	1356.5118	6.934991644	1346.2532	7.811643809	1341.3912	7.836091558
1333.2323	20.75591406	1351.0332	94.53487874	1376.4791	453.4351558	1380.2821	43.77989048	1386.2144	260.6060735	1374.3507	24.72069541
1383.6439	12.00269984	1387.0188	22.47866969	1379.0097	17.38109492	1394.0543	13.09696195	1395.1334	84.85623429	1394.879	14.01644068
1405.4656	259.3608903	1408.5882	562.9543997	1401.8287	63.29545421	1410.1432	492.5896223	1409.7775	586.2119411	1412.8465	368.1687693
1409.1473	318.2572182	1416.5872	6.858581256	1417.84	74.52320614	1414.0991	11.42964069	1422.0893	64.42247789	1417.4813	53.40009026
1433.097	73.71172469	1431.619	112.5727462	1435.3562	8.513790585	1422.0556	128.5876705	1430.2315	65.48107671	1424.4031	233.4831476
1456.1814	30.58741448	1460.9601	9.898945562	1481.9177	5.359872694	1478.3154	25.5615081	1482.7067	19.9401703	1482.6311	19.88764103
1483.6615	9.050791999	1484.3199	26.57591632	1484.6354	20.33829384	1489.5587	12.93911861	1496.7033	19.85978257	1487.9649	37.78943944
1491.1039	5.878800865	1499.4688	43.08000307	1489.9078	21.42546078	1495.6315	34.08974439	1497.9599	24.73386069	1497.238	15.22631099
1500.6693	26.31695039	1505.6615	9.786024509	1505.274	42.07531331	1521.9589	20.46049946	1515.2785	12.3988218	1523.664	17.90911788
1737.6142	19.13958372	1755.496	23.89916961	1756.1708	67.35065276	1757.0821	55.17825783	1772.7708	7.5378529	1769.4972	6.686281197
3050.9534	28.33299968	3028.1765	25.38863668	3019.8274	33.48194047	3058.7451	14.34333315	3040.5448	11.77278033	3052.0917	15.65556154
3074.9189	3.650362457	3058.4376	10.92688044	3062.9319	17.11480417	3069.3433	16.10384697	3059.5198	4.564665168	3062.2722	26.73270962
3119.4711	15.73572562	3099.1912	15.88593572	3080.8978	18.30625694	3087.9148	23.94427967	3072.2628	36.91396203	3093.548	24.74355197
3149.6309	5.917286312	3115.0946	6.761407018	3107.906	25.93828551	3113.2468	44.63811268	3107.5093	14.01131227	3105.2706	11.50092505
3166.8794	4.049008342	3118.6408	11.38561117	3116.6772	4.348471132	3119.3293	7.823457994	3115.9623	5.254391849	3112.0459	25.43164871
3174.4849	3.767104904	3157.5686	13.51514038	3159.4052	6.054166383	3150.9416	4.719756028	3130.2362	11.5822712	3146.3676	11.3604662
3185.4236	5.107252479	3165.3513	3.22292411	3174.7044	15.78892905	3155.6829	9.280199985	3163.1283	10.49308953	3155.0641	7.315179667
3268.6073	3.446745727	3250.5982	6.731268077	3210.4417	0.622434338	3178.0123	17.54687851	3175.5424	15.15875392	3165.0541	19.9005135
3878.683	60.36485513	3876.1148	61.93047253	3820.7717	75.72800643	3848.7856	67.21664299	3874.2316	40.4799746	3851.9519	52.39691498

Table S39: Vibrational frequencies of $ISOPOOSO_2$s calculated by G16 at the M06-2X/aug-cc-pVTZ level of theory.

1,2-ISOPOOSO$_2$		4,3-ISOPOOSO$_2$		*E*-1,4-ISOPOOSO$_2$		*Z*-1,4-ISOPOOSO$_2$		*E*-4,1-ISOPOOSO$_2$		*Z*-4,1-ISOPOOSO$_2$	
Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity
34.47	52.52070026	39.82	96.73938034	42.761	106.8323696	32.8965	261.4606656	23.4191	185.1001623	31.9984	40.08298111
50.2308	43.33228256	44.7665	46.22430677	71.771	79.15872471	44.4195	150.0755985	31.6829	224.0053141	46.6237	223.480936
66.9213	12.81089131	54.3541	6.319433415	77.0617	107.9536318	61.0311	40.6776545	43.4424	112.5767054	51.3308	17.48685807
81.4112	30.76901734	69.8678	102.6415711	85.7712	109.210377	98.4302	21.08787206	61.5878	101.7303526	84.3935	53.41666191
145.3297	81.89083381	165.8039	64.09593334	131.2991	23.33494441	123.1617	76.90076019	83.008	15.42258125	128.2889	14.76484624
186.8417	10.87871697	182.4503	10.35557961	149.3914	83.80620201	145.6729	9.609745849	118.1709	14.43896311	148.7449	16.25316109
220.6428	20.49819812	198.7059	17.48095206	156.5154	50.36341672	178.4251	9.826757308	161.9478	106.0536399	161.704	53.47683295
254.9195	16.80301422	213.0623	6.442958908	249.1575	11.50749991	247.1165	15.80638683	222.8187	19.05368225	201.366	6.904368128
273.9093	32.45590112	244.5822	18.04167458	267.7836	64.05624535	261.4315	58.23452163	260.7285	18.23415881	285.7344	266.0036668
288.1815	71.79991961	287.1896	46.10476826	317.802	33.03471402	289.0941	67.2429345	271.8297	252.616618	295.8577	19.37136772
319.4138	132.5486839	329.3516	227.9317532	369.074	4.671739419	323.4794	863.7996206	304.1196	440.3533385	353.8797	368.7027918
367.6428	507.7121685	357.1429	79.34383867	374.809	30.72975628	362.3658	93.12004607	335.9749	915.2871915	363.2962	480.3447226
394.9158	395.4174113	388.9829	532.1556768	437.358	13.96423176	402.9056	63.8373924	375.2913	51.45304518	398.5001	14.30576524
413.3338	642.3012638	439.6175	9.413187415	440.962	858.4991181	431.8607	63.93501033	432.2884	43.44065541	455.3766	274.7560499
445.5392	66.16892268	462.5716	234.3341346	452.7924	150.636641	448.5607	196.8049839	452.9967	98.7043991	461.2359	64.12811789
488.5338	144.7295701	514.8405	229.1661871	481.2826	136.7874815	497.6146	69.00589159	478.9375	70.23005353	486.2423	112.7165165
503.5653	101.3405284	536.498	60.795966	510.2602	280.2482943	523.8555	179.8991053	517.0783	201.1663414	508.1408	14.28012654
528.5903	122.595843	555.5947	52.20085815	578.9971	90.17736917	569.2756	71.21866616	534.3493	84.88651421	532.5162	162.696536
614.7529	56.47947712	571.9162	20.76255463	609.5457	20.87551751	646.1011	90.23024728	621.8758	35.87774732	664.162	103.6095329
684.5014	141.861399	701.0008	827.6817802	692.9255	522.0206998	712.2083	468.3398255	681.1552	602.280493	706.9376	455.3161984
701.4985	704.1139381	741.4851	4.327359141	813.9355	16.22401814	790.4261	12.66177983	834.7279	25.00518693	797.588	36.9229886
789.7329	5.050062593	867.3217	60.78101708	876.1418	22.40121219	886.8938	17.0057743	897.1776	39.42540816	905.5678	3.124316736
879.7499	26.36879745	888.3984	18.38161719	922.963	246.7154352	921.7599	131.9986207	967.782	112.4014454	928.2712	91.46975411
943.4203	24.68180377	973.6978	42.76658421	973.2724	23.55995952	954.8877	92.09614734	979.1152	117.8876947	969.5438	78.4705146
978.0805	54.48627814	978.117	125.3002222	996.3472	69.91905553	994.7828	33.1966272	1003.2033	21.09418747	995.9297	42.70478693
996.897	148.6862368	993.2991	2.862424343	1003.3296	89.59437913	1023.8786	173.0173796	1047.9202	234.2339103	1029.6587	156.082474
1002.9067	29.83813829	1045.0291	177.899646	1036.0303	30.93425354	1056.33	84.02649145	1061.737	16.44700173	1065.9371	17.6385933
1038.3561	29.58134142	1067.3373	129.4978251	1071.8772	49.45930757	1073.0599	6.718394783	1082.7071	123.6926162	1080.4856	12.82937887
1051.1009	63.69252896	1087.2875	157.4078079	1129.702	318.6105737	1106.6176	181.5485819	1091.5891	296.4313399	1091.2394	302.3036597
1118.9085	418.4638925	1110.2464	60.30594238	1131.4038	42.32082689	1121.4492	9.892659621	1139.7383	313.363513	1134.1494	35.03242555
1140.3283	400.8120125	1134.328	221.8290057	1143.8071	153.6926908	1135.0429	366.8338962	1142.1431	60.00950583	1139.3884	348.9459259
1167.3086	45.61543102	1141.0389	312.3539224	1227.2804	31.5620236	1201.7624	68.23815828	1196.868	5.147790181	1187.0471	27.85981078
1217.8729	39.39007489	1225.2115	130.2285725	1239.8461	17.34412745	1261.3906	21.61545876	1249.5713	7.282349922	1253.5542	13.25116447
1232.8117	42.49891118	1296.1274	3.281387743	1290.413	29.33649131	1298.0265	9.675781566	1250.1167	40.41552461	1300.2077	16.19129779
1278.8637	110.2881794	1314.5904	6.145586234	1321.0644	369.7006639	1330.0178	399.5666965	1337.5713	447.8782228	1335.699	374.6108785
1333.7034	11.08605154	1338.3257	428.5179762	1346.7639	14.85222436	1351.5975	28.71184888	1346.4938	5.422227844	1340.5554	20.34463951
1337.3069	384.6743092	1356.5997	27.45027143	1378.3293	10.46517996	1386.4892	57.42503901	1386.7922	153.8202113	1380.0242	46.85725249
1382.8828	9.753936873	1390.3622	42.49208226	1399.694	64.43886304	1401.6382	64.82309464	1399.7752	55.33270811	1398.9044	45.86038717
1410.1006	58.35138378	1416.3715	9.827510969	1418.5011	81.38055012	1413.8766	31.11437233	1420.9487	64.17462347	1416.2369	27.10561802
1430.9637	48.65348268	1435.2343	99.94602573	1436.1081	7.939303285	1415.7986	38.87369823	1430.2317	66.29611166	1420.0555	103.3677081
1456.0276	27.56166519	1461.25	5.358419345	1481.0382	7.036350498	1477.0731	22.32142389	1483.4719	20.46907547	1482.5354	15.58666763
1485.5893	9.584988344	1485.3064	27.24075472	1485.1165	21.41614529	1490.0628	9.146312077	1495.25	18.70541127	1489.2495	32.93715101
1493.5941	6.213826167	1500.3596	39.22605363	1491.614	14.56266157	1496.541	33.27516786	1512.1636	38.7262095	1498.0391	17.1987008
1503.2493	29.19420214	1506.3323	6.947329781	1503.353	42.75242383	1513.9301	21.04886383	1515.4057	1.637715973	1518.6251	16.73858961
1735.4011	18.93410849	1751.6576	21.12789723	1760.5381	51.43820627	1759.356	55.99785568	1771.1523	6.728685523	1771.7433	8.863734858
3053.5216	29.18386537	3011.738	40.50531089	3011.6906	36.06775146	3057.8063	18.03705419	3031.5045	24.62223729	3052.6213	16.96364204
3071.353	4.759969204	3058.5881	12.5154037	3060.0776	15.90438541	3060.1851	12.83726074	3059.0507	6.117018095	3052.7795	25.89950176
3118.7071	15.52199141	3092.6738	20.42469579	3081.9473	17.54070429	3081.9671	27.5334786	3072.3726	39.0392843	3086.6408	31.48307159
3146.1976	12.25426347	3115.4556	8.27253131	3098.272	20.4520431	3103.953	55.43289925	3107.5964	14.53315174	3105.9646	27.16070758
3157.3277	7.069863305	3117.2133	15.33221313	3111.9968	6.882743137	3119.9973	8.368535471	3117.0652	5.96950854	3106.5804	8.652010427
3173.9267	3.710702894	3157.1195	12.79743167	3148.4092	8.719146933	3136.281	5.290947612	3124.3837	21.45263547	3133.3941	15.54383378
3185.4965	4.529671102	3166.9099	3.205213616	3172.6683	16.68089504	3156.1165	9.350342218	3164.306	10.39841022	3154.2771	6.534119582
3269.3124	2.572299212	3252.2794	6.500981532	3204.3487	0.172182778	3175.1081	15.89786701	3174.3421	14.20783743	3163.1862	19.58548914
3882.3757	66.82703764	3876.1727	66.24718815	3827.6643	62.80756473	3846.2177	94.71015267	3873.5424	40.28685964	3844.8386	60.07101823

Table S40: Vibrational frequencies of $ISOPOOSO_2$s calculated by G16 at the M06-2X/aug-cc-pV(T+*d*)Z level of theory.

