Multi and single-reference methods for the analysis of multi-state peroxidation of enolates

P. Ortega[1], S. Gil-Guerrero[1], A. Veselinova[1], A. Zanchet[2], L. González-Sánchez[1], P. G. Jambrina[1], and C. Sanz-Sanz[3]

1) Departamento de Química-Física. Universidad de Salamanca, Salamanca, 37008 (Spain)
2) Instituto de Física Fundamental (CSIC), Madrid, 28006 (Spain)
3) Departamento de Química Física Aplicada. Universidad Autónoma de Madrid, Madrid, 28049 (Spain)

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Table S1. Optimized geometries along the MEP for the addition of O_2 to oxobutenide. Geometries are shown in Cartesian coordinates (in Å).

12

r(C-O) = 1.20

C	-1.246591	0.831537	0.022189
C	-0.041892	-0.142320	0.172417
C	1.283460	0.615870	0.014653
C	2.486220	0.029905	0.036243
O	-1.203040	2.052034	-0.054030
H	-0.085573	-0.317007	1.304975
H	2.583012	-1.056574	0.089941
O	-1.149786	-2.045793	0.169574
O	-0.119723	-1.161276	-0.456606
H	-2.210841	0.283558	-0.078511
H	1.200370	1.704712	-0.032439
H	3.406246	0.615632	-0.028482

12

r(C-O) = 1.25

C	-1.243535	0.824945	0.023362
C	-0.041397	-0.133806	0.170676
C	1.282774	0.616800	0.014638
C	2.483354	0.027053	0.036825
O	-1.209046	2.046271	-0.052406
H	-0.078265	-0.400461	1.271192
H	2.577294	-1.059209	0.097529
O	-1.122225	-2.073724	0.103255
O	-0.146822	-1.153120	-0.545134
H	-2.195626	0.264895	-0.112948
H	1.205462	1.705892	-0.043269
H	3.404808	0.609538	-0.036237

12

r(C-O) = 1.30

C	-1.241531	0.818423	0.024545
C	-0.040164	-0.125180	0.168883
C	1.282354	0.617957	0.014612
C	2.480539	0.023792	0.037462
O	-1.212265	2.040764	-0.050354
H	-0.076657	-0.469428	1.238203
H	2.571409	-1.062059	0.107916
O	-1.124231	-2.083702	0.011996
O	-0.167754	-1.145468	-0.626562
H	-2.185695	0.250425	-0.124108
H	1.210381	1.706700	-0.058101
H	3.403602	0.602344	-0.045700

12

r(C-O) = 1.35

C	-1.240374	0.812234	0.025680
C	-0.038378	-0.116900	0.167137
C	1.282164	0.619336	0.014567
C	2.477784	0.020321	0.038117
O	-1.215972	2.035620	-0.048257
H	-0.075693	-0.532506	1.203380
H	2.564957	-1.064966	0.120076
O	-1.136574	-2.085973	-0.087480
O	-0.188157	-1.135588	-0.705984
H	-2.178558	0.237264	-0.126364
H	1.214767	1.707229	-0.074847
H	3.402827	0.594002	-0.055921

12

r(C-O) = 1.40

C	-1.239768	0.806490	0.026740
C	-0.036167	-0.109107	0.165475
C	1.281987	0.620783	0.014525
C	2.475145	0.016826	0.038762
O	-1.220169	2.030962	-0.046224
H	-0.075052	-0.592405	1.165624
H	2.558582	-1.067632	0.134140
O	-1.153513	-2.082996	-0.193016
O	-0.209201	-1.122377	-0.784968
H	-2.173339	0.225349	-0.124015
H	1.218727	1.707227	-0.094137
H	3.402196	0.585105	-0.067226

12

r(C-O) = 1.45

C	-1.239450	0.800822	0.027791
C	-0.033770	-0.101202	0.163796
C	1.281690	0.622035	0.014520
C	2.472728	0.013337	0.039395
O	-1.224832	2.026458	-0.044179
H	-0.074307	-0.648089	1.125549
H	2.552901	-1.070034	0.148679
O	-1.171754	-2.076160	-0.301393
O	-0.231235	-1.106411	-0.862392
H	-2.169542	0.214289	-0.118137
H	1.222211	1.706581	-0.113553
H	3.401517	0.576401	-0.078132

12

r(C-O) = 1.50

C	-1.239270	0.795390	0.028798
C	-0.031181	-0.093488	0.162156
C	1.281165	0.623184	0.014541
C	2.470483	0.009906	0.040007
O	-1.230578	2.022238	-0.042246
H	-0.073016	-0.701442	1.081905
H	2.547522	-1.072136	0.163658
O	-1.188897	-2.066169	-0.412894
O	-0.254658	-1.087147	-0.939071
H	-2.166566	0.203812	-0.111023
H	1.225060	1.705274	-0.133950
H	3.400898	0.567644	-0.088957

12

r(C-O) = 1.55

C	-1.239192	0.790222	0.029766
C	-0.028823	-0.085707	0.160537
C	1.280325	0.623563	0.014660
C	2.468886	0.006914	0.040539
O	-1.236891	2.018346	-0.040446
H	-0.071788	-0.751969	1.034791
H	2.544580	-1.073615	0.177604
O	-1.203482	-2.053323	-0.529194
O	-0.278920	-1.064270	-1.015203
H	-2.164817	0.194761	-0.101833
H	1.227231	1.702958	-0.153379
H	3.400064	0.560644	-0.099073

12

r(C-O) = 1.60

C	-1.239158	0.784980	0.030746
C	-0.026278	-0.077678	0.158872
C	1.279169	0.623861	0.014810
C	2.467464	0.003829	0.041075
O	-1.244893	2.014394	-0.038685
H	-0.070180	-0.798230	0.985123
H	2.541464	-1.075262	0.189928
O	-1.214885	-2.038363	-0.644019
O	-0.303200	-1.040712	-1.088477
H	-2.163643	0.185800	-0.091204
H	1.228969	1.700511	-0.170493
H	3.399501	0.553686	-0.107018

12

r(C-O) = 1.65

C	-1.239125	0.780009	0.031691
C	-0.024374	-0.069438	0.157223
C	1.277695	0.622937	0.015100
C	2.467000	0.001484	0.041488
O	-1.253478	2.010632	-0.037101
H	-0.070034	-0.841155	0.932217
H	2.542188	-1.076110	0.200348
O	-1.220909	-2.021518	-0.764813
O	-0.326496	-1.013068	-1.162165
H	-2.163477	0.178157	-0.078289
H	1.230201	1.697149	-0.184802
H	3.398573	0.549837	-0.114096

12

r(C-O) = 1.70

C	-1.238904	0.774930	0.032649
C	-0.022614	-0.061180	0.155572
C	1.276078	0.622234	0.015372
C	2.466637	-0.000993	0.041909
O	-1.262928	2.006850	-0.035541
H	-0.069336	-0.879924	0.877607
H	2.541582	-1.077548	0.207879
O	-1.226026	-2.003798	-0.877524
O	-0.350139	-0.987194	-1.231952
H	-2.163010	0.170455	-0.066116
H	1.231472	1.694524	-0.195305
H	3.398323	0.545654	-0.117920

12

r(C-O) = 1.75

C	-1.239022	0.770350	0.033535
C	-0.021376	-0.053197	0.154016
C	1.274504	0.620695	0.015724
C	2.467092	-0.002855	0.042227
O	-1.273311	2.003381	-0.034203
H	-0.069807	-0.915409	0.820712
H	2.544018	-1.078652	0.212456
O	-1.225358	-1.984590	-0.995140
O	-0.371217	-0.956815	-1.303239
H	-2.163287	0.163579	-0.053687
H	1.232250	1.691892	-0.201298
H	3.398049	0.544150	-0.119884