1,2-ISOPOOSO$_2$		4,3-ISOPOOSO$_2$		*E*-1,4-ISOPOOSO$_2$		*Z*-1,4-ISOPOOSO$_2$		*E*-4,1-ISOPOOSO$_2$		*Z*-4,1-ISOPOOSO$_2$	
Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity
34.3755	48.11578479	37.8418	89.00866822	32.4872	120.9202275	33.168	140.6175981	21.673	217.9967395	34.3942	39.28595222
50.6369	39.75460437	45.5175	37.34568529	70.8057	92.85870838	49.2905	159.3476551	32.3626	201.4878299	50.9206	44.11632372
67.5244	11.67437142	54.5304	5.391828926	77.5303	121.7499891	59.635	66.97049942	44.9453	107.7205554	53.2729	147.2858958
79.8446	31.33774916	68.8404	104.1328665	93.3935	92.03590859	95.8373	25.45477082	61.6095	99.17563121	85.1141	57.46405363
145.1837	80.76139322	165.3632	65.08459133	146.9562	62.23957485	122.3066	76.67514638	83.3922	16.55228545	129.2105	14.21184518
187.8848	10.1664609	182.8604	10.0160141	150.0181	28.20163659	143.7627	8.208413932	117.9569	14.75263545	149.0254	15.48639623
222.8118	19.9208639	199.5677	17.79927033	158.6511	47.27648307	178.7628	8.36430255	162.3269	107.5164728	163.913	53.21614152
253.7648	16.33710339	213.4836	6.245241366	250.9484	12.85295222	249.5169	12.96186538	223.3845	18.45894029	201.5803	7.069206414
274.9149	21.64664082	246.3101	12.09403526	267.6382	69.50338994	261.9366	62.16437264	261.9054	21.3844961	288.3198	260.1951763
288.4129	81.01821529	289.1866	44.55723276	318.2762	33.43798698	289.9868	68.98394789	274.6115	270.3335492	298.0121	15.63699963
319.6849	142.1450621	330.3376	323.6828834	372.2432	3.980360669	333.3122	835.9151298	306.9172	461.2987544	355.5868	527.5545634
368.4241	622.6160552	356.3528	93.48449893	381.8803	42.78350597	366.542	78.4226746	336.8069	869.6435724	368.1712	330.3711321
398.7427	358.5460888	383.4057	463.7496271	432.999	849.3842847	404.333	94.49452985	375.901	48.13902503	400.6045	25.86904944
413.8897	556.9352781	443.2525	9.111885265	438.9042	206.5940891	437.5236	57.86365781	439.4921	51.08699006	462.0616	261.0263537
449.856	67.74923607	469.9994	233.6567573	453.8513	19.87704856	456.5892	195.853814	455.6494	89.71055933	463.7519	45.21011776
492.2433	112.7793073	523.7292	184.1708467	486.6216	107.8811097	500.6703	62.6628322	482.8803	78.48090224	490.0517	112.0658178
506.9247	106.4807921	536.7083	69.7133998	523.411	282.807575	533.9142	177.3452558	525.9175	117.1822785	508.9698	18.52867597
538.7249	141.6818577	557.9117	79.10196328	579.6188	83.09804923	571.131	87.52588307	538.6165	163.2040179	543.3358	170.2853086
615.8103	59.48430194	574.2845	25.01863575	610.2076	21.04639158	646.6269	81.82243127	622.5584	35.32832708	665.5722	83.51771076
684.6	121.0886419	717.79	888.9138161	713.821	550.1992887	724.2048	534.3421407	699.2277	675.838309	721.2792	532.9270696
717.4714	789.0030358	741.6482	11.61831099	814.5551	21.06180977	790.6489	11.46842972	834.7865	29.26959436	797.693	36.29348245
791.137	8.97282484	867.2142	63.08269346	877.882	21.93418296	887.4755	18.19305337	897.2542	39.20906799	905.7844	4.911297916
879.831	27.26052626	888.9647	18.26624186	925.2389	272.1265178	922.8278	142.8449156	968.1068	116.7899113	929.0751	99.9699103
943.7381	26.44554682	973.7578	54.0284012	973.6861	23.84412911	954.3227	94.06025345	979.0237	122.7718534	969.8204	81.36422447
978.5744	55.15957047	978.3559	119.3672207	997.9689	66.98159119	995.0517	28.04220237	1003.1417	17.44786723	995.9519	38.99543896
996.9925	151.3665585	993.2869	3.823172722	1005.8147	86.88969337	1024.9394	162.4625376	1047.9657	214.0846185	1029.9111	144.5022486
1002.8303	20.3672713	1044.9774	164.5996064	1036.2669	33.07844653	1056.5568	86.72819735	1061.9439	14.16160624	1066.2359	16.7525103
1038.3611	29.52702658	1067.8325	125.1899658	1072.6248	51.12082932	1072.7902	6.28499453	1082.9498	126.0766955	1080.5735	13.14657928
1051.1903	56.43804604	1087.3424	145.4783635	1130.3563	178.9926596	1106.4463	206.1073558	1091.6251	294.8848263	1091.1415	312.6170482
1119.1041	421.538839	1110.3224	59.11648115	1143.3683	124.7302196	1121.6758	11.35599693	1141.1533	77.16227024	1135.147	30.98253315
1159.5428	395.5626217	1134.1637	237.2483543	1154.7037	232.7296495	1160.5275	363.7845452	1163.1897	321.7865733	1162.5279	365.7957978
1170.6247	83.75819722	1162.7296	342.6848698	1226.8979	33.68833846	1201.1185	68.43649192	1196.87	4.883126141	1187.1678	29.92633266
1218.0011	38.67451977	1224.8093	133.4473914	1239.3937	13.78077609	1260.911	19.88068744	1249.5482	6.924266764	1253.6066	12.97565675
1232.722	37.32497345	1296.4568	3.615963817	1291.3632	24.92965586	1298.5454	12.50172294	1250.1319	40.3990773	1300.6003	16.47382104
1278.7659	108.1886163	1314.7503	8.282833684	1346.4542	18.05852601	1351.3956	18.9433524	1346.4939	6.174483354	1340.658	18.40590117
1334.0413	14.94871238	1356.1571	100.7062009	1358.1992	400.4074345	1370.3441	443.0825165	1373.7432	495.4485827	1374.0655	410.3413525
1373.54	397.7852151	1374.6759	370.7859754	1378.3897	11.99143558	1385.5483	40.73506394	1386.9139	132.724014	1380.0144	29.36454929
1383.0287	7.917765489	1391.0235	40.28793105	1399.0294	72.27130554	1400.3549	67.23194364	1399.9061	48.54025908	1399.0385	49.55898559
1410.5234	60.06708149	1416.3949	9.448236197	1419.3711	71.05145068	1413.9671	29.76910203	1420.9297	64.38015537	1416.2731	27.42773366
1430.8704	53.49929101	1435.0264	101.4795066	1436.1014	7.341806349	1416.331	42.84698729	1430.3087	65.58185797	1420.1068	107.5876416
1456.0054	26.62282694	1461.2853	5.197489335	1482.1011	4.083335374	1477.2087	22.46736954	1483.4846	20.44066356	1482.5822	15.41853604
1485.4871	9.267137758	1485.4466	27.38965463	1485.7368	24.09018651	1489.7743	9.05194835	1495.2358	17.86381206	1489.2906	33.62601329
1493.461	6.245366374	1500.5203	38.50374427	1491.5017	13.66771607	1496.5056	33.42950556	1512.6287	38.84168816	1498.1241	17.09094155
1502.9731	29.15656687	1505.7916	6.923065804	1503.973	43.2759243	1514.2864	21.26415593	1515.6498	1.412141316	1519.0722	16.57031299
1735.25	18.73505162	1751.4724	21.04653826	1761.5259	50.35036937	1759.5721	55.50283852	1771.1757	6.736930509	1771.7819	8.795092199
3053.6159	29.15539802	3012.642	39.76126074	3011.6985	37.13173512	3057.9048	18.01807807	3032.9815	23.70437313	3052.5957	17.60494302
3071.7103	4.722401025	3058.8491	12.51707466	3059.5038	15.26843954	3060.6571	13.62490786	3059.2619	6.011620644	3053.4197	25.55450325
3118.8452	15.37829777	3093.0185	19.94828646	3081.1673	17.31480547	3083.4781	26.76104451	3072.3277	39.20138741	3087.0782	30.10012609
3146.5388	12.38707514	3115.6639	8.397204544	3098.4002	20.19406977	3104.396	53.44121084	3107.5646	14.56963115	3106.1547	26.26603506
3157.8058	7.124632747	3117.3669	15.38546241	3111.1745	7.697656144	3119.9394	8.394136464	3117.3018	5.921448398	3106.6141	9.453233985
3174.0717	3.60960667	3157.0793	12.80985188	3148.2775	8.531083752	3136.2715	5.29706933	3124.6073	21.20149223	3134.0895	15.32806436
3185.5403	4.467492478	3166.7716	3.183055702	3172.5918	16.6497351	3155.9812	9.410533831	3164.3615	10.38045158	3154.2004	6.524792554
3269.2501	2.551725515	3252.1596	6.487850069	3204.0979	0.236567524	3175.2116	15.77635561	3174.3115	14.21136768	3163.1174	19.61214859
3882.5946	66.77127804	3877.5334	65.68955645	3830.2169	62.49438126	3846.8722	87.30516394	3873.5312	40.27894281	3846.1377	58.65822319

Table S41: Vibrational frequencies of transition state of ISOPO-OSO_2s calculated by G16 at the M06-2X/aug-cc-pVTZ level of theory.

1,2-ISOPO-OSO_2		4,3-ISOPO-OSO_2		*E*-1,4-ISOPO-OSO_2		*Z*-1,4-ISOPO-OSO_2		*E*-4,1-ISOPO-OSO_2		*Z*-4,1-ISOPO-OSO_2	
Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity
-908.64	641.0871	-892.44	594.8134	-908.23	285.0772	-923.11	305.2112	-473.25	1530.8424	-1021.35	580.5528
28.6296	113.2597802	24.3169	98.00862791	39.6236	53.74424156	32.2389	12.33736016	34.1381	511.0779619	59.7015	30.18367719
55.1763	35.65247861	49.6362	97.39568629	73.4599	72.02756559	60.9799	26.54150832	49.5805	383.2534713	72.6031	73.29517866
65.0445	44.67521563	55.4124	59.9643598	76.725	40.38533668	88.064	19.76940661	52.0211	130.8375043	99.7952	25.01688348
86.4394	6.332127741	83.3127	27.58633245	113.2855	28.73931098	116.3655	156.6919817	88.8436	51.06886324	120.0034	61.09589006
131.0313	115.8262531	160.6592	14.55121695	139.4707	75.40543938	142.2476	103.7625414	102.1103	318.2913252	134.6168	47.98533514
151.5966	22.97112855	171.1811	74.23848429	150.8956	20.44989308	162.4169	4.165833717	118.7331	75.41454282	148.2221	35.5950837
193.4556	75.90462067	178.3567	21.36993044	157.5254	62.37904951	173.019	31.39287913	161.107	377.0472939	151.1712	187.8435222
231.3524	5.885313189	189.1067	102.9780777	188.7222	96.41706413	203.8294	96.71621086	184.0719	10.29035873	194.4285	783.3954111
248.2065	2.915623433	209.1194	1.772265118	255.8234	97.0888091	265.303	47.86771627	221.3096	38.67366428	217.2701	1232.93567
301.6135	12.06421253	261.8594	73.96535834	287.5027	97.0600864	271.8206	20.29184263	267.9436	557.7875064	246.42	107.9704939
313.6222	25.88091003	328.6368	543.2814856	316.1322	15.26063549	309.9382	51.63052129	303.474	1301.431889	290.6507	225.4645779
352.5854	1207.476307	358.7792	107.7833547	419.2519	10.95806612	390.5576	77.36144455	333.3811	135.1577722	343.6935	10.572045
387.08	72.9146165	374.5019	271.011333	443.1378	8.800952873	450.4861	56.38551813	357.6069	172.4276656	409.3425	35.98076487
419.5902	457.2720627	475.2686	199.3319566	452.5392	416.7258858	457.0164	14.39972383	437.3315	94.79906116	458.8064	8.023028835
479.974	381.1211283	490.8633	222.9361316	459.9759	620.1383502	474.0664	772.0666441	454.972	52.0766774	486.11	185.5946683
492.2192	153.4666662	492.4281	177.1445753	484.0231	143.9056973	486.9466	137.4346553	466.3037	365.4534501	500.4732	230.5987201
499.3652	18.68292935	515.3324	71.06455991	503.2851	73.80722582	501.2987	79.41969367	498.006	100.9641832	520.5172	126.4133496
517.8767	46.16246279	535.065	6.632779051	548.9824	127.134326	525.6815	129.1056017	526.8641	90.27828681	528.212	100.4403519
567.0901	29.0764683	540.2043	277.2003552	594.9178	59.40664665	632.9915	19.0466347	559.6453	253.2335192	647.7205	64.73126719
652.3577	364.6927251	708.9875	213.0448918	795.9209	78.42200489	779.7425	24.63447807	725.0723	589.7226961	796.4029	24.28894984
780.5136	17.86585097	842.4694	19.9439232	816.8642	77.58348093	810.3227	126.9555815	806.0564	12.46277752	852.0363	32.33849425
871.8203	17.96331012	881.1554	131.2868839	875.2758	62.47478806	877.4022	51.76473397	903.2242	1686.321948	898.6176	38.31540041
880.4199	76.17021176	888.8306	7.53282532	928.664	14.55690327	926.5398	41.45953312	971.9496	4.767823367	943.7604	24.713067
941.6002	57.54967204	975.839	94.59702289	982.3853	34.50490535	953.5429	84.1522067	980.6507	78.74238604	976.6473	32.17301753
983.6458	5.262303891	981.9383	69.43125218	994.5529	82.60681969	1032.9873	147.5535194	1023.6616	96.16145118	1018.0702	123.4433507
998.4619	184.948888	1028.7153	18.13797322	1054.0539	31.77615842	1053.8178	14.96320535	1054.2351	19.8729101	1035.4376	221.1835169
1037.4144	28.4468466	1071.743	43.65826997	1070.4792	34.84986151	1071.9882	30.05627219	1078.4753	867.5046215	1071.6832	17.14272832
1047.0895	66.86184308	1091.0302	202.0703657	1126.7987	132.6607162	1113.2343	73.51023036	1087.1494	216.1596623	1086.0902	117.5690906
1119.0731	269.1512309	1098.0609	4.505443833	1144.2796	177.2885224	1127.5644	149.9665932	1105.9149	88.11835686	1124.9059	5.345175765
1146.3768	93.01184296	1128.9595	292.6637162	1179.7244	357.3245269	1181.5979	434.4362223	1155.8925	285.444461	1173.2765	43.91145206
1184.8632	644.249273	1186.6247	599.3122816	1215.9275	90.55750241	1205.3703	16.3531593	1186.9752	4.60622019	1192.2809	513.9110756
1196.1789	51.24641771	1231.7678	90.64311058	1228.1686	78.77198658	1232.5818	157.7372633	1210.4792	98.52975694	1237.4223	75.96063919
1263.2857	69.33570947	1281.0386	25.87922901	1242.91	28.92442303	1251.05	16.3341915	1237.6193	120.5078361	1281.9918	36.57759345
1270.8992	119.4820407	1288.2802	69.44284144	1323.616	26.36328065	1335.2199	28.67112556	1245.8506	494.6120298	1342.5011	87.4472221
1337.472	17.7637044	1349.0296	440.792716	1340.6992	452.2325502	1346.898	478.6016284	1306.346	59.09798741	1351.2105	322.4604975
1350.0134	482.2843979	1356.3162	95.30083868	1378.4491	16.14456017	1385.5582	16.89786502	1349.4551	154.0035495	1359.6739	150.6035961
1395.145	36.67204827	1405.0988	33.89613656	1402.8589	51.16810128	1401.2843	46.58021684	1386.4131	61.97492164	1401.0962	43.64858481
1410.6554	51.02840126	1412.5589	18.43377774	1417.4416	62.80344204	1415.0188	57.0058988	1407.8094	171.5885662	1413.4897	15.95036769
1429.1801	40.12426074	1427.8683	121.3098216	1428.3344	5.398390801	1420.851	97.31528431	1430.1444	15.61398484	1424.0211	111.8331425
1450.4368	18.71839157	1452.5886	4.29867397	1438.6124	29.46710015	1432.3592	24.56150655	1454.2224	127.6743872	1459.9659	23.76698022
1482.628	18.76913332	1484.5501	20.36821631	1483.9236	18.89119936	1472.8089	15.01107339	1482.3731	38.06062905	1483.0543	27.56645298
1495.8411	27.73832498	1495.78	13.05306248	1487.8443	8.210760161	1487.8747	45.65402547	1491.4307	27.9038079	1496.1779	27.0057556
1507.8352	3.073865031	1502.8888	22.73116063	1492.8191	53.22709475	1493.5305	23.42277364	1530.1149	8.480874115	1528.8689	17.79021966
1709.5872	0.92898397	1724.5119	21.32074714	1768.7585	59.36578229	1753.9064	65.59383341	1629.9646	136.1065102	1768.2298	23.45632279
3053.4072	34.22794029	3057.8557	16.69742054	2987.152	16.44237219	2990.5581	15.17168836	2991.671	40.66565787	3007.8941	13.55036982
3078.7347	5.687745985	3065.2171	17.40620651	3015.0088	36.94316756	3059.108	21.82367202	3066.5412	6.875747541	3051.8772	57.2203521
3122.0419	16.14061434	3076.9716	38.26784064	3062.399	13.6131196	3064.6219	10.70904591	3067.3245	14.13166376	3053.2892	17.5141868
3155.1729	9.915922559	3121.815	7.546311841	3081.369	18.18706553	3092.0772	22.77589713	3092.7956	26.38593874	3108.8612	8.36322305
3173.4077	3.89485127	3123.8826	13.89317712	3104.2676	23.26283886	3111.1345	27.3739563	3134.2024	3.965337308	3127.9543	7.302183363
3176.8048	1.174288551	3155.1721	10.05728491	3118.8095	5.166067136	3123.1727	7.951401422	3157.8297	3.087717547	3136.6687	11.52290692
3194.6305	11.90201735	3165.7673	5.607367791	3170.7425	15.43975621	3159.0349	7.759475325	3158.3373	2.971139452	3152.4706	17.31813244
3261.8071	2.515352512	3253.6595	3.66023215	3187.2954	0.103511951	3167.2349	9.129336565	3191.3418	0.524153924	3167.8865	16.24138342
3877.3523	49.6629188	3888.1135	41.36262548	3820.6849	73.20119466	3853.8193	75.97353044	3872.1301	61.59857401	3870.6759	44.92720002

Table S42: Vibrational frequencies of transition state of ISOPO-OSO_2s calculated by G16 at the M06-2X/aug-cc-pV(T+*d*)Z level of theory.

1,2-ISOPO-OSO_2		4,3-ISOPO-OSO_2		*E*-1,4-ISOPO-OSO_2		*Z*-1,4-ISOPO-OSO_2		*E*-4,1-ISOPO-OSO_2		*Z*-4,1-ISOPO-OSO_2	
Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity
-912.31	605.5097	-897.5	553.014	-915.1	288.9773	-931.67	310.0693	-476.87	1538.3224	-1024.25	578.4861
29.5375	108.4954017	17.7124	93.3135736	36.1537	56.30929866	31.437	15.29161136	33.1515	544.4107753	56.7419	30.22531745
56.112	39.06071659	50.4386	106.3104257	71.1319	62.44448778	62.1301	24.71457567	49.4651	341.2736471	71.6322	77.86409602
65.936	36.06648549	56.7294	40.28117393	75.3342	57.96563034	86.7121	20.78153803	53.4532	160.1335571	98.143	27.00301285
87.2573	5.43152734	81.9019	25.86959468	112.6882	28.69339105	117.1411	159.4858509	89.9387	49.06311142	120.7283	61.60802815
131.9328	110.6926181	160.2061	17.74243081	139.783	75.25980221	143.3784	97.54906129	104.0596	288.8739662	131.8719	44.29809995
154.4784	24.40716293	168.7101	63.11477848	150.8477	30.63829865	164.0369	3.879059435	118.5634	75.11871021	149.5824	92.55370807
195.8979	71.20509201	178.8828	21.14650828	158.0517	47.70818674	174.9761	29.33861578	162.2205	374.5674051	151.0832	151.120179
231.5419	6.233705337	190.797	109.7854262	192.3284	95.52189872	205.3191	94.93804821	184.4235	8.894963001	193.5784	883.818132
249.2511	2.716139419	208.2667	2.018961675	257.4413	108.7424525	266.4518	59.76494655	222.2899	41.65278052	216.0742	1197.397852
303.2965	15.67497441	263.9309	77.06994308	290.8337	86.62902653	274.0585	8.643790189	269.543	579.0541282	250.2215	80.82060605
313.7898	24.96823525	320.6764	672.5795449	317.1153	15.82221074	313.3239	50.05528777	305.4636	1254.750343	292.4449	209.0565268
352.881	1230.387809	358.7755	108.3838063	420.9638	27.8078276	390.8077	82.13525574	334.9126	111.091425	345.9065	10.72353858
388.1259	64.31844462	372.0957	189.1259965	445.1593	116.7820943	460.0708	41.18939209	357.8792	173.0845865	409.9946	36.79635095
420.5292	441.6729427	486.5534	146.9593374	455.2295	891.1448799	462.0146	31.29591991	440.4617	102.5060863	459.2661	8.64042347
492.0453	299.0994237	499.1345	247.9889306	462.0539	49.83143107	474.6347	805.7237118	456.1946	72.64164755	495.5517	162.5354864
500.2513	268.3116973	502.3993	180.2092086	498.4748	153.7568275	500.3797	111.3584528	475.6172	329.7500193	514.451	250.5068383
506.7339	0.689654298	516.7265	61.46383359	510.424	53.15794027	502.3085	89.03440926	501.4804	128.1183594	526.0297	117.3423331
524.7729	14.78084207	538.6623	91.99437349	553.0072	126.9780524	534.8819	122.3277598	531.1175	56.84722753	536.0805	107.435604
569.9457	30.85917886	544.5036	184.0151417	594.8713	57.9104159	632.777	18.71453487	574.8573	251.8524526	648.4887	64.73948186
654.2881	329.5882646	710.9956	184.998648	802.9003	61.75986335	779.8541	25.84948131	727.751	496.5769203	796.9456	24.23786925
780.5472	19.34319076	844.0635	19.19445843	818.8412	96.03060428	818.0376	129.2519976	807.0562	9.943140095	859.4178	39.59838216
873.6432	9.82778905	888.2926	12.48611397	875.4572	62.88654881	878.7239	49.81730623	920.9825	1676.27701	899.7526	39.20749365
890.3676	67.9812856	891.7106	102.4449146	931.3616	13.70817573	928.823	39.27878528	972.2611	17.43046198	946.7789	21.09775868
941.8101	56.15044151	976.5385	110.2729733	981.9806	35.79803317	953.9645	85.81872776	982.6158	52.17922841	977.3204	31.97370162
983.3809	6.099831636	982.5409	52.82432529	994.6193	79.60349902	1032.7554	145.7981441	1023.8819	97.30927488	1018.4686	123.6586805
998.188	187.4371878	1029.1909	21.83838391	1052.7287	26.63997458	1052.9902	10.2543243	1054.9787	8.149501338	1035.7177	218.7359572
1037.2683	30.05812234	1071.5206	52.47250503	1070.4383	35.46799207	1071.9545	32.21054108	1087.1406	209.6548015	1072.1897	17.43452616
1047.2501	67.37004926	1089.7588	194.6872442	1127.6848	138.2638281	1114.1689	77.77572735	1095.3828	591.7563088	1086.7764	122.5294326
1119.2866	275.8088456	1099.7501	6.082674194	1144.3345	173.4549406	1127.9004	151.0307716	1113.2903	456.792311	1125.3899	5.389669661
1147.0897	93.02915881	1129.0255	288.4223237	1195.7749	329.5862565	1197.3814	389.5929967	1155.6471	292.2128301	1174.9645	15.7944166
1193.2243	209.6450499	1204.0266	610.0853302	1219.3802	90.15975128	1209.0328	43.74425504	1187.8788	3.907858958	1210.6306	578.9874426
1208.6891	505.581053	1231.4813	100.4459023	1230.4116	112.599226	1236.585	173.3418389	1210.5651	92.89935225	1239.8822	58.00523584
1263.4033	82.51879918	1282.1136	16.06010241	1243.2781	29.44979917	1252.2539	21.82414194	1237.9371	57.03581284	1282.8967	36.18329619
1271.3069	98.59340639	1289.6	70.878005	1323.7344	25.51888237	1335.628	26.97416496	1276.6358	576.9708089	1344.5335	11.01841436
1337.9023	12.09907396	1354.934	47.8736285	1367.6943	460.4776103	1375.4841	492.9641218	1306.6591	59.06489703	1357.9704	14.90151726
1379.7044	501.8690448	1378.2774	514.6875932	1377.7185	29.33588031	1385.4427	42.74346022	1349.6518	154.7410594	1381.2373	506.785934
1394.9523	40.99982411	1405.4371	34.65722337	1401.9943	53.15623318	1401.9812	33.14260515	1386.4917	62.5931998	1402.1385	78.38533809
1410.8038	50.40715019	1412.4858	15.56911525	1417.2767	58.12714838	1415.187	54.99679516	1407.8804	167.5672243	1413.7641	15.60752391
1429.697	39.41606564	1428.2768	116.2980043	1428.879	3.263821188	1421.0262	94.48408915	1430.0639	14.36565235	1424.7348	120.3373017
1451.0985	19.36279712	1452.9775	3.7917709	1440.4219	27.20498334	1435.7591	23.57834924	1454.4561	124.3028971	1462.1646	21.30240269
1482.907	17.26632312	1484.3744	20.40556596	1484.3168	19.22161991	1472.9981	15.17733395	1482.5885	37.32696006	1483.2219	28.05716393
1496.2735	27.0418905	1495.7592	12.78279612	1487.7655	8.536993557	1488.2378	45.28877714	1491.4023	28.00919653	1496.2716	26.73664203
1507.5789	3.287938206	1502.3345	22.97614947	1492.9269	53.41057251	1493.6895	22.9061447	1531.0966	8.026755214	1530.638	16.33798297
1711.4009	0.838253213	1726.1387	19.89384512	1768.9367	60.86653549	1754.073	67.39822315	1633.0293	144.2166934	1768.4972	23.03003697
3053.0719	34.14389023	3057.6312	17.32831146	2992.8598	14.79411964	2996.5343	13.53397393	2992.9268	40.36254567	3011.4748	12.60495859
3079.0638	5.625205861	3065.373	17.28350652	3015.596	36.89932901	3059.224	22.23010099	3066.5849	6.592438156	3051.8741	57.55152295
3122.1149	16.11634233	3078.4622	36.15227628	3062.5659	13.84685155	3064.6246	10.59278955	3067.4019	14.23665404	3053.3078	17.39348257
3155.439	9.827344454	3121.4662	9.639965903	3081.7001	18.06200033	3092.9197	23.60216119	3092.658	25.80650285	3108.8794	8.371258419
3173.5831	3.884328081	3123.7793	11.87644757	3106.8879	23.3408071	3113.3351	26.60781329	3134.2681	3.90924957	3130.2951	6.771268084
3177.1679	1.233420828	3155.5182	10.18007936	3118.8231	5.013827482	3123.1437	7.90778934	3158.0032	1.99494933	3137.2398	11.81735261
3194.2446	11.25425989	3165.5568	5.543971943	3171.548	15.73143449	3158.9562	7.928390033	3159.4706	3.745484922	3152.4965	17.30166556
3262.1815	2.596999679	3253.3261	3.801871471	3187.8442	0.082344786	3167.4717	9.269716882	3191.3814	0.557773859	3167.8759	16.72577562
3878.5281	49.96219887	3889.9363	41.07628764	3821.2038	71.7686783	3855.3587	76.28249514	3872.1945	62.09393258	3870.6339	44.63672565