12

r(C-O) = 1.80

C	-1.239236	0.765779	0.034415
C	-0.020229	-0.045491	0.152503
C	1.273235	0.619607	0.016015
C	2.467427	-0.004903	0.042568
O	-1.283605	1.999694	-0.032815
H	-0.070119	-0.945185	0.764826
H	2.544752	-1.080433	0.214640
O	-1.224520	-1.965321	-1.104952
O	-0.390528	-0.929300	-1.371230
H	-2.163408	0.156431	-0.041090
H	1.233843	1.690524	-0.203168
H	3.398285	0.541912	-0.119856

12

r(C-O) = 1.85

C	-1.239367	0.761593	0.035224
C	-0.019481	-0.038367	0.151121
C	1.272053	0.618393	0.016303
C	2.467993	-0.006627	0.042854
O	-1.293375	1.996309	-0.031573
H	-0.071421	-0.970268	0.711205
H	2.546077	-1.082174	0.214667
O	-1.223752	-1.947397	-1.209062
O	-0.408616	-0.904229	-1.436759
H	-2.163364	0.149785	-0.029077
H	1.235249	1.689590	-0.202283
H	3.398600	0.540754	-0.118403

12

r(C-O) = 1.90

C	-1.239221	0.757957	0.035918
C	-0.018868	-0.032248	0.149935
C	1.270887	0.617376	0.016552
C	2.468400	-0.008093	0.043096
O	-1.302045	1.993355	-0.030532
H	-0.072327	-0.990343	0.662139
H	2.546973	-1.083915	0.213217
O	-1.223927	-1.931513	-1.305474
O	-0.425853	-0.883685	-1.499132
H	-2.163021	0.143972	-0.019255
H	1.236420	1.689274	-0.199314
H	3.398885	0.539949	-0.115983

12

r(C-O) = 1.95

C	-1.239617	0.754620	0.036569
C	-0.018404	-0.026638	0.148845
C	1.270230	0.616590	0.016754
C	2.468987	-0.009580	0.043334
O	-1.311046	1.990581	-0.029540
H	-0.073549	-1.007984	0.613468
H	2.547573	-1.085922	0.210459
O	-1.226800	-1.916757	-1.396940
O	-0.442157	-0.864957	-1.560000
H	-2.162745	0.137951	-0.010342
H	1.238158	1.689600	-0.194274
H	3.399620	0.538949	-0.112619

12

r(C-O) = 2.00

C	-1.239620	0.751832	0.037104
C	-0.018098	-0.022014	0.147951
C	1.269495	0.615927	0.016925
C	2.469419	-0.010753	0.043521
O	-1.318317	1.988314	-0.028744
H	-0.074822	-1.021518	0.571144
H	2.548003	-1.087684	0.207069
O	-1.233829	-1.906767	-1.477197
O	-0.458298	-0.855077	-1.616200
H	-2.162229	0.133014	-0.002981
H	1.239465	1.690138	-0.188580
H	3.400188	0.538415	-0.108904

12

r(C-O) = 2.05

C	-1.239279	0.749669	0.037513
C	-0.017998	-0.018376	0.147260
C	1.268649	0.615193	0.017087
C	2.469825	-0.011494	0.043642
O	-1.323865	1.986658	-0.028183
H	-0.076223	-1.032078	0.534539
H	2.548835	-1.089001	0.203373
O	-1.245028	-1.901214	-1.548164
O	-0.474005	-0.853024	-1.668758
H	-2.161700	0.129393	0.002663
H	1.240072	1.690590	-0.182835
H	3.400486	0.538681	-0.105367

12

r(C-O) = 2.10

C	-1.239224	0.747670	0.037895
C	-0.017905	-0.015079	0.146628
C	1.268093	0.614716	0.017210
C	2.470234	-0.012314	0.043769
O	-1.329448	1.985095	-0.027643
H	-0.077583	-1.040835	0.500565
H	2.549212	-1.090455	0.199416
O	-1.258272	-1.899076	-1.613833
O	-0.490419	-0.854390	-1.719462
H	-2.161166	0.125619	0.007798
H	1.241059	1.691357	-0.176497
H	3.401025	0.538557	-0.101503

12

r(C-O) = 2.15

C	-1.239120	0.746016	0.038210
C	-0.017831	-0.012363	0.146107
C	1.267570	0.614335	0.017312
C	2.470578	-0.012996	0.043874
O	-1.334083	1.983867	-0.027204
H	-0.078798	-1.047877	0.470345
H	2.549549	-1.091678	0.195939
O	-1.274562	-1.900552	-1.673059
O	-0.508910	-0.859740	-1.767865
H	-2.160691	0.122530	0.012324
H	1.241921	1.692037	-0.170980
H	3.401480	0.538484	-0.098086

12

r(C-O) = 2.20

C	-1.238950	0.744703	0.038458
C	-0.017834	-0.010176	0.145693
C	1.267052	0.613950	0.017404
C	2.470929	-0.013486	0.043947
O	-1.337790	1.982978	-0.026875
H	-0.080076	-1.053524	0.443995
H	2.550032	-1.092672	0.192511
O	-1.296210	-1.907006	-1.722726
O	-0.529714	-0.872061	-1.812657
H	-2.160281	0.120131	0.016132
H	1.242475	1.692652	-0.165654
H	3.401850	0.538696	-0.094870

12

r(C-O) = 2.25

C	-1.238802	0.743602	0.038667
C	-0.017849	-0.008332	0.145345
C	1.266583	0.613620	0.017483
C	2.471266	-0.013898	0.044007
O	-1.340951	1.982282	-0.026605
H	-0.081221	-1.058069	0.420784
H	2.550496	-1.093537	0.189350
O	-1.322331	-1.917571	-1.764390
O	-0.553757	-0.889153	-1.854520
H	-2.159922	0.118119	0.019541
H	1.242948	1.693232	-0.160690
H	3.402193	0.538948	-0.091860

12

r(C-O) = 2.30

C	-1.238698	0.742655	0.038847
C	-0.017868	-0.006748	0.145045
C	1.266177	0.613354	0.017549
C	2.471586	-0.014269	0.044060
O	-1.343723	1.981723	-0.026371
H	-0.082270	-1.061755	0.400250
H	2.550894	-1.094320	0.186424
O	-1.351542	-1.932250	-1.799550
O	-0.580287	-0.910552	-1.893783
H	-2.159609	0.116374	0.022647
H	1.243410	1.693788	-0.156075
H	3.402537	0.539163	-0.089042

12

r(C-O) = 2.35

C	-1.238587	0.741869	0.038997
C	-0.017912	-0.005422	0.144797
C	1.265804	0.613111	0.017608
C	2.471892	-0.014566	0.044101
O	-1.346066	1.981316	-0.026184
H	-0.083291	-1.064760	0.382187
H	2.551299	-1.094979	0.183783
O	-1.383084	-1.951767	-1.828089
O	-0.608597	-0.937101	-1.930189
H	-2.159328	0.114923	0.025355
H	1.243761	1.694272	-0.151928
H	3.402836	0.539417	-0.086558

12

r(C-O) = 2.40

C	-1.238515	0.741180	0.039128
C	-0.017950	-0.004266	0.144579
C	1.265483	0.612922	0.017656
C	2.472179	-0.014843	0.044139
O	-1.348137	1.980989	-0.026019
H	-0.084226	-1.067246	0.366085
H	2.551645	-1.095578	0.181406
O	-1.417372	-1.975470	-1.850074
O	-0.639823	-0.967731	-1.963740
H	-2.159062	0.113619	0.027805
H	1.244134	1.694731	-0.148138
H	3.403135	0.539608	-0.084277