Table S43: Vibrational frequencies of ISOPOs calculated by G16 at the M06-2X/aug-cc-pVTZ level of theory.

1,2-ISOPO		4,3-ISOPO		*E*-1,4-ISOPO		*Z*-1,4-ISOPO		*E*-4,1-ISOPO		*Z*-4,1-ISOPO	
Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity
97.1063	1.696719085	51.7695	58.63553788	52.5874	510.757631	39.0696	752.1832057	20.459	574.8444949	40.9182	648.481089
147.0623	228.5336103	124.5729	199.0360966	85.5578	100.1851292	70.4028	28.8313163	65.2228	25.15744722	74.2814	28.89412153
217.2819	9.29774105	169.247	147.6350701	138.3289	127.2937342	149.1538	46.97820361	226.1857	65.69693583	146.8918	15.7846644
220.2894	17.59367255	190.3486	19.86015643	151.8359	66.4716083	192.6467	97.75795944	251.8139	0.711334613	192.6706	10.3404726
303.7492	2.202547178	264.3234	248.2836666	224.0814	186.2585451	257.7652	83.27172848	310.6867	947.6823069	251.6763	271.001809
317.2476	201.7990164	296.8405	216.321363	308.3336	8.985840308	264.7594	12.91479172	347.3643	418.6461035	283.4803	41.8134789
337.1826	156.3884252	332.6407	233.4171548	333.2508	1311.825638	307.8268	1180.532023	371.5184	98.60034848	324.2989	1291.361123
384.9462	69.71643107	395.8495	888.0630529	405.5186	341.8997777	393.1346	254.049785	420.887	63.43802229	389.324	18.5562661
434.6441	925.2553747	453.2918	258.6800932	433.6028	22.15775762	444.3729	49.55000866	441.7583	39.48503567	433.135	55.49244547
497.5534	36.25030914	527.7856	51.07218041	494.4498	29.8577611	491.588	16.1089242	458.9303	23.78963397	497.5556	12.85685203
554.4986	11.25595669	570.5581	75.66637262	586.3038	22.08069176	628.0323	39.44980789	593.4922	134.2263334	612.4311	37.24464442
689.637	70.30704279	709.4632	124.7776166	732.3478	65.75457465	707.9249	95.65763972	756.6741	11.86368348	739.3363	57.23503244
769.3304	25.81675425	784.5499	303.1825453	842.6968	5.007714002	824.7189	2.236275191	803.2005	130.4713924	784.8414	25.76095757
888.1342	42.87909259	844.9171	16.54227826	876.3397	78.93668741	898.3581	39.43221875	898.2722	119.5230783	901.8657	38.21102475
928.422	7.866454923	895.6114	31.43770836	978.251	22.29574357	953.2172	116.3881085	939.7579	46.32628882	967.265	120.2632575
960.6979	13.67826044	956.3415	186.6346251	990.7943	66.13426549	1017.7384	55.8702315	976.8651	57.21553206	1027.4354	106.1227015
980.9038	166.5136868	975.8508	3.620032277	1052.7537	20.96609964	1059.8197	156.0706968	1050.1078	236.0933752	1057.3758	32.49278952
1036.6819	39.16427515	1034.9618	44.13207301	1069.0202	58.0399705	1073.1328	4.229055786	1081.2202	198.1913457	1070.2828	20.61936202
1045.1679	39.64518624	1068.2225	18.16926461	1099.508	33.59596047	1090.6995	257.1101414	1099.2014	59.84923224	1081.0292	323.715908
1091.4917	166.4993055	1071.3691	38.09325311	1137.9708	225.9967478	1114.0073	21.92685929	1137.2417	37.16752849	1114.9072	113.9201943
1138.0824	318.840543	1129.3641	595.8277047	1151.6198	81.59348293	1139.7869	29.493109	1147.2465	11.65752594	1163.1408	3.910027944
1181.797	27.89243318	1191.1216	28.99001084	1217.5512	81.23578761	1201.821	70.66600394	1165.6815	7.509029547	1201.1885	34.01382421
1227.9093	17.65731147	1218.4533	37.52076287	1229.5874	7.93150684	1240.1012	13.63876529	1193.4074	39.55442599	1248.1204	8.336333055
1243.9688	33.31262444	1302.3437	35.42336135	1312.1832	12.60224269	1328.343	18.04766221	1278.1514	29.14037567	1329.0399	8.4804418
1322.9212	0.588946123	1319.7761	15.78104573	1370.8427	38.13963959	1363.6419	61.94141974	1339.8593	58.85485252	1357.8244	51.54157102
1365.9521	5.84382516	1362.1749	60.61055365	1372.476	50.00451909	1372.8496	36.7724414	1365.5084	38.22873873	1367.7671	49.27219715
1376.128	30.18121668	1410.1179	26.54622968	1388.8805	44.43462339	1389.2608	13.4198351	1398.6979	93.84638639	1385.0329	42.08786285
1418.0325	134.2280483	1411.9317	114.8674272	1420.5505	59.62596098	1413.045	31.63776536	1426.5213	48.00936658	1415.7021	11.54463446
1457.7123	29.60372261	1452.6992	2.056901146	1429.4089	24.25691458	1421.2678	98.42018352	1456.7538	46.07533158	1422.3373	141.0966547
1478.163	19.41526542	1477.7747	18.60130899	1488.0538	23.17573782	1479.0135	21.26067762	1488.2603	19.18543083	1479.6162	22.64138882
1494.7703	11.3193527	1492.1041	39.64227177	1491.7151	7.759415725	1496.6642	37.58285093	1500.1666	10.66805953	1496.6008	32.87052711
1519.1433	2.32539708	1510.9598	6.311125283	1499.8606	25.64117614	1514.4578	9.617231297	1510.3618	5.878857492	1512.6009	5.850637959
1731.2201	18.69939186	1744.1734	27.04949665	1778.0009	21.61094517	1767.5671	15.53131377	1526.5981	7.315559393	1767.8626	15.21391894
3039.4607	44.37364543	2988.1268	7.195964048	2916.2116	28.56685549	2915.7933	26.61250779	3038.1392	32.45918093	2913.1485	20.62001112
3078.2644	8.546530332	3057.8186	30.38005878	3011.245	57.34315351	3039.4437	5.486950416	3066.1427	6.071382479	3047.388	4.47287122
3118.7987	17.30914139	3061.7469	30.87230565	3041.512	8.067561976	3057.8116	21.60813193	3072.4391	37.89814373	3056.3024	23.77711874
3163.1326	6.953090693	3117.6125	11.08929279	3058.0747	29.32448551	3072.882	36.91080795	3111.0443	27.48567184	3071.6819	46.05854423
3168.8973	8.345274047	3150.5966	8.819710426	3080.0053	18.6739744	3107.7022	33.12877874	3134.8053	14.53312565	3103.5789	20.19392292
3177.9988	9.861774001	3156.5911	2.406965964	3104.8008	14.91423651	3118.4473	11.33552985	3157.7583	13.49676771	3118.4889	10.38347189
3178.5365	0.599187178	3157.4435	15.55204223	3172.5022	15.73273888	3153.5768	9.788744675	3190.3645	4.657558244	3154.8509	2.652347544
3255.011	6.857573233	3241.9945	9.912598778	3184.04	2.175973435	3164.9952	14.29113976	3204.2142	18.21877329	3159.5919	23.24566054
3836.2135	53.75871381	3857.1104	62.46025996	3867.9529	38.63955827	3869.4984	38.3147266	3864.7744	34.63546165	3873.6994	37.18182388

Table S44: Vibrational frequencies of ISOPOs calculated by G16 at the M06-2X/aug-cc-pV(T+*d*)Z level of theory.

1,2-ISOPO		4,3-ISOPO		*E*-1,4-ISOPO		*Z*-1,4-ISOPO		*E*-4,1-ISOPO		*Z*-4,1-ISOPO	
Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity	Freq.	Intensity
97.1099	1.696656185	51.7701	58.6425643	52.5828	510.8174864	39.0668	752.2575398	20.4534	575.0018834	40.9069	648.6407187
147.0641	228.5389512	124.5723	199.0306503	85.5648	100.1909204	70.4012	28.82630488	65.2201	25.15237188	74.2755	28.91252995
217.2817	9.299585657	169.247	147.6114986	138.3313	127.2857578	149.1523	46.97065192	226.1855	65.69346638	146.8911	15.78473962
220.2895	17.59366456	190.3481	19.86230444	151.8363	66.46880576	192.6459	97.75008202	251.8117	0.711340828	192.6705	10.34254854
303.7492	2.203860563	264.3238	248.247068	224.0806	186.2716725	257.7661	83.2420318	310.6907	947.5866432	251.6753	271.0076412
317.2474	201.7752511	296.8422	216.2784618	308.3336	8.985840308	264.7602	12.89968473	347.3661	418.7185847	283.4806	41.81906381
337.1898	156.4253123	332.6426	233.3810417	333.246	1311.858899	307.8398	1180.451067	371.5184	98.60142229	324.2965	1291.365759
384.947	69.70384999	395.8557	888.0652685	405.5182	341.8794556	393.1363	254.1024688	420.8864	63.44190415	389.3274	18.55507936
434.6479	925.2491212	453.294	258.749245	433.6028	22.15867768	444.3727	49.55182648	441.7581	39.48415047	433.1344	55.49068023
497.5478	36.2475099	527.7862	51.07061061	494.4496	29.85696634	491.5878	16.10974229	458.9302	23.79137771	497.5558	12.85764866
554.4984	11.25596075	570.5578	75.66641241	586.3035	22.08002263	628.0323	39.45044311	593.4888	134.2271023	612.4341	37.23273677
689.6394	70.31084744	709.4641	124.7740844	732.3464	65.75633457	707.9247	95.65879381	756.6738	11.86368818	739.4327	57.24105873
769.3299	25.81832669	784.551	303.1821202	842.6963	5.007716974	824.7186	2.235792277	803.2001	130.4714574	784.8409	25.74267494
888.1385	42.87169801	844.9173	16.54321867	876.3385	78.9367955	898.3576	39.43312885	898.2718	119.5253521	901.8667	38.21496352
928.4238	7.867728759	895.6118	31.43635801	978.2514	22.29573445	953.2177	116.3842808	939.7583	46.32329751	967.2654	120.2830049
960.6956	13.68120002	956.3412	186.635518	990.7936	66.13431221	1017.7381	55.87024797	976.8642	57.21517639	1027.4396	106.1036299
980.9027	166.5106199	975.8508	3.620032277	1052.7549	20.96531784	1059.8212	156.0674645	1050.1082	236.0799886	1057.3827	32.49823683
1036.6817	39.15658623	1034.9612	44.13171313	1069.0205	58.0403274	1073.1327	4.229427933	1081.2211	198.2055706	1070.2792	20.64142325
1045.1658	39.6479378	1068.2225	18.16851769	1099.5075	33.59488724	1090.701	257.1061301	1099.2012	59.84851726	1081.0295	323.6874024
1091.4904	166.5108343	1071.369	38.09400139	1137.9717	225.9944657	1114.0073	21.93044041	1137.2401	37.16863317	1114.9079	113.9290684
1138.0812	318.8426319	1129.3654	595.8227799	1151.6193	81.59802177	1139.7868	29.49451163	1147.2463	11.65752797	1163.1406	3.909685632
1181.7975	27.89208381	1191.1213	28.99102293	1217.5507	81.23647629	1201.8214	70.66797209	1165.6818	7.508685377	1201.1857	34.0168926
1227.9085	17.6560234	1218.454	37.52106873	1229.5871	7.931184325	1240.1013	13.63844249	1193.4071	39.55443594	1248.1146	8.339887767
1243.9661	33.31333814	1302.3431	35.42368399	1312.1827	12.6022475	1328.3429	18.0479639	1278.1506	29.14070604	1329.0391	8.488551537
1322.9202	0.588645008	1319.776	15.78074464	1370.8424	38.14866949	1363.642	61.94258541	1339.8586	58.85518102	1357.8141	51.52550863
1365.9513	5.842368282	1362.1754	60.60877419	1372.4754	49.99582079	1372.8497	36.7692422	1365.5082	38.2269914	1367.7789	49.24960517
1376.128	30.18817428	1410.1184	26.53377212	1388.8801	44.43463619	1389.2612	13.41925692	1398.6976	93.84840308	1385.0314	42.10288634
1418.0325	134.2283296	1411.9324	114.8840406	1420.5509	59.62510169	1413.0448	31.63438192	1426.5214	48.00992254	1415.703	11.54434533
1457.7122	29.60536669	1452.6992	2.056901146	1429.4089	24.25719367	1421.2683	98.42716621	1456.7523	46.07510516	1422.3363	141.0947906
1478.163	19.41553531	1477.7742	18.60131529	1488.0541	23.17573314	1479.0134	21.26067905	1488.2602	19.18516406	1479.6161	22.64139035
1494.7703	11.3193527	1492.1042	39.64226912	1491.7154	7.759949038	1496.6641	37.58285344	1500.1661	10.66832901	1496.6007	32.86839679
1519.1433	2.325134472	1510.9597	6.3111257	1499.8611	25.64090161	1514.4579	9.617230662	1510.3614	5.879123184	1512.6004	5.850903637
1731.2184	18.69871891	1744.1721	27.04974554	1778.0008	21.61094638	1767.5678	15.53108192	1526.5981	7.315559393	1767.8616	15.21279924
3039.4675	44.37315239	2988.1298	7.195956823	2916.2134	28.56697466	2915.7944	26.61249775	3038.1439	32.45808023	2913.1529	20.62039081
3078.2637	8.546402677	3057.8204	30.36321086	3011.2433	57.34331837	3039.4433	5.487082392	3066.1454	6.071767466	3047.3894	4.476927436
3118.798	17.30876154	3061.746	30.88912319	3041.5129	8.066903764	3057.8115	21.60813264	3072.4445	37.89833681	3056.3031	23.77659118
3163.1307	6.954860575	3117.6092	11.08879268	3058.0734	29.32593298	3072.8808	36.90965393	3111.0424	27.4855604	3071.6865	46.05730637
3168.9001	8.343881859	3150.596	8.82059847	3080.0024	18.67373293	3107.7015	33.13045503	3134.8077	14.53324179	3103.5831	20.19261018
3178.0008	9.863650769	3156.5903	2.40721934	3104.7985	14.91399058	3118.4483	11.33539828	3157.7576	13.49651803	3118.4893	10.38385434
3178.5381	0.596676668	3157.4494	15.55176048	3172.4992	15.73300525	3153.5779	9.78874126	3190.3685	4.65692718	3154.8519	2.646656329
3255.0134	6.8578133	3241.9961	9.912347779	3184.0461	2.175593387	3164.9969	14.29075394	3204.2122	18.21940719	3159.5911	23.25033816
3836.2095	53.75876987	3857.1017	62.46019398	3867.956	38.63963044	3869.4891	38.31471559	3864.7724	34.6355828	3873.7004	37.1817113

Table S45: Vibrational frequencies of the complexes of *E*-1,4-ISOPOO-SO_2 and *E*-1,4-ISOPO-SO_3 calculated by G16 at the M06-2X/aug-cc-pVTZ level of theory.

E-1,4-ISOPOO_SO_2		*E*-1,4-ISOPO_SO_3	
Freq.	Intensity	Freq.	Intensity
27.9789	333.5797764	15.9142	204.581268
57.1054	235.9180569	64.811	270.0942252
75.1137	78.61025466	89.3352	93.10880336
82.6254	0.878749544	134.201	36.34129638
86.6241	38.60257015	141.7573	54.6554476
107.4875	34.64313087	154.1849	509.8907786
121.0581	33.20815175	173.2564	88.74440715
131.2182	54.53953787	201.0246	19.61312917
159.5269	32.18988351	210.6557	52.09275332
163.9178	804.6220211	216.8134	142.6563026
181.3958	19.01715436	272.3866	664.8312175
244.5846	63.27817531	300.5258	427.2775608
331.3016	17.46993598	402.0126	167.0324214
359.6597	25.8835194	454.843	560.3977021
435.0821	25.40445682	468.2048	1064.866779
469.1436	128.2764162	481.5592	638.5042961
489.178	804.6867149	487.7545	1151.642317
540.479	290.5479188	522.2754	149.1293695
577.0063	85.90800388	529.1169	99.44599367
599.3537	21.34831948	589.7568	35.09546913
808.803	5.264426369	671.5821	27.33665456
871.2356	19.75705876	859.3977	18.67696583
910.1294	208.2375377	880.2386	87.80368357
979.837	32.67412135	987.2902	77.28387614
986.2252	100.1433705	994.6652	87.62061182
1024.1888	15.93750916	1058.1467	42.18297113
1071.673	34.77344204	1073.481	7.269490793
1133.9076	124.4272711	1081.5265	123.4882818
1148.4085	154.4570408	1105.5437	50.78477155
1219.692	22.4303271	1153.7813	238.5672722
1230.3791	153.9316197	1162.9111	45.41777006
1244.4123	67.68860735	1208.1116	65.58947515
1255.4437	33.13969913	1237.8447	98.42994338
1297.4784	42.8236271	1306.2421	0.716797881
1351.6273	2.833194151	1359.1374	24.51455546
1390.3956	52.38654287	1374.5915	518.2557032
1396.0647	644.5372936	1394.2877	229.5081112
1412.3476	22.49754482	1399.1953	267.6509161
1420.9684	32.44286044	1411.0982	205.9349861
1431.7656	7.002092839	1412.9861	17.88131569
1478.2151	5.543861736	1425.0463	15.58809884
1487.4751	23.21747461	1470.2267	13.6902062
1489.8918	14.15964056	1477.8906	49.24949023
1505.503	38.49714443	1493.7458	41.05906021
1769.1597	41.46884993	1705.367	175.5488126
3024.636	30.97899167	2946.5977	11.9172949
3062.5195	15.68340998	2989.4699	1.391732542
3076.4446	24.16167287	3028.0789	24.6889572
3106.8039	17.94918394	3059.1565	3.17453196
3118.8027	5.605848067	3072.8351	9.341507158
3161.8061	6.125904841	3123.9684	2.258425307
3174.7447	15.164699	3172.0344	4.981913489
3192.5555	0.820483256	3186.4354	4.441573239
3839.2493	128.2835817	3850.3167	79.39553333

Table S46: Vibrational frequencies of the complexes of *E*-1,4-ISOPOO-SO_2 and *E*-1,4-ISOPO-SO_3 calculated by G16 at the M06-2X/aug-cc-pV(T+*d*)Z level of theory.

E-1,4-ISOPOO_SO_2		*E*-1,4-ISOPO_SO_3	
Freq.	Intensity	Freq.	Intensity
20.0422	529.2736164	22.5981	145.0603298
58.1403	240.9407935	65.7407	278.7390316
72.1879	53.65036234	93.3083	91.0938265
79.4522	7.832961123	136.0329	37.95756063
87.2886	26.27039067	142.8017	57.52150876
103.9025	8.746514537	154.1842	493.1576418
112.8743	63.19103289	174.4243	89.2434695
129.2663	56.76729023	202.5261	26.17495355
155.9806	39.52040738	213.6357	39.72857982
162.7906	761.2199954	219.7297	151.3623703
181.5352	17.33677879	271.7982	663.1206176
245.209	60.0047122	301.5141	412.2303611
331.8542	18.55163521	402.3986	167.3361732
360.7006	24.10556463	455.2103	539.4521283
435.0606	24.34202115	472.2488	662.0177874
468.136	112.239085	484.1875	161.117481
491.7529	810.6732206	494.7703	2011.967907
545.219	292.2519561	535.0377	139.89719
576.8714	94.15970211	541.815	101.7327077
599.8885	20.08303409	589.943	40.35496293
808.5265	4.580378754	671.1627	27.75495748
870.837	19.22232458	859.0695	18.5266744
909.6563	206.5705445	880.516	86.08967673
978.9	32.55705279	987.963	72.07390881
986.913	101.3691353	995.3559	92.02513495
1024.6225	15.70221302	1058.416	41.67658647
1071.1072	34.63537941	1073.4117	5.395327999
1133.645	125.9914721	1105.0804	82.31567724
1147.9679	158.0012353	1105.9865	88.96392642
1219.4929	20.9870677	1153.9774	239.8611661
1239.9586	104.3587204	1163.1357	46.28224335
1249.983	87.28824468	1208.1335	65.65796086
1254.5707	60.31520821	1238.2264	93.90026757
1296.8815	44.13162713	1306.1901	0.745230702
1352.1912	4.832919985	1359.4326	39.05606799
1388.8234	40.94722262	1385.9801	217.3740444
1410.5916	80.48217394	1400.2096	188.4246541
1416.9655	355.7677497	1408.2764	238.937266
1429.9105	276.0738143	1421.6191	151.9222713
1431.7151	4.391718181	1425.0475	30.20838988
1478.194	3.73383419	1430.2442	438.1337022
1487.2666	23.4347825	1470.1951	15.00411337
1489.0474	15.79579613	1478.0373	43.44014834
1505.153	39.0645552	1494.2257	41.69411919
1769.5444	42.03810797	1705.1719	168.7396449
3023.284	31.4281674	2947.323	12.03442354
3062.694	15.68551233	2990.4761	1.388863007
3076.902	24.64299567	3028.7027	24.71890963
3107.0426	18.10971555	3059.0207	3.240792888
3117.9073	5.448414708	3073.2095	9.288963523
3162.2646	5.777203601	3124.2052	2.328740772
3175.4767	15.29839283	3172.1431	4.953194464
3192.2536	0.975400158	3186.4639	4.43890435
3839.8155	126.1667028	3850.9013	80.12201956

Table S47: Vibrational frequencies of SO_2 and SO_3 calculated by G16 at the M06-2X/aug-cc-pVTZ level of theory.

SO_2		SO_3	
Freq.	Intensity	Freq.	Intensity
535.5235	259.5333667	502.1363	322.9343028
1234.5494	118.5920085	527.6276	223.545788
1419.1182	714.5343309	527.8038	224.146889
-	-	1108.5291	0.007197641
-	-	1429.2422	605.8856566
-	-	1430.1431	605.5608929

Table S48: Vibrational frequencies of SO_2 and SO_3 calculated by G16 at the M06-2X/aug-cc-pV(T+*d*)Z level of theory.

SO_2		SO_3	
Freq.	Intensity	Freq.	Intensity
540.39	260.197831	519.6272	314.109445
1254.613	125.3591387	541.8686	222.6491038
1454.322	714.8541964	541.8969	222.4814036
-	-	1134.3342	0
-	-	1459.7754	615.4021105
-	-	1459.7966	615.2229171

Table S49: Rotational constants of the optimised molecules at the M06-2X/aug-cc-pVTZ level of theory (GHz).