12

r(C-O) = 2.45

C	-1.238425	0.740751	0.039213
C	-0.018104	-0.003455	0.144435
C	1.265161	0.612623	0.017707
C	2.472565	-0.014927	0.044147
O	-1.349453	1.980929	-0.025937
H	-0.085149	-1.069122	0.352636
H	2.552392	-1.095958	0.178882
O	-1.455656	-2.002783	-1.864750
O	-0.674575	-1.002678	-1.994045
H	-2.159069	0.113064	0.029836
H	1.244180	1.695103	-0.144092
H	3.403380	0.540246	-0.082025

12

r(C-O) = 2.50

C	-1.238357	0.740198	0.039318
C	-0.018090	-0.002543	0.144262
C	1.264871	0.612519	0.017742
C	2.472773	-0.015182	0.044181
O	-1.351045	1.980731	-0.025798
H	-0.086052	-1.071037	0.339498
H	2.552588	-1.096425	0.177375
O	-1.498147	-2.034046	-1.871193
O	-0.713186	-1.042395	-2.020351
H	-2.158739	0.111971	0.032011
H	1.244506	1.695421	-0.141603
H	3.403604	0.540289	-0.080385

12

r(C-O) = 2.55

C	-1.238321	0.739814	0.039393
C	-0.018148	-0.001863	0.144136
C	1.264621	0.612372	0.017775
C	2.473045	-0.015331	0.044198
O	-1.352129	1.980686	-0.025707
H	-0.086740	-1.072451	0.328646
H	2.553016	-1.096766	0.175846
O	-1.542237	-2.070729	-1.868462
O	-0.755277	-1.087158	-2.042477
H	-2.158631	0.111374	0.033823
H	1.244740	1.695718	-0.138937
H	3.403828	0.540529	-0.078858

12

r(C-O) = 2.60

C	-1.238242	0.739520	0.039450
C	-0.018224	-0.001314	0.144038
C	1.264351	0.612199	0.017809
C	2.473311	-0.015413	0.044205
O	-1.352926	1.980748	-0.025646
H	-0.087760	-1.073742	0.318782
H	2.553482	-1.096990	0.174595
O	-1.588120	-2.110148	-1.860166
O	-0.800025	-1.134830	-2.061394
H	-2.158530	0.110991	0.035638
H	1.244706	1.695899	-0.136723
H	3.403991	0.540883	-0.077529

12

r(C-O) = 2.65

C	-1.238129	0.739212	0.039508
C	-0.018268	-0.000775	0.143939
C	1.264081	0.612070	0.017838
C	2.473513	-0.015516	0.044217
O	-1.353609	1.980761	-0.025576
H	-0.088430	-1.074698	0.310230
H	2.553870	-1.097219	0.173537
O	-1.637123	-2.153428	-1.843312
O	-0.847503	-1.188067	-2.075341
H	-2.158326	0.110551	0.037084
H	1.244812	1.696110	-0.134663
H	3.404122	0.541121	-0.076408

12

r(C-O) = 2.70

C	-1.238031	0.739005	0.039548
C	-0.018344	-0.000376	0.143869
C	1.263831	0.611921	0.017865
C	2.473741	-0.015558	0.044220
O	-1.354076	1.980885	-0.025539
H	-0.089242	-1.075585	0.302641
H	2.554307	-1.097360	0.172624
O	-1.687073	-2.200953	-1.816772
O	-0.897540	-1.246452	-2.084204
H	-2.158221	0.110351	0.038398
H	1.244746	1.696256	-0.132853
H	3.404232	0.541462	-0.075410

12

r(C-O) = 2.75

C	-1.237989	0.738750	0.039598
C	-0.018375	0.000059	0.143788
C	1.263632	0.611863	0.017883
C	2.473928	-0.015679	0.044233
O	-1.354641	1.980922	-0.025470
H	-0.089856	-1.076293	0.295808
H	2.554593	-1.097564	0.171952
O	-1.737551	-2.251285	-1.784461
O	-0.950030	-1.307750	-2.088734
H	-2.158065	0.109981	0.039612
H	1.244973	1.696464	-0.131208
H	3.404406	0.541519	-0.074610

12

r(C-O) = 2.80

C	-1.237828	0.738658	0.039615
C	-0.018481	0.000283	0.143754
C	1.263366	0.611686	0.017910
C	2.474140	-0.015635	0.044223
O	-1.354714	1.981174	-0.025477
H	-0.090790	-1.076988	0.289979
H	2.555054	-1.097573	0.171301
O	-1.790295	-2.304926	-1.741627
O	-1.003924	-1.376003	-2.086658
H	-2.157997	0.110085	0.040639
H	1.244628	1.696512	-0.129832
H	3.404429	0.542018	-0.073835

12

r(C-O) = 2.85

C	-1.237843	0.738400	0.039665
C	-0.018461	0.000700	0.143672
C	1.263218	0.611693	0.017921
C	2.474283	-0.015801	0.044243
O	-1.355411	1.981151	-0.025396
H	-0.091172	-1.077475	0.284347
H	2.555218	-1.097803	0.170869
O	-1.842815	-2.361475	-1.689909
O	-1.059184	-1.448841	-2.078541
H	-2.157781	0.109534	0.041339
H	1.245046	1.696737	-0.128486
H	3.404626	0.541881	-0.073243

12

r(C-O) = 2.90

C	-1.237688	0.738325	0.039678
C	-0.018542	0.000876	0.143646
C	1.262978	0.611560	0.017942
C	2.474450	-0.015768	0.044236
O	-1.355462	1.981394	-0.025405
H	-0.092004	-1.077997	0.279630
H	2.555555	-1.097802	0.170429
O	-1.895151	-2.421594	-1.627313
O	-1.115969	-1.527751	-2.062926
H	-2.157676	0.109595	0.042051
H	1.244756	1.696793	-0.127334
H	3.404638	0.542266	-0.072688

12

r(C-O) = 2.95

C	-1.237635	0.738163	0.039709
C	-0.018553	0.001154	0.143594
C	1.262801	0.611526	0.017955
C	2.474583	-0.015851	0.044244
O	-1.355857	1.981464	-0.025366
H	-0.092579	-1.078345	0.275399
H	2.555772	-1.097921	0.170109
O	-1.945151	-2.485416	-1.553265
O	-1.173495	-1.612361	-2.039335
H	-2.157467	0.109258	0.042604
H	1.244928	1.696938	-0.126255
H	3.404743	0.542324	-0.072199

12

r(C-O) = 3.00

C	-1.237507	0.738050	0.039728
C	-0.018579	0.001341	0.143560
C	1.262607	0.611488	0.017966
C	2.474676	-0.015887	0.044247
O	-1.356073	1.981622	-0.025355
H	-0.093258	-1.078720	0.271566
H	2.555862	-1.097982	0.169872
O	-1.992160	-2.551611	-1.468971
O	-1.230681	-1.702044	-2.008018
H	-2.157261	0.109075	0.043056
H	1.244870	1.697069	-0.125205
H	3.404786	0.542425	-0.071860

Table S2. Optimized geometries along the MEP for the addition of O_2 to S-methyl-butenthioate. Geometries are shown in Cartesian coordinates (in Å).