Species	Coordinate	1,2-isomer	4,3-isomer	*E*-1,4-isomer	*Z*-1,4-isomer	*E*-4,1-isomer	*Z*-4,1-isomer	SO_2	SO_3
ISOPOO	X	2.8148848	2.9576288	3.3873656	2.8931585	4.7760783	2.4120726	-	-
	Y	1.6810235	1.4225951	1.1545784	1.5166968	0.8955393	1.7363124	-	-
	Z	1.4652277	1.2370739	1.0144532	1.1604781	0.8398830	1.1804250	-	-
ISOPOO-SO_2 (complex)	X	-	-	0.9197172	-	-	-	-	-
	Y	-	-	0.8892175	-	-	-	-	-
	Z	-	-	0.6279472	-	-	-	-	-
ISOPOO-SO_2 (TS)	X	1.4941990	1.6547757	1.1767346	1.6324150	3.0069918	1.4160253	-	-
	Y	0.6452438	0.5834069	0.8824476	0.6084895	0.3280560	0.6534188	-	-
	Z	0.5258287	0.5092739	0.7182876	0.4814527	0.3117069	0.4949039	-	-
$ISOPOOSO_2$	X	1.4982629	1.6563408	1.2081587	1.6190497	3.0414101	1.3634829	-	-
	Y	0.6865762	0.6030143	0.8582783	0.6548547	0.3363734	0.7182649	-	-
	Z	0.5448706	0.5114211	0.7219976	0.5054440	0.3213419	0.5177009	-	-
ISOPO-SO_3 (TS)	X	1.6447592	1.4979183	1.2180790	1.2979951	1.6461870	1.4618900	-	-
	Y	0.5794076	0.5985448	0.8204675	0.7742485	0.4719647	0.7300960	-	-
	Z	0.5306003	0.5267972	0.7057158	0.6574845	0.3877219	0.5665557	-	-
ISOPO-SO_3 (complex)	X	-	-	1.0487077	-	-	-	-	-
	Y	-	-	0.9200571	-	-	-	-	-
	Z	-	-	0.7248919	-	-	-	-	-
ISOPO	X	3.7597207	4.4763937	3.9443592	4.2438549	5.4681125	4.3974923	-	-
	Y	2.0990515	1.7356070	1.5380095	1.4629537	1.4942408	1.4330600	-	-
	Z	1.7867971	1.4978162	1.1593200	1.2022347	1.3400175	1.1956059	-	-
SO_2	X	-	-	-	-	-	-	57.6553304	-
	Y	-	-	-	-	-	-	10.4334157	-
	Z	-	-	-	-	-	-	8.8346763	-
SO_3	X	-	-	-	-	-	-	-	10.3556149
	Y	-	-	-	-	-	-	-	10.3494440
	Z	-	-	-	-	-	-	-	5.1762643

Table S50: Rotational constants of the optimised molecules at the M06-2X/aug-cc-pV(T+*d*)Z level of theory (GHz).

Species	Coordinate	1,2-isomer	4,3-isomer	*E*-1,4-isomer	*Z*-1,4-isomer	*E*-4,1-isomer	*Z*-4,1-isomer	SO_2	SO_3
ISOPOO	X	2.8148848	2.9576288	3.3873656	2.8931585	4.7760783	2.4120726	-	-
	Y	1.6810235	1.4225951	1.1545784	1.5166968	0.8955393	1.7363124	-	-
	Z	1.4652277	1.2370739	1.0144532	1.1604781	0.8398830	1.1804250	-	-
ISOPOO-SO_2 (complex)	X	-	-	0.9197172	-	-	-	-	-
	Y	-	-	0.8892175	-	-	-	-	-
	Z	-	-	0.6279472	-	-	-	-	-
ISOPOO-SO_2 (TS)	X	1.4941990	1.6547757	1.1767346	1.6324150	3.0069918	1.4160253	-	-
	Y	0.6452438	0.5834069	0.8824476	0.6084895	0.3280560	0.6534188	-	-
	Z	0.5258287	0.5092739	0.7182876	0.4814527	0.3117069	0.4949039	-	-
$ISOPOOSO_2$	X	1.4982629	1.6563408	1.2081587	1.6190497	3.0414101	1.3634829	-	-
	Y	0.6865762	0.6030143	0.8582783	0.6548547	0.3363734	0.7182649	-	-
	Z	0.5448706	0.5114211	0.7219976	0.5054440	0.3213419	0.5177009	-	-
ISOPO-SO_3 (TS)	X	1.6447592	1.4979183	1.2180790	1.2979951	1.6461870	1.4618900	-	-
	Y	0.5794076	0.5985448	0.8204675	0.7742485	0.4719647	0.7300960	-	-
	Z	0.5306003	0.5267972	0.7057158	0.6574845	0.3877219	0.5665557	-	-
ISOPO-SO_3 (complex)	X	-	-	1.0487077	-	-	-	-	-
	Y	-	-	0.9200571	-	-	-	-	-
	Z	-	-	0.7248919	-	-	-	-	-
ISOPO	X	3.7597207	4.4763937	3.9443592	4.2438549	5.4681125	4.3974923	-	-
	Y	2.0990515	1.7356070	1.5380095	1.4629537	1.4942408	1.4330600	-	-
	Z	1.7867971	1.4978162	1.1593200	1.2022347	1.3400175	1.1956059	-	-
SO_2	X	-	-	-	-	-	-	57.6553304	-
	Y	-	-	-	-	-	-	10.4334157	-
	Z	-	-	-	-	-	-	8.8346763	-
SO_3	X	-	-	-	-	-	-	-	10.3535751
	Y	-	-	-	-	-	-	-	10.3535751
	Z	-	-	-	-	-	-	-	5.1767876

Table S51: Electronic state (point group) of the optimised molecules at the M06-2X/aug-cc-pVTZ and M06-2X/aug-cc-pV(T+*d*)Z levels of theory.

Species	1,2-isomer	4,3-isomer	*E*-1,4-isomer	*Z*-1,4-isomer	*E*-4,1-isomer	*Z*-4,1-isomer	SO_2	SO_3
ISOPOO	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	-	-
ISOPOO-SO_2 (complex)	-	-	^{2}A (C1)	-	-	-	-	-
ISOPOO-SO_2 (TS)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	-	-
ISOPOOSO_2	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	-	-
ISOPO-SO_3 (TS)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	-	-
ISOPO-SO_3 (complex)	-	-	^{2}A (C1)	-	-	-	-	-
ISOPO	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	^{2}A (C1)	-	-
SO_2	-	-	-	-	-	-	^{1}A (C2v)	-
SO_3	-	-	-	-	-	-	-	^{1}A (Cs)

Table S52: Spin contamination of the open-shell molecules at the M06-2X/aug-cc-pVTZ level of theory. “Before” and “After” indicate the values before and after the annihilation of spin contamination.

Species		1,2-isomer	4,3-isomer	*E*-1,4-isomer	*Z*-1,4-isomer	*E*-4,1-isomer	*Z*-4,1-isomer
ISOPOO	Before	0.7557	0.7558	0.7557	0.7558	0.7557	0.7558
	After	0.7500	0.7500	0.7500	0.7500	0.7500	0.7500
ISOPOO-SO_2 (complex)	Before	-	-	0.7562	-	-	-
	After	-	-	0.7500	-	-	-
ISOPOO-SO_2 (TS)	Before	0.7641	0.7685	0.7754	0.7644	0.7763	0.7690
	After	0.7501	0.7502	0.7503	0.7501	0.7502	0.7502
ISOPOOSO_2	Before	0.7579	0.7582	0.7578	0.7580	0.7581	0.7579
	After	0.7500	0.7501	0.7500	0.7500	0.7500	0.7500
ISOPO-SO_3 (TS)	Before	1.0050	0.9294	0.7602	0.8004	0.7701	0.7592
	After	0.7573	0.7571	0.7501	0.7504	0.7502	0.7500
ISOPO-SO_3 (complex)	Before	-	-	0.7543	-	-	-
	After	-	-	0.7500	-	-	-
ISOPO	Before	0.7552	0.7559	0.7546	0.7544	0.7567	0.7544
	After	0.7500	0.7500	0.7500	0.7500	0.7500	0.7500

Table S53: Spin contamination of the open-shell molecules at the CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ level of theory. “Before” and “After” indicate the values before and after the annihilation of spin contamination.

Species		1,2-isomer	4,3-isomer	*E*-1,4-isomer	*Z*-1,4-isomer	*E*-4,1-isomer	*Z*-4,1-isomer
ISOPOO	Before	0.7649	0.7663	0.7666	0.7687	0.7648	0.7701
	After	0.7502	0.7502	0.7502	0.7503	0.7502	0.7503
ISOPOO-SO_2 (complex)	Before	-	-	0.7688	-	-	-
	After	-	-	0.7503	-	-	-
ISOPOO-SO_2 (TS)	Before	0.8903	0.8891	0.8992	0.8899	0.8916	0.8921
	After	0.7562	0.7565	0.7576	0.7562	0.7563	0.7563
ISOPOOSO_2	Before	0.7866	0.7871	0.7848	0.7872	0.7872	0.7873
	After	0.751	0.751	0.7509	0.751	0.7511	0.751
ISOPO-SO_3 (TS)	Before	1.2981	1.296	1.1724	1.176	1.8284	1.2255
	After	0.8771	0.8618	0.7833	0.7844	1.3822	0.7995
ISOPO-SO_3 (complex)	Before	-	-	0.7604	-	-	-
	After	-	-	0.7501	-	-	-
ISOPO	Before	0.7696	0.7648	0.7656	0.7671	0.7704	0.7652
	After	0.7503	0.7502	0.7502	0.7502	0.7503	0.7502

Table S54: Spin contamination of the open-shell molecules at the M06-2X/aug-cc-pV(T+*d*)Z level of theory. "Before" and "After" indicate the values before and after the annihilation of spin contamination.

Species		1,2-isomer	4,3-isomer	*E*-1,4-isomer	*Z*-1,4-isomer	*E*-4,1-isomer	*Z*-4,1-isomer
ISOPOO	Before	0.7556	0.7557	0.7557	0.7557	0.7557	0.7557
	After	0.7500	0.7500	0.7500	0.7500	0.7500	0.7500
ISOPOO-SO_2 (complex)	Before	-	-	0.7562	-	-	-
	After	-	-	0.75	-	-	-
ISOPOO-SO_2 (TS)	Before	0.7750	0.7741	0.7754	0.7755	0.7761	0.7762
	After	0.7502	0.7502	0.7502	0.7502	0.7502	0.7502
ISOPOOSO_2	Before	0.7575	0.7577	0.7575	0.7576	0.7578	0.7576
	After	0.7500	0.7500	0.7500	0.7500	0.7500	0.7500
ISOPO-SO_3 (TS)	Before	0.8061	0.8072	0.7996	0.8004	0.8399	0.8053
	After	0.7506	0.7506	0.7504	0.7504	0.7516	0.7505
ISOPO-SO_3 (complex)	Before	-	-	0.7544	-	-	-
	After	-	-	0.75	-	-	-
ISOPO	Before	0.7545	0.7557	0.7545	0.7545	0.7568	0.7545
	After	0.7500	0.7500	0.7500	0.7500	0.7500	0.7500

Table S55: Spin contamination of the open-shell molecules at the CCSD(T)/aug-cc-pV(T+*d*)Z//M06-2X/aug-cc-pV(T+*d*)Z level of theory. "Before" and "After" indicate the values before and after the annihilation of spin contamination.

Species		1,2-isomer	4,3-isomer	*E*-1,4-isomer	*Z*-1,4-isomer	*E*-4,1-isomer	*Z*-4,1-isomer
ISOPOO	Before	0.7649	0.7663	0.7666	0.7687	0.7648	0.7701
	After	0.7502	0.7502	0.7502	0.7503	0.7502	0.7503
ISOPOO-SO_2 (complex)	Before	-	-	0.7679	-	-	-
	After	-	-	0.7502	-	-	-
ISOPOO-SO_2 (TS)	Before	0.8856	0.8846	0.8958	0.8853	0.8866	0.8868
	After	0.7555	0.7558	0.7569	0.7556	0.7556	0.7557
ISOPOOSO_2	Before	0.7817	0.7821	0.7801	0.7823	0.7821	0.7823
	After	0.7508	0.7508	0.7507	0.7508	0.7508	0.7508
ISOPO-SO_3 (TS)	Before	1.2716	1.2683	1.1511	1.1546	1.9148	1.2023
	After	0.8631	0.8487	0.7789	0.7789	1.38558	0.7938
ISOPO-SO_3 (complex)	Before	-	-	0.7604	-	-	-
	After	-	-	0.7501	-	-	-
ISOPO	Before	0.7696	0.7648	0.7656	0.7671	0.7704	0.7652
	After	0.7503	0.7502	0.7502	0.7502	0.7503	0.7502

Table S56: Results of T_1-diagnostic at the CCSD(T)/aug-cc-pVTZ//M06-2X/aug-cc-pVTZ level of theory.