16

r(C-O) = 1.20

C	3.102210	-0.718728	-0.039245
S	1.764298	0.566184	0.114431
C	0.361844	-0.564162	0.036959
C	-1.055231	0.150300	0.190041
C	-2.153248	-0.911637	0.028982
C	-3.458863	-0.631863	0.104508
O	0.519608	-1.757512	-0.172884
H	-1.813038	-1.942239	-0.086729
H	4.054478	-0.172391	0.004937
H	-4.213463	-1.417883	0.026250
H	3.026148	-1.254069	-0.993881
H	3.054176	-1.446606	0.780989
H	-1.044941	0.363951	1.309458
H	-3.813790	0.394363	0.220533
O	-1.235757	1.131464	-0.476839
O	-0.316177	2.185106	0.022231

16

r(C-O) = 1.25

C	3.091765	-0.712986	-0.034752
S	1.751536	0.573724	0.111945
C	0.358304	-0.562123	0.031833
C	-1.047546	0.134572	0.187635
C	-2.151420	-0.912781	0.027562
C	-3.454391	-0.622773	0.108966
O	0.517555	-1.755100	-0.183126
H	-1.821863	-1.944926	-0.105422
H	4.042597	-0.165135	0.022002
H	-4.215315	-1.401620	0.021422
H	3.026439	-1.243110	-0.993094
H	3.036517	-1.445387	0.781100
H	-1.047544	0.398751	1.287659
H	-3.800312	0.404730	0.238722
O	-1.223882	1.142580	-0.530226
O	-0.296468	2.180506	-0.022837

16

r(C-O) = 1.30

C	3.083799	-0.708067	-0.030098
S	1.741674	0.580355	0.109028
C	0.355669	-0.560293	0.026104
C	-1.041970	0.120832	0.185630
C	-2.150201	-0.914086	0.025943
C	-3.450585	-0.614476	0.113666
O	0.516355	-1.752795	-0.194667
H	-1.830115	-1.946605	-0.126626
H	4.033272	-0.159227	0.038851
H	-4.217847	-1.385805	0.015657
H	3.028667	-1.233318	-0.991732
H	3.020396	-1.444304	0.781724
H	-1.051979	0.435736	1.264550
H	-3.787874	0.413711	0.258886
O	-1.211316	1.153576	-0.585576
O	-0.279941	2.180341	-0.072202

16

r(C-O) = 1.35

C	3.077095	-0.703942	-0.025596
S	1.734204	0.586234	0.106118
C	0.353650	-0.558644	0.020347
C	-1.037950	0.108863	0.183937
C	-2.149005	-0.915114	0.024318
C	-3.447078	-0.607253	0.118239
O	0.516109	-1.750394	-0.206360
H	-1.836893	-1.946853	-0.149166
H	4.025833	-0.155308	0.054456
H	-4.220231	-1.371089	0.008879
H	3.030957	-1.224910	-0.990014
H	3.006083	-1.443742	0.782431
H	-1.057018	0.474432	1.239895
H	-3.776419	0.420970	0.279989
O	-1.198053	1.163799	-0.643093
O	-0.266064	2.183106	-0.126062

16

r(C-O) = 1.40

C	3.071612	-0.700145	-0.021094
S	1.729145	0.590897	0.103023
C	0.351897	-0.557315	0.014425
C	-1.034791	0.097837	0.182412
C	-2.147988	-0.915834	0.022673
C	-3.444018	-0.600633	0.122829
O	0.516585	-1.748223	-0.218488
H	-1.843476	-1.946145	-0.171909
H	4.019681	-0.151790	0.068774
H	-4.222274	-1.357484	0.002232
H	3.034042	-1.217863	-0.987624
H	2.994040	-1.442936	0.783669
H	-1.062931	0.513077	1.214053
H	-3.766321	0.426986	0.301362
O	-1.183557	1.173089	-0.701727
O	-0.254161	2.188353	-0.185566

16

r(C-O) = 1.45

C	3.066838	-0.696769	-0.016684
S	1.724529	0.595042	0.100008
C	0.350042	-0.556005	0.008542
C	-1.032315	0.087756	0.181041
C	-2.146864	-0.916615	0.020970
C	-3.440989	-0.594458	0.127376
O	0.516618	-1.746185	-0.230702
H	-1.849209	-1.944612	-0.195517
H	4.014078	-0.148877	0.083631
H	-4.224505	-1.343891	-0.004391
H	3.037249	-1.210438	-0.985568
H	2.981196	-1.442461	0.784515
H	-1.069464	0.551939	1.186599
H	-3.756264	0.432147	0.323274
O	-1.168511	1.181609	-0.760998
O	-0.244478	2.196180	-0.250095

16

r(C-O) = 1.50

C	3.062591	-0.693579	-0.013028
S	1.722232	0.597461	0.097523
C	0.347925	-0.555391	0.003741
C	-1.030270	0.078705	0.179761
C	-2.145324	-0.916711	0.019624
C	-3.438210	-0.589115	0.131146
O	0.517702	-1.744883	-0.240831
H	-1.853822	-1.941908	-0.217609
H	4.009584	-0.146958	0.095680
H	-4.225602	-1.332419	-0.011227
H	3.039510	-1.204114	-0.983684
H	2.970446	-1.441852	0.785004
H	-1.076933	0.592963	1.156045
H	-3.748163	0.435799	0.343515
O	-1.152480	1.186470	-0.824191
O	-0.239631	2.206036	-0.329585

16

r(C-O) = 1.55

C	3.059771	-0.689893	-0.009797
S	1.720442	0.598202	0.095375
C	0.345062	-0.555891	-0.000419
C	-1.028603	0.069695	0.178433
C	-2.143769	-0.916479	0.018489
C	-3.435749	-0.583522	0.134540
O	0.518427	-1.744875	-0.249677
H	-1.858248	-1.938167	-0.240003
H	4.005933	-0.143946	0.108090
H	-4.227152	-1.320169	-0.019111
H	3.043133	-1.196108	-0.982670
H	2.960653	-1.441221	0.784325
H	-1.085010	0.635744	1.121340
H	-3.740432	0.439500	0.362930
O	-1.137660	1.186304	-0.891049
O	-0.240065	2.215945	-0.424274

16

r(C-O) = 1.60

C	3.057640	-0.684684	-0.008825
S	1.719268	0.595786	0.095441
C	0.340787	-0.559358	-0.000922
C	-1.026526	0.060869	0.176856
C	-2.141695	-0.915542	0.018450
C	-3.433493	-0.577376	0.135686
O	0.519848	-1.748523	-0.250962
H	-1.861974	-1.934352	-0.256804
H	4.003156	-0.139300	0.115562
H	-4.228045	-1.308401	-0.027695
H	3.045153	-1.186451	-0.983914
H	2.955047	-1.439878	0.780969
H	-1.092782	0.681752	1.080492
H	-3.734131	0.444048	0.376086
O	-1.125840	1.176757	-0.965478
O	-0.251586	2.224421	-0.549855

16

r(C-O) = 1.65

C	3.057894	-0.675355	-0.010909
S	1.716194	0.590294	0.099230
C	0.335338	-0.568134	0.003809
C	-1.023263	0.049233	0.174391
C	-2.140755	-0.913863	0.020033
C	-3.432502	-0.567971	0.133922
O	0.523549	-1.758479	-0.241127
H	-1.868395	-1.932051	-0.264430
H	4.001419	-0.127357	0.115036
H	-4.230723	-1.293160	-0.036671
H	3.045308	-1.172481	-0.988170
H	2.957293	-1.434197	0.775196
H	-1.098819	0.730496	1.029535
H	-3.728283	0.453596	0.379518
O	-1.122219	1.149174	-1.051511
O	-0.277745	2.222119	-0.718891

16

r(C-O) = 1.70

C	3.060393	-0.660967	-0.017019
S	1.709981	0.582966	0.107698
C	0.329561	-0.583086	0.015429
C	-1.018642	0.034084	0.170823
C	-2.141754	-0.912004	0.023682
C	-3.432846	-0.554116	0.128330
O	0.530006	-1.775617	-0.216154
H	-1.879209	-1.933172	-0.259282
H	4.000190	-0.106543	0.106858
H	-4.236125	-1.272754	-0.045475
H	3.045360	-1.152136	-0.997185
H	2.968886	-1.425153	0.764576
H	-1.100924	0.778435	0.967960
H	-3.721721	0.470480	0.369301
O	-1.126127	1.102464	-1.147135
O	-0.313249	2.197768	-0.919708