Species	1,2-isomer	4,3-isomer	*E*-1,4-isomer	*Z*-1,4-isomer	*E*-4,1-isomer	*Z*-4,1-isomer	SO_2	SO_3
ISOPOO	0.02068415	0.02076303	0.02061027	0.02107679	0.02026341	0.02103601	-	-
ISOPOO-SO_2 (complex)	-	-	0.02141138	-	-	-	-	-
ISOPOO-SO_2 (TS1)	0.02401188	0.02392258	0.02446145	0.0247022	0.02392523	0.02413011	-	-
ISOPOOSO$_2$	0.01791046	0.01795712	0.01783919	0.01787137	0.01777258	0.01782545	-	-
ISOPO-SO_3 (TS2)	0.03395381	0.03411182	0.03101153	0.03106571	0.04792527	0.03276026	-	-
ISOPO-SO_3 (complex)	-	-	0.01714205	-	-	-	-	-
ISOPO	0.01677333	0.01858451	0.01583723	0.01599266	0.01372785	0.01530928	-	-
SO_2	-	-	-	-	-	-	0.02109463	-
SO_3	-	-	-	-	-	-	-	0.01833553

Table S57: Results of T_1-diagnostic at the CCSD(T)/aug-cc-pV(T+*d*)Z//M06-2X/aug-cc-pV(T+*d*)Z level of theory.

Species	1,2-isomer	4,3-isomer	*E*-1,4-isomer	*Z*-1,4-isomer	*E*-4,1-isomer	*Z*-4,1-isomer	SO_2	SO_3
ISOPOO	0.02068415	0.02075969		0.02107679	0.02026341	0.02103601	-	-
ISOPOO-SO_2 (complex)	-	-	0.02119027	-	-	-	-	-
ISOPOO-SO_2 (TS1)	0.02386706	0.02379334	0.02436636	0.02392955	0.02377627	0.0239619	-	-
ISOPOOSO$_2$	0.01748244	0.01751658	0.01742283	0.01746881	0.01734652	0.01742249	-	-
ISOPO-SO_3 (TS2)	0.03332761	0.03341617	0.03060486	0.03062592	0.13040866	0.03212904	-	-
ISOPO-SO_3 (complex)	-	-	0.01688054	-	-	-	-	-
ISOPO	0.01677337	0.01858449	0.0158383	0.01599316	0.01372785	0.01530928	-	-
SO_2	-	-	-	-	-	-	0.0204715	-
SO_3	-	-	-	-	-	-	-	0.01782716

Table S58: Kinetic parameters of ISOPOOs + SO_2 reactions used in Fig. 3 of the main manuscript.

ISOPOOs	A	E a/R	k_{TS1} (298K)
1,2-ISOPOO	7.317×10^{-15}	4603	1.440×10^{-21}
4,3-ISOPOO	2.915×10^{-15}	4734	3.701×10^{-22}
Z-1,4-ISOPOO	1.281×10^{-14}	4681	1.939×10^{-21}
Z-4,1-ISOPOO	5.776×10^{-15}	4671	9.057×10^{-22}
E-1,4-ISOPOO	3.399×10^{-16}	7020	2.015×10^{-26}
E-4,1-ISOPOO	7.383×10^{-15}	4216	5.323×10^{-21}

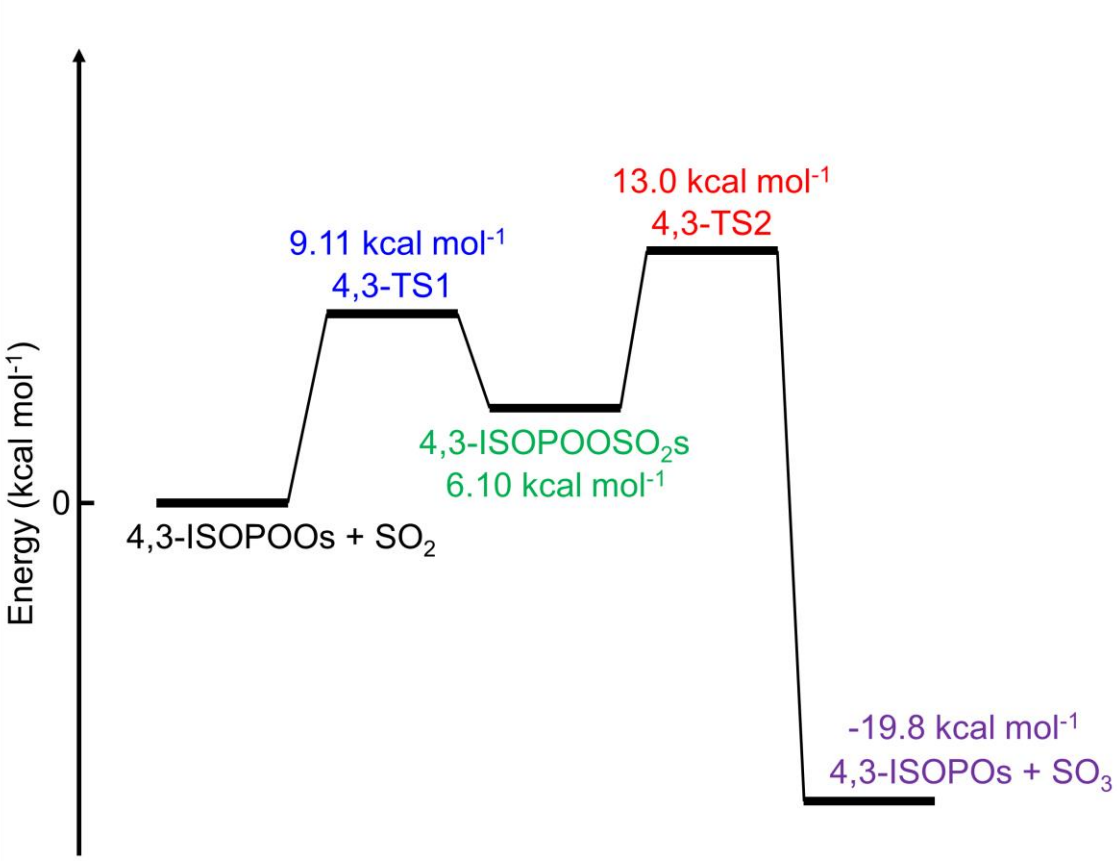

Figure S10: Potential diagram of the entire 4,3-ISOPOO + SO_2 reaction obtained from the quantum chemical calculations for evaluated by CCSD(T)/aug-cc-pV(T+d)Z//M06-2X/aug-cc-pV(T+d)Z level of theory.

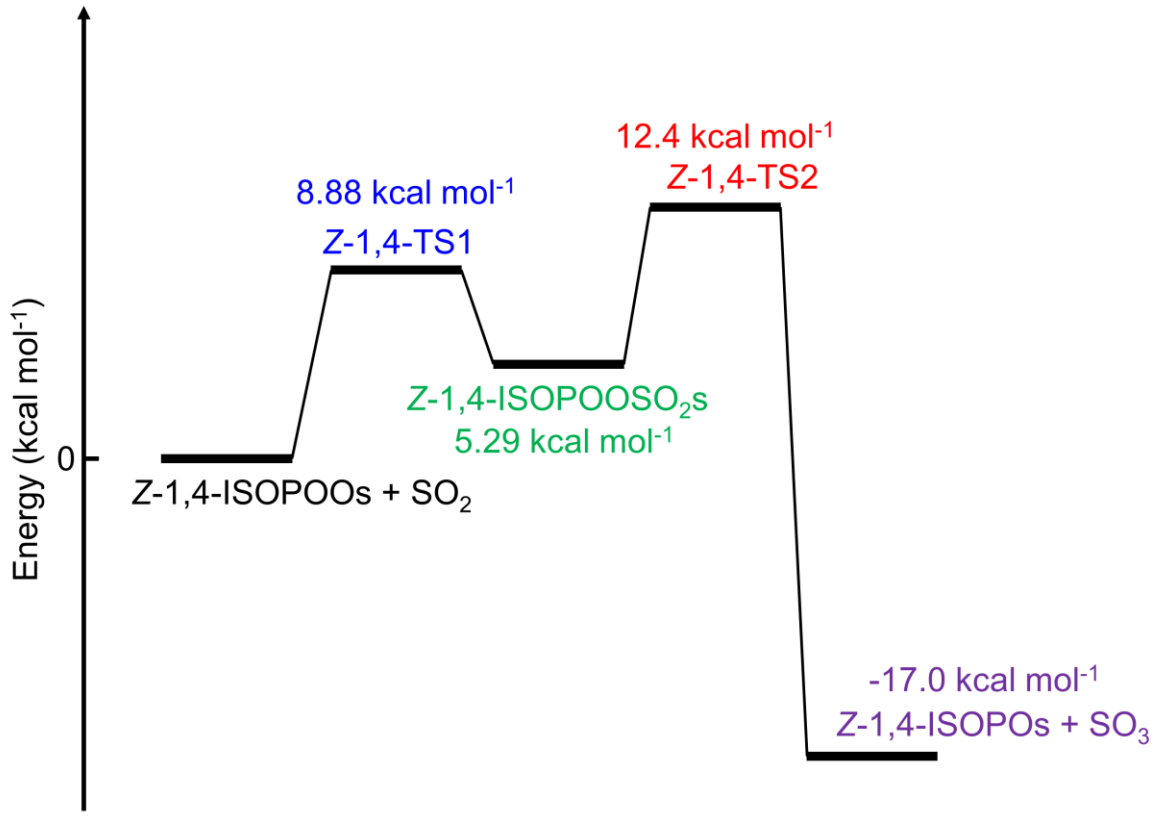

Figure S11: Potential diagram of the entire *Z*-1,4-ISOPOO + SO_2 reaction obtained from the quantum chemical calculations for evaluated by CCSD(T)/aug-cc-pV(T+d)Z//M06-2X/aug-cc-pV(T+d)Z level of theory.

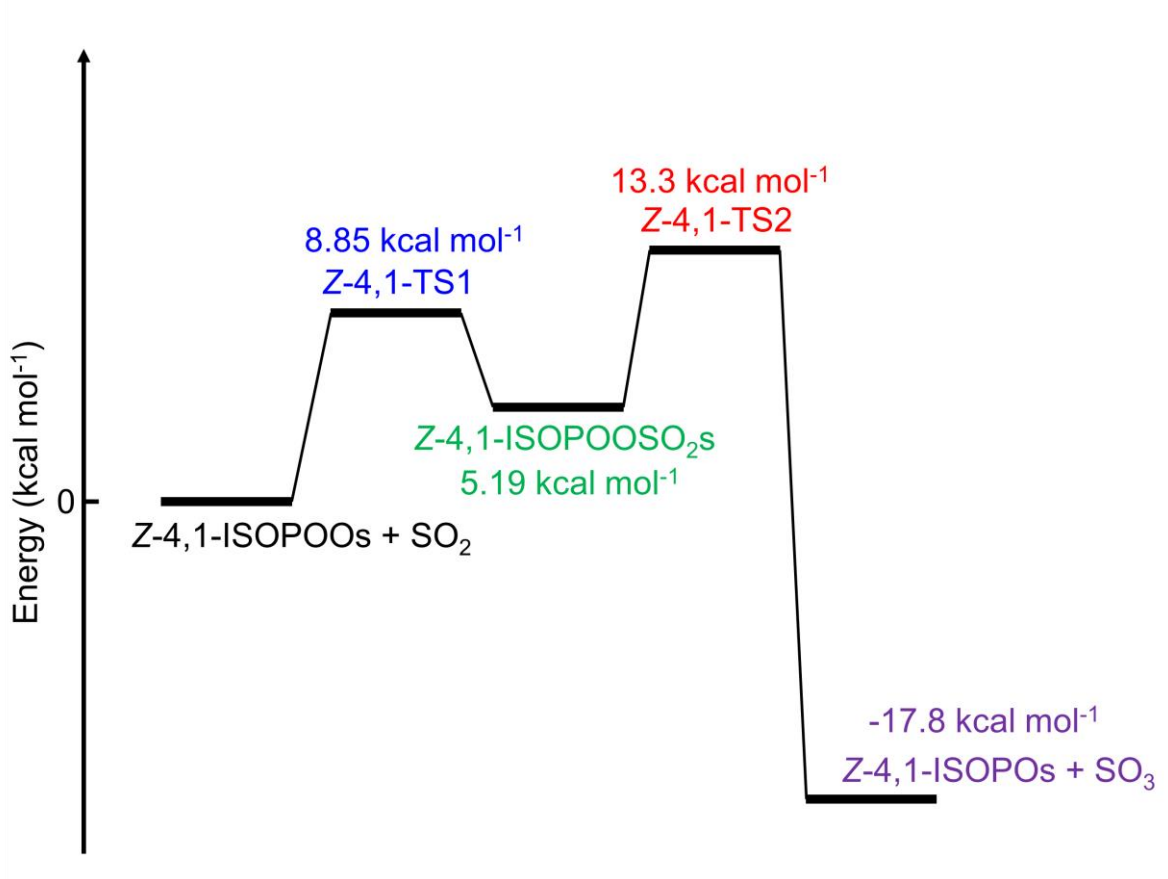

Figure S12: Potential diagram of the entire *Z*-4,1-ISOPOO + SO_2 reaction obtained from the quantum chemical calculations for evaluated by CCSD(T)/aug-cc-pV(T+d)Z//M06-2X/aug-cc-pV(T+d)Z level of theory.