16

r(C-O) = 1.75

C	3.064521	-0.643793	-0.024918
S	1.701856	0.576764	0.117674
C	0.324910	-0.600784	0.030153
C	-1.013143	0.016027	0.166565
C	-2.144911	-0.909821	0.028456
C	-3.434664	-0.537719	0.120989
O	0.538639	-1.795500	-0.183570
H	-1.893957	-1.937067	-0.243298
H	3.999144	-0.081134	0.099329
H	-4.243440	-1.250469	-0.050771
H	3.048398	-1.125750	-1.009569
H	2.983137	-1.415668	0.749815
H	-1.099377	0.820674	0.899506
H	-3.715661	0.491772	0.349956
O	-1.129220	1.042352	-1.246122
O	-0.342408	2.147968	-1.124913

16

r(C-O) = 1.80

C	3.068844	-0.625885	-0.033822
S	1.693297	0.572641	0.127421
C	0.321602	-0.618775	0.046545
C	-1.007715	-0.003183	0.162067
C	-2.149205	-0.908089	0.033810
C	-3.436814	-0.520159	0.112645
O	0.548608	-1.815373	-0.146342
H	-1.910903	-1.942799	-0.221284
H	3.997941	-0.055741	0.096518
H	-4.252172	-1.226456	-0.053737
H	3.055453	-1.094640	-1.024917
H	2.994878	-1.408430	0.730580
H	-1.096201	0.856755	0.826449
H	-3.708213	0.515519	0.324668
O	-1.128089	0.975091	-1.344084
O	-0.359663	2.079017	-1.318313

16

r(C-O) = 1.85

C	3.072850	-0.608634	-0.042406
S	1.685197	0.569931	0.135166
C	0.319437	-0.635814	0.062277
C	-1.002567	-0.022081	0.157739
C	-2.153928	-0.906405	0.039165
C	-3.439080	-0.503156	0.104471
O	0.558679	-1.833734	-0.109491
H	-1.928693	-1.948856	-0.196572
H	3.996468	-0.033651	0.104029
H	-4.260754	-1.203621	-0.054564
H	3.068852	-1.058381	-1.042495
H	2.999863	-1.406070	0.706326
H	-1.091461	0.885913	0.752528
H	-3.701086	0.538615	0.297700
O	-1.119793	0.903833	-1.439584
O	-0.362064	1.997034	-1.495926

16

r(C-O) = 1.90

C	3.076722	-0.592582	-0.051026
S	1.677923	0.568373	0.141203
C	0.317817	-0.651513	0.077852
C	-0.998144	-0.039857	0.153698
C	-2.158636	-0.905089	0.044560
C	-3.441047	-0.487049	0.096161
O	0.567923	-1.850390	-0.072210
H	-1.945912	-1.955057	-0.169565
H	3.994639	-0.019255	0.132404
H	-4.269129	-1.181732	-0.053975
H	3.094286	-1.008627	-1.065640
H	2.990857	-1.414369	0.669209
H	-1.086565	0.909097	0.678989
H	-3.693306	0.560776	0.268701
O	-1.106687	0.831515	-1.531215
O	-0.354188	1.908350	-1.657822

16

r(C-O) = 1.95

C	3.099152	-0.560683	-0.056475
S	1.665158	0.554740	0.140613
C	0.309965	-0.688646	0.088400
C	-0.993797	-0.067332	0.148255
C	-2.172016	-0.902571	0.050090
C	-3.446592	-0.456857	0.090975
O	0.555419	-1.890475	-0.041103
H	-1.983688	-1.961686	-0.141288
H	3.816173	-0.393482	0.757279
H	-4.288429	-1.136988	-0.047915
H	3.585051	-0.382525	-1.024232
H	2.708466	-1.586853	-0.018843
H	-1.069223	0.918334	0.601817
H	-3.677621	0.599107	0.242526
O	-1.091606	0.736436	-1.625692
O	-0.335298	1.785325	-1.829416

16

r(C-O) = 2.00

C	3.100260	-0.550194	-0.060590
S	1.660957	0.556114	0.141270
C	0.309486	-0.697984	0.096155
C	-0.990734	-0.080396	0.145601
C	-2.174917	-0.901547	0.053232
C	-3.447383	-0.445969	0.086847
O	0.564431	-1.899201	-0.020779
H	-1.996273	-1.965280	-0.122484
H	3.819238	-0.380912	0.751022
H	-4.293807	-1.121793	-0.044241
H	3.581698	-0.369379	-1.029995
H	2.713780	-1.578141	-0.021579
H	-1.064390	0.929100	0.542741
H	-3.671236	0.613530	0.224209
O	-1.075856	0.680928	-1.701867
O	-0.318747	1.710425	-1.947619

16

r(C-O) = 2.10

C	3.102633	-0.534372	-0.067052
S	1.655382	0.559204	0.140868
C	0.308838	-0.712176	0.108129
C	-0.986474	-0.100168	0.141638
C	-2.179348	-0.899819	0.058270
C	-3.448937	-0.429556	0.080260
O	0.578991	-1.911815	0.011344
H	-2.016174	-1.970627	-0.089841
H	3.825350	-0.358936	0.739910
H	-4.302032	-1.099330	-0.036697
H	3.576873	-0.352999	-1.039909
H	2.722148	-1.564582	-0.022680
H	-1.055566	0.941184	0.446129
H	-3.662146	0.635087	0.193360
O	-1.044389	0.593383	-1.839683
O	-0.283048	1.587981	-2.144793

16

r(C-O) = 2.20

C	3.104704	-0.524527	-0.069492
S	1.652803	0.561889	0.138960
C	0.308136	-0.720809	0.112986
C	-0.983934	-0.112993	0.139264
C	-2.182006	-0.898500	0.060817
C	-3.450188	-0.419261	0.077670
O	0.588787	-1.918868	0.026062
H	-2.029002	-1.973530	-0.068687
H	3.826564	-0.349195	0.738297
H	-4.307604	-1.085091	-0.028727
H	3.579042	-0.340486	-1.041804
H	2.726543	-1.555922	-0.026729
H	-1.049315	0.946231	0.376180
H	-3.656584	0.648339	0.175325
O	-1.017066	0.543273	-1.960312
O	-0.250855	1.512094	-2.296910

16

r(C-O) = 2.30

C	3.106691	-0.518192	-0.069598
S	1.651878	0.564181	0.136875
C	0.307433	-0.726390	0.113725
C	-0.982343	-0.121409	0.137839
C	-2.183654	-0.897374	0.061829
C	-3.451414	-0.412726	0.077450
O	0.595736	-1.922959	0.030338
H	-2.037582	-1.975006	-0.055582
H	3.825251	-0.345856	0.741822
H	-4.311386	-1.076300	-0.021287
H	3.584804	-0.330079	-1.039266
H	2.729109	-1.550155	-0.032037
H	-1.044470	0.947873	0.327489
H	-3.653777	0.656509	0.165948
O	-0.989711	0.520626	-2.070722
O	-0.217697	1.471250	-2.419989

16

r(C-O) = 2.40

C	3.108522	-0.514516	-0.068357
S	1.652164	0.566033	0.135130
C	0.306721	-0.729626	0.112048
C	-0.981409	-0.126535	0.137075
C	-2.184508	-0.896357	0.061853
C	-3.452614	-0.409057	0.078626
O	0.600253	-1.925006	0.028126
H	-2.042692	-1.975519	-0.048356
H	3.822178	-0.348290	0.748682
H	-4.313793	-1.071745	-0.014736
H	3.592945	-0.320669	-1.033757
H	2.729774	-1.546472	-0.039600
H	-1.041120	0.948567	0.294309
H	-3.653223	0.660938	0.162503
O	-0.961157	0.520951	-2.173845
O	-0.182910	1.459724	-2.522381

16

r(C-O) = 2.50

C	3.110018	-0.512111	-0.067205
S	1.652799	0.567508	0.133874
C	0.306128	-0.731752	0.110397
C	-0.980762	-0.129962	0.136589
C	-2.184991	-0.895547	0.061723
C	-3.453681	-0.406718	0.079741
O	0.603475	-1.926278	0.025433
H	-2.046053	-1.975768	-0.043219
H	3.820311	-0.349926	0.753610
H	-4.315509	-1.069052	-0.009435
H	3.598882	-0.314763	-1.029659
H	2.730435	-1.543996	-0.044106
H	-1.038649	0.948824	0.270510
H	-3.653367	0.663740	0.160473
O	-0.925816	0.534770	-2.272791
O	-0.139022	1.465412	-2.608734

16

r(C-O) = 2.60

C	3.111146	-0.510522	-0.066097
S	1.653482	0.568663	0.132926
C	0.305616	-0.733192	0.108749
C	-0.980231	-0.132272	0.136281
C	-2.185199	-0.894802	0.061497
C	-3.454621	-0.405301	0.080815
O	0.605792	-1.927108	0.022406
H	-2.048177	-1.975784	-0.039478
H	3.818483	-0.352123	0.758023
H	-4.316654	-1.067737	-0.005083
H	3.603879	-0.310083	-1.025941
H	2.730540	-1.542211	-0.048168
H	-1.036613	0.948925	0.253489
H	-3.654175	0.665375	0.159551
O	-0.880642	0.557263	-2.368639
O	-0.082874	1.482000	-2.681898

16

r(C-O) = 2.70

C	3.112055	-0.509043	-0.065460
S	1.653951	0.569642	0.132201
C	0.305271	-0.734562	0.107842
C	-0.979761	-0.134282	0.135989
C	-2.185445	-0.894272	0.061449
C	-3.455410	-0.403932	0.081425
O	0.607830	-1.928043	0.020976
H	-2.050169	-1.975915	-0.035874
H	3.817601	-0.352753	0.760624
H	-4.317770	-1.066246	-0.001637
H	3.607091	-0.306706	-1.023728
H	2.731066	-1.540695	-0.050521
H	-1.034891	0.948687	0.239866
H	-3.654541	0.667008	0.158195
O	-0.823596	0.586467	-2.461344
O	-0.012135	1.506531	-2.740824

16

r(C-O) = 2.80

C	3.112207	-0.506768	-0.067638
S	1.653444	0.570412	0.132005
C	0.305217	-0.736815	0.111513
C	-0.978969	-0.136781	0.135391
C	-2.185863	-0.893956	0.062817
C	-3.455880	-0.401769	0.079162
O	0.610317	-1.930282	0.030290
H	-2.052875	-1.976696	-0.026313
H	3.821527	-0.345304	0.754202
H	-4.318944	-1.063614	0.000131
H	3.602142	-0.308339	-1.029356
H	2.732765	-1.538913	-0.045735
H	-1.032582	0.947985	0.223312
H	-3.653922	0.669867	0.149409
O	-0.736888	0.605336	-2.553597
O	0.094521	1.519078	-2.781024

16

r(C-O) = 2.90

C	3.111522	-0.502582	-0.072958
S	1.651293	0.571191	0.131854
C	0.305550	-0.740989	0.120372
C	-0.977572	-0.141012	0.134262
C	-2.186835	-0.893880	0.065912
C	-3.455952	-0.397626	0.073658
O	0.614350	-1.934580	0.052247
H	-2.057780	-1.978280	-0.009231
H	3.830111	-0.327831	0.738014
H	-4.320783	-1.057793	0.000466
H	3.588444	-0.314061	-1.043181
H	2.736464	-1.535830	-0.033505
H	-1.028732	0.945726	0.200780
H	-3.651127	0.675324	0.131692
O	-0.604307	0.593147	-2.646328
O	0.252417	1.496683	-2.798831

16

r(C-O) = 3.00

C	3.111522	-0.502582	-0.072958
S	1.651293	0.571191	0.131854
C	0.305550	-0.740989	0.120372
C	-0.977572	-0.141012	0.134262
C	-2.186835	-0.893880	0.065912
C	-3.455952	-0.397626	0.073658
O	0.614350	-1.934580	0.052247
H	-2.057780	-1.978280	-0.009231
H	3.830111	-0.327831	0.738014
H	-4.320783	-1.057793	0.000466
H	3.588444	-0.314061	-1.043181
H	2.736464	-1.535830	-0.033505
H	-1.028732	0.945726	0.200780
H	-3.651127	0.675324	0.131692
O	-0.624584	0.656459	-2.734642
O	0.232140	1.559995	-2.887144

16

r(C-O) = 3.50

C	3.111522	-0.502582	-0.072958
S	1.651293	0.571191	0.131854
C	0.305550	-0.740989	0.120372
C	-0.977572	-0.141012	0.134262
C	-2.186835	-0.893880	0.065912
C	-3.455952	-0.397626	0.073658
O	0.614350	-1.934580	0.052247
H	-2.057780	-1.978280	-0.009231
H	3.830111	-0.327831	0.738014
H	-4.320783	-1.057793	0.000466
H	3.588444	-0.314061	-1.043181
H	2.736464	-1.535830	-0.033505
H	-1.028732	0.945726	0.200780
H	-3.651127	0.675324	0.131692
O	-0.666477	0.856036	-3.204803
O	0.190247	1.759572	-3.357305

16

r(C-O) = 4.00

C	3.111522	-0.502582	-0.072958
S	1.651293	0.571191	0.131854
C	0.305550	-0.740989	0.120372
C	-0.977572	-0.141012	0.134262
C	-2.186835	-0.893880	0.065912
C	-3.455952	-0.397626	0.073658
O	0.614350	-1.934580	0.052247
H	-2.057780	-1.978280	-0.009231
H	3.830111	-0.327831	0.738014
H	-4.320783	-1.057793	0.000466
H	3.588444	-0.314061	-1.043181
H	2.736464	-1.535830	-0.033505
H	-1.028732	0.945726	0.200780
H	-3.651127	0.675324	0.131692
O	-0.741239	1.119709	-3.656931
O	0.115485	2.023245	-3.809433

16

r(C-O) = 5.00

C	3.111522	-0.502582	-0.072958
S	1.651293	0.571191	0.131854
C	0.305550	-0.740989	0.120372
C	-0.977572	-0.141012	0.134262
C	-2.186835	-0.893880	0.065912
C	-3.455952	-0.397626	0.073658
O	0.614350	-1.934580	0.052247
H	-2.057780	-1.978280	-0.009231
H	3.830111	-0.327831	0.738014
H	-4.320783	-1.057793	0.000466
H	3.588444	-0.314061	-1.043181
H	2.736464	-1.535830	-0.033505
H	-1.028732	0.945726	0.200780
H	-3.651127	0.675324	0.131692
O	-0.871231	1.603992	-4.551090
O	-0.014508	2.507528	-4.703592

Table S3. Optimized geometries along the MEP for the addition of O_2 to DPA. Geometries are shown in Cartesian coordinates (in Å).