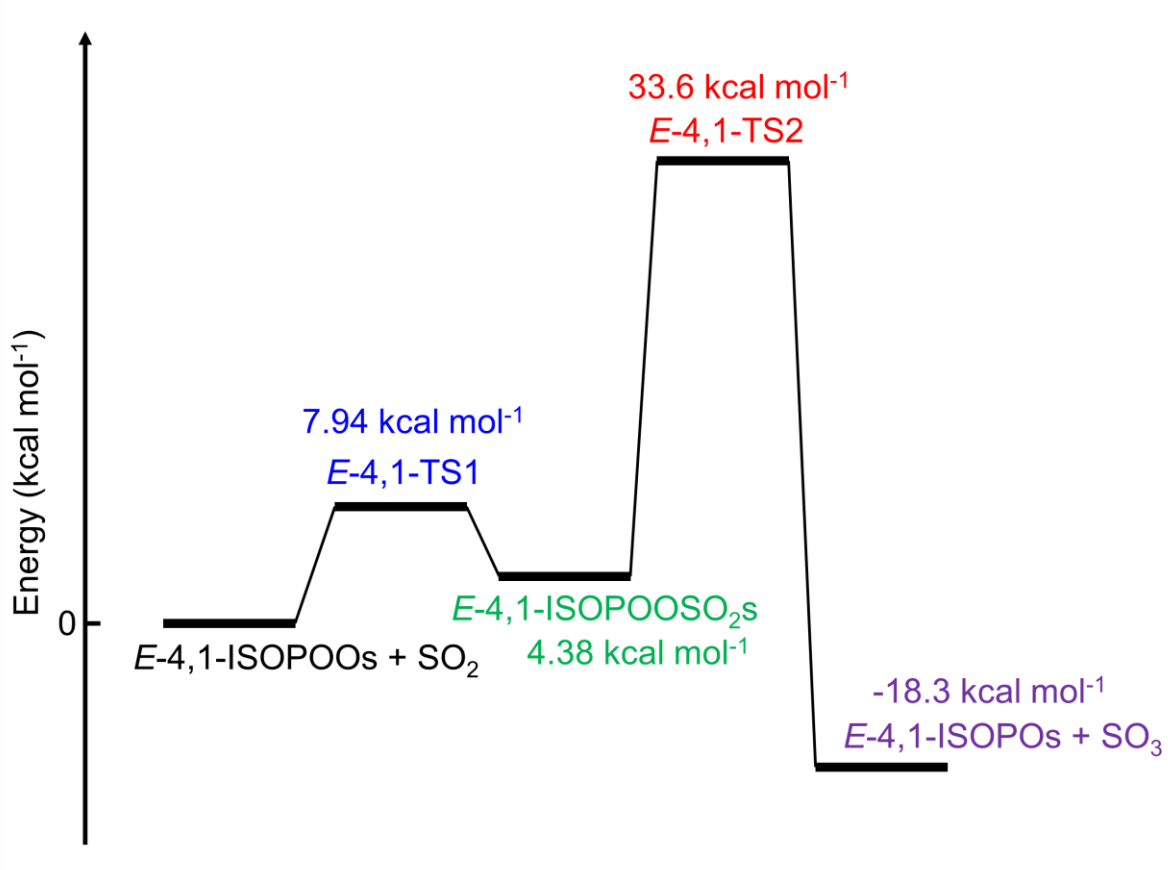

Figure S13: Potential diagram of the entire *E*-4,1-ISOPOO + SO_2 reaction obtained from the quantum chemical calculations for evaluated by CCSD(T)/aug-cc-pV(T+d)Z//M06-2X/aug-cc-pV(T+d)Z level of theory.

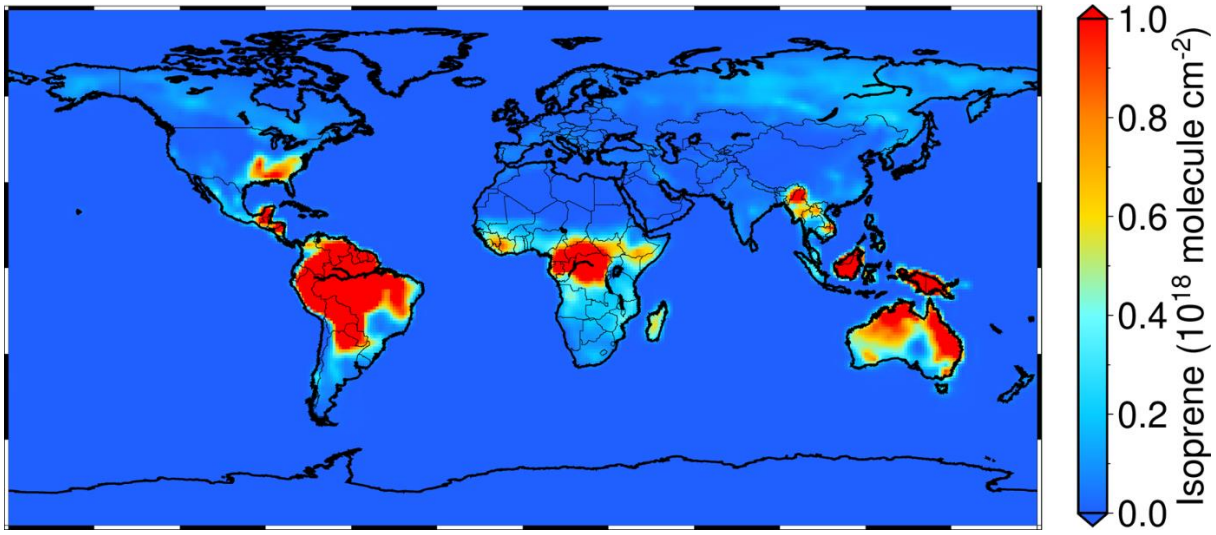

Figure S14: Calculated annual-mean column concentration of isoprene.

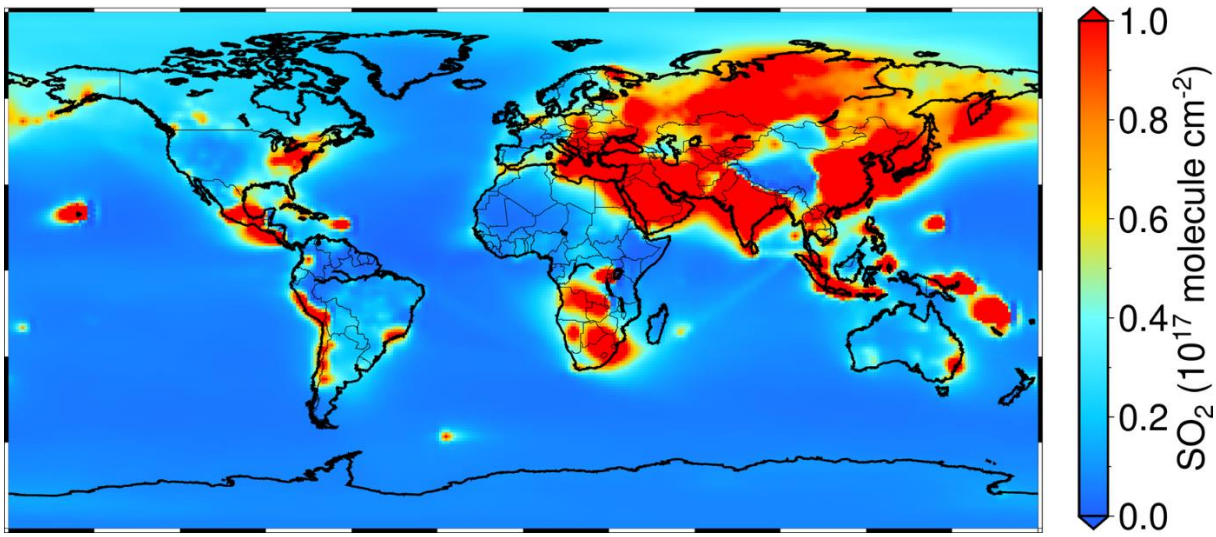

Figure S15: Calculated annual-mean column concentrations of SO_2.

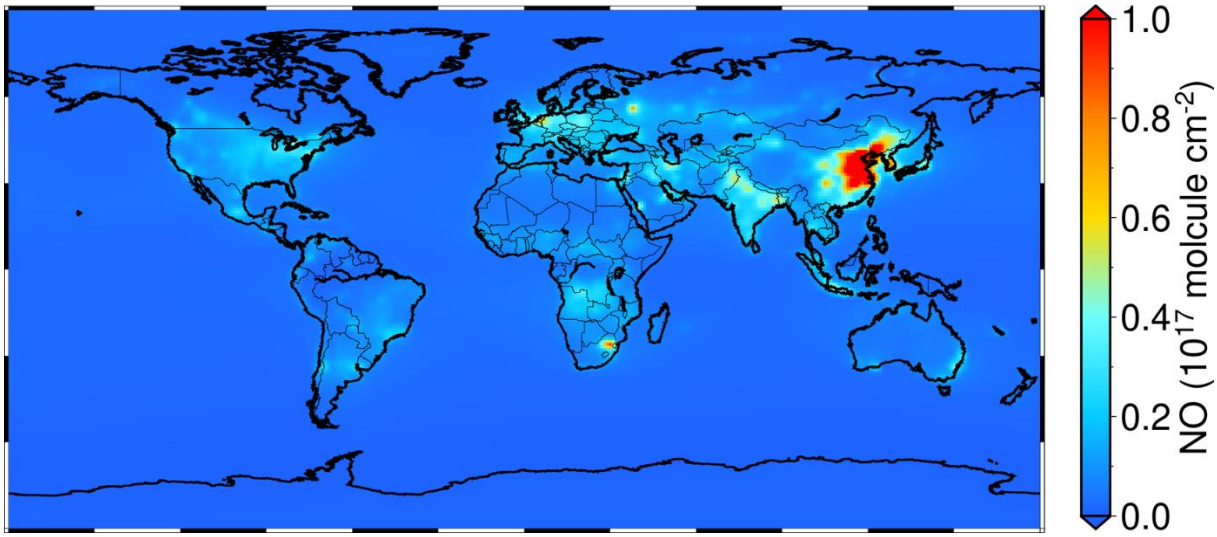

Figure S16: Calculated annual-mean column concentration of NO.

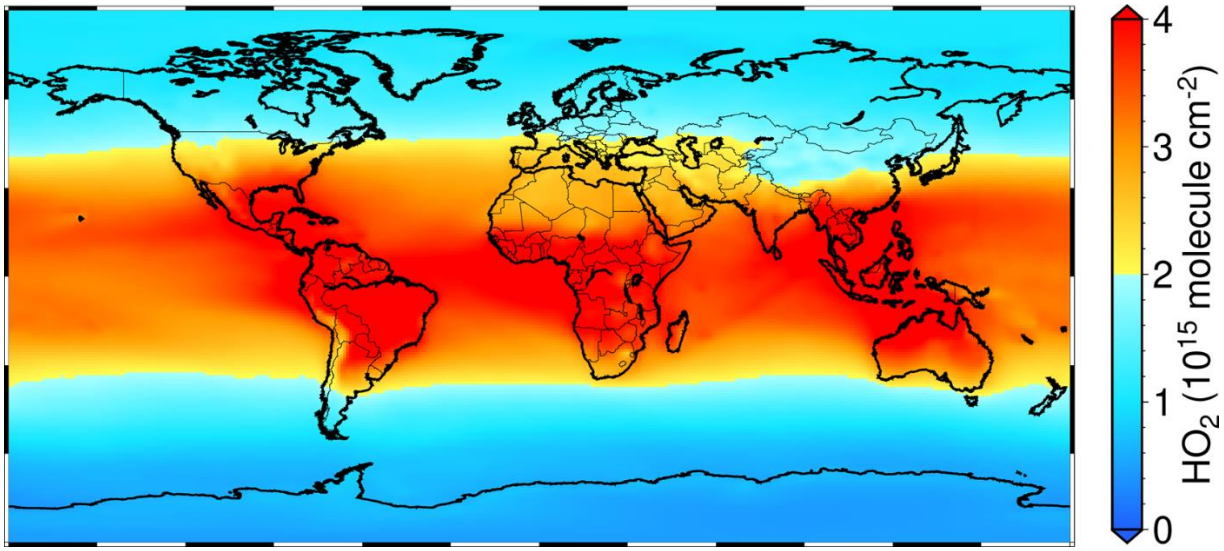

Figure S17: Calculated results of annual-mean column concentration of HO_2.