24

r(C-O) = 1.30

C	-2.568133	1.438905	0.047772
C	-1.201166	1.144399	0.032045
C	-0.777108	-0.189080	-0.051412
C	-1.739269	-1.211356	-0.123124
C	-3.095151	-0.894260	-0.107475
C	-3.532589	0.434174	-0.022192
C	0.685832	-0.665261	-0.138548
O	0.902187	-1.622863	0.713620
O	2.014857	-2.415282	0.154033
O	-4.000670	-1.938264	-0.182197
O	-3.021343	2.743480	0.136958
C	1.796596	0.429423	-0.073955
O	1.631921	1.629394	0.102535
S	3.457504	-0.265961	-0.186779
C	4.366421	1.353138	-0.068975
H	0.780413	-1.065611	-1.181479
H	-0.462525	1.940430	0.093068
H	-1.421671	-2.251093	-0.171641
H	-4.593021	0.691775	-0.007247
H	-4.892536	-1.572823	-0.157354
H	-2.248880	3.320026	0.184706
H	5.432521	1.101460	-0.151111
H	4.174980	1.842004	0.894183
H	4.082442	2.037015	-0.879071

24

r(C-O) = 1.35

C	-2.571291	1.437654	0.048091
C	-1.203444	1.147604	0.030122
C	-0.775651	-0.184567	-0.055060
C	-1.733963	-1.210465	-0.124788
C	-3.090914	-0.897798	-0.105944
C	-3.532141	0.429320	-0.020060
C	0.684324	-0.650746	-0.135393
O	0.913362	-1.615113	0.781142
O	2.018974	-2.414829	0.227862
O	-3.993048	-1.944644	-0.178315
O	-3.029085	2.740515	0.137318
C	1.794857	0.427254	-0.074565
O	1.632866	1.629313	0.096249
S	3.451556	-0.275871	-0.180588
C	4.363655	1.341825	-0.068267
H	0.790065	-1.107663	-1.147625
H	-0.466306	1.945201	0.090064
H	-1.412564	-2.249069	-0.172245
H	-4.593410	0.683398	-0.003430
H	-4.886130	-1.582649	-0.147489
H	-2.258811	3.319962	0.185304
H	5.428944	1.086999	-0.151296
H	4.174693	1.832512	0.894406
H	4.080277	2.025110	-0.879102

24

r(C-O) = 1.40

C	-2.574144	1.436448	0.048624
C	-1.205598	1.150520	0.027698
C	-0.774411	-0.180516	-0.059858
C	-1.729243	-1.209748	-0.126558
C	-3.087151	-0.901141	-0.104035
C	-3.531708	0.424754	-0.017485
C	0.682469	-0.637637	-0.131778
O	0.923924	-1.602125	0.853850
O	2.019821	-2.416268	0.314984
O	-3.986193	-1.950586	-0.173493
O	-3.036251	2.737623	0.138206
C	1.793125	0.426087	-0.075278
O	1.633659	1.630568	0.087830
S	3.446686	-0.283857	-0.171975
C	4.362096	1.331315	-0.067194
H	0.800395	-1.152670	-1.108873
H	-0.469656	1.949418	0.086162
H	-1.404425	-2.247350	-0.172669
H	-4.593734	0.675551	0.001268
H	-4.880336	-1.591729	-0.137027
H	-2.267998	3.319777	0.185890
H	5.426737	1.073399	-0.149166
H	4.174498	1.825976	0.893695
H	4.080523	2.012494	-0.880444

24

r(C-O) = 1.45

C	-2.576939	1.435195	0.049272
C	-1.207756	1.153354	0.024554
C	-0.773207	-0.176595	-0.065524
C	-1.724844	-1.209051	-0.128467
C	-3.083642	-0.904425	-0.101810
C	-3.531426	0.420282	-0.014240
C	0.680563	-0.625613	-0.127922
O	0.932994	-1.582166	0.932162
O	2.015122	-2.418972	0.419065
O	-3.979738	-1.956439	-0.167611
O	-3.043104	2.734797	0.139621
C	1.791065	0.425845	-0.076006
O	1.635147	1.632921	0.077783
S	3.442852	-0.290748	-0.161687
C	4.361619	1.321089	-0.065720
H	0.811723	-1.199897	-1.064617
H	-0.473064	1.953652	0.080843
H	-1.397235	-2.245864	-0.173032
H	-4.594140	0.667952	0.007512
H	-4.874849	-1.600615	-0.125740
H	-2.276816	3.319587	0.186567
H	5.425454	1.060026	-0.146902
H	4.175245	1.820134	0.893026
H	4.080847	1.998950	-0.881920

24

r(C-O) = 1.50

C	-2.579487	1.433782	0.050216
C	-1.209813	1.156037	0.020502
C	-0.771867	-0.172972	-0.072817
C	-1.720706	-1.208483	-0.130575
C	-3.080285	-0.907711	-0.099028
C	-3.531171	0.415812	-0.010217
C	0.678563	-0.613969	-0.123360
O	0.938909	-1.550129	1.019367
O	2.002160	-2.419209	0.549955
O	-3.973538	-1.962267	-0.160529
O	-3.049613	2.731847	0.141752
C	1.787962	0.427043	-0.076893
O	1.635980	1.637156	0.064688
S	3.439105	-0.295506	-0.148053
C	4.362237	1.310543	-0.063694
H	0.824352	-1.251489	-1.011134
H	-0.476444	1.957785	0.074015
H	-1.390792	-2.244658	-0.173261
H	-4.594484	0.660486	0.015471
H	-4.869454	-1.609362	-0.111647
H	-2.285143	3.318915	0.190069
H	5.425205	1.045916	-0.143226
H	4.177364	1.816337	0.891717
H	4.082638	1.983439	-0.884220

24

r(C-O) = 1.55

C	-2.582097	1.432049	0.051487
C	-1.212067	1.158602	0.015605
C	-0.770192	-0.169559	-0.081172
C	-1.716611	-1.208102	-0.132682
C	-3.076836	-0.911231	-0.096021
C	-3.531075	0.411044	-0.005600
C	0.676683	-0.601427	-0.118303
O	0.938785	-1.502002	1.115701
O	1.973238	-2.415179	0.715216
O	-3.967264	-1.968493	-0.152477
O	-3.056129	2.728587	0.144856
C	1.783028	0.430135	-0.077874
O	1.636417	1.643798	0.049342
S	3.434642	-0.298547	-0.132210
C	4.364600	1.298571	-0.061304
H	0.838287	-1.304213	-0.947764
H	-0.480131	1.961968	0.065636
H	-1.384850	-2.243819	-0.173009
H	-4.594995	0.652545	0.024542
H	-4.863795	-1.618551	-0.094736
H	-2.293393	3.317980	0.192053
H	5.426307	1.029459	-0.140725
H	4.182909	1.811790	0.890630
H	4.085315	1.965966	-0.886156

24

r(C-O) = 1.60

C	-2.584855	1.429711	0.052989
C	-1.214604	1.160973	0.010126
C	-0.768037	-0.166425	-0.090509
C	-1.712631	-1.207970	-0.134735
C	-3.073321	-0.915149	-0.092621
C	-3.531356	0.405797	-0.000649
C	0.674796	-0.587094	-0.112876
O	0.929638	-1.432297	1.221547
O	1.923628	-2.396243	0.919618
O	-3.960868	-1.975326	-0.143964
O	-3.062809	2.724756	0.148823
C	1.776103	0.435851	-0.079067
O	1.636849	1.653344	0.031811
S	3.429156	-0.299908	-0.114304
C	4.369339	1.284389	-0.058522
H	0.853961	-1.356956	-0.871793
H	-0.484589	1.966364	0.056297
H	-1.379656	-2.243412	-0.172618
H	-4.595821	0.644101	0.034223
H	-4.857818	-1.628248	-0.076479
H	-2.301641	3.316372	0.193509
H	5.429312	1.008999	-0.137457
H	4.192037	1.807110	0.888957
H	4.091326	1.945336	-0.888645

24

r(C-O) = 1.65

C	-2.587817	1.426946	0.054419
C	-1.217407	1.162899	0.004946
C	-0.765595	-0.163875	-0.098852
C	-1.709048	-1.208221	-0.136277
C	-3.069924	-0.919252	-0.089642
C	-3.532076	0.400399	0.003818
C	0.672974	-0.570899	-0.108081
O	0.912568	-1.349573	1.326755
O	1.859226	-2.356704	1.138337
O	-3.954854	-1.982322	-0.136057
O	-3.069332	2.720689	0.152376
C	1.768166	0.443280	-0.080285
O	1.637994	1.664275	0.015585
S	3.422591	-0.301212	-0.098208
C	4.376161	1.268804	-0.055909
H	0.870155	-1.401804	-0.790036
H	-0.489636	1.970602	0.047437
H	-1.375372	-2.243553	-0.171833
H	-4.597087	0.635395	0.043145
H	-4.851987	-1.637705	-0.059464
H	-2.309492	3.313940	0.197834
H	5.433816	0.985504	-0.135769
H	4.204866	1.799722	0.888013
H	4.099405	1.924714	-0.890098

24

r(C-O) = 1.70

C	-2.590903	1.424008	0.055346
C	-1.220416	1.164532	0.001134
C	-0.763128	-0.161789	-0.104654
C	-1.705849	-1.208663	-0.137199
C	-3.066831	-0.923290	-0.087403
C	-3.533190	0.395059	0.006964
C	0.671221	-0.553923	-0.104808
O	0.892636	-1.266493	1.422680
O	1.797297	-2.297035	1.342690
O	-3.949233	-1.989191	-0.130199
O	-3.075859	2.716562	0.154930
C	1.760683	0.451143	-0.081269
O	1.640517	1.674902	0.004002
S	3.415791	-0.303482	-0.086938
C	4.383847	1.253005	-0.053974
H	0.884638	-1.435163	-0.710779
H	-0.494920	1.974515	0.041028
H	-1.371756	-2.243928	-0.171497
H	-4.598704	0.626989	0.049286
H	-4.846527	-1.646751	-0.046383
H	-2.317227	3.311327	0.200817
H	5.438828	0.961375	-0.137434
H	4.220344	1.788899	0.888439
H	4.107365	1.906816	-0.889630

24

r(C-O) = 1.75

C	-2.594078	1.421197	0.055822
C	-1.223474	1.165974	-0.000970
C	-0.760836	-0.159967	-0.107750
C	-1.702988	-1.209149	-0.137510
C	-3.064053	-0.927064	-0.086124
C	-3.534530	0.390039	0.008528
C	0.669613	-0.537548	-0.102974
O	0.874355	-1.189362	1.508149
O	1.743596	-2.228702	1.521097
O	-3.944085	-1.995577	-0.126814
O	-3.082311	2.712633	0.156318
C	1.754264	0.458517	-0.081890
O	1.643883	1.684225	-0.002594
S	3.409653	-0.306630	-0.080867
C	4.391516	1.238084	-0.052996
H	0.896630	-1.457944	-0.638740
H	-0.500264	1.978183	0.037728
H	-1.368397	-2.244297	-0.171557
H	-4.600557	0.619102	0.052205
H	-4.841650	-1.654952	-0.038909
H	-2.324839	3.308898	0.201921
H	5.443839	0.938607	-0.141102
H	4.236115	1.776217	0.889492
H	4.115167	1.892408	-0.888111

24

r(C-O) = 1.80

C	-2.597230	1.418634	0.055941
C	-1.226465	1.167410	-0.001668
C	-0.758711	-0.158145	-0.108548
C	-1.700197	-1.209506	-0.137375
C	-3.061448	-0.930525	-0.085771
C	-3.535863	0.385338	0.008842
C	0.668272	-0.522599	-0.102277
O	0.857569	-1.123734	1.583785
O	1.708037	-2.154213	1.674837
O	-3.939162	-2.001490	-0.125838
O	-3.088712	2.708993	0.156757
C	1.748747	0.465303	-0.082091
O	1.647723	1.692402	-0.004727
S	3.403887	-0.310378	-0.079139
C	4.398326	1.224173	-0.052918
H	0.906272	-1.472707	-0.575499
H	-0.505399	1.981673	0.036796
H	-1.364892	-2.244436	-0.172101
H	-4.602414	0.611687	0.052746
H	-4.837122	-1.662572	-0.035601
H	-2.332413	3.306663	0.203463
H	5.448004	0.918000	-0.148587
H	4.252341	1.761205	0.891697
H	4.120281	1.881758	-0.884785

24

r(C-O) = 1.85

C	-2.615570	1.410517	0.055816
C	-1.242726	1.173379	-0.001484
C	-0.760058	-0.148019	-0.107606
C	-1.692714	-1.208420	-0.136672
C	-3.056322	-0.942825	-0.085923
C	-3.544482	0.368103	0.008258
C	0.666472	-0.490545	-0.102096
O	0.830194	-1.032483	1.659152
O	1.679849	-2.032160	1.840747
O	-3.923398	-2.022796	-0.126354
O	-3.119946	2.695970	0.156873
C	1.736114	0.495597	-0.081930
O	1.633224	1.722275	-0.003830
S	3.389698	-0.310485	-0.080849
C	4.444719	1.182294	-0.054228
H	0.921328	-1.464364	-0.512625
H	-0.530738	1.995585	0.037518
H	-1.348798	-2.240505	-0.172668
H	-4.613203	0.583809	0.051692
H	-4.824552	-1.692454	-0.036353
H	-2.369517	3.300918	0.204383
H	5.134576	1.166333	-0.907255
H	5.012717	1.224351	0.883621
H	3.773934	2.049443	-0.120109

24

r(C-O) = 1.90

C	-2.602803	1.414361	0.055613
C	-1.231721	1.170117	0.000800
C	-0.754867	-0.154695	-0.105522
C	-1.694646	-1.209756	-0.136039
C	-3.056728	-0.936320	-0.087417
C	-3.538070	0.377064	0.006169
C	0.666663	-0.498158	-0.102725
O	0.822279	-1.043832	1.710566
O	1.710521	-1.989341	1.926821
O	-3.929926	-2.011767	-0.129513
O	-3.100635	2.702618	0.156484
C	1.738710	0.477978	-0.081546
O	1.654227	1.706905	-0.000433
S	3.391642	-0.317777	-0.084429
C	4.408895	1.199491	-0.055197
H	0.921220	-1.485028	-0.480250
H	-0.514235	1.987700	0.041687
H	-1.357415	-2.244020	-0.173542
H	-4.605628	0.598683	0.048116
H	-4.829214	-1.675899	-0.041393
H	-2.346729	3.303122	0.205582
H	5.451859	0.883602	-0.185366
H	4.294774	1.721480	0.902244
H	4.113885	1.873895	-0.867330

24

r(C-O) = 1.95

C	-2.620368	1.406732	0.055115
C	-1.247307	1.176477	0.003833
C	-0.755779	-0.143830	-0.101964
C	-1.685710	-1.207911	-0.134804
C	-3.050792	-0.948084	-0.089082
C	-3.545625	0.359939	0.003304
C	0.666121	-0.468975	-0.103307
O	0.783118	-1.012895	1.765639
O	1.767919	-1.811286	2.074172
O	-3.912747	-2.032737	-0.133676
O	-3.131821	2.689816	0.155716
C	1.725655	0.508713	-0.080561
O	1.640113	1.737177	0.005385
S	3.373590	-0.318736	-0.090912
C	4.449237	1.157020	-0.058397
H	0.935418	-1.464421	-0.446392
H	-0.538795	2.001740	0.047663
H	-1.338802	-2.238845	-0.174594
H	-4.615386	0.570946	0.043207
H	-4.815708	-1.705811	-0.049589
H	-2.384225	3.297989	0.206699
H	5.117738	1.153067	-0.928377
H	5.039551	1.172303	0.866294
H	3.784485	2.031291	-0.089578

24

r(C-O) = 2.00

C	-2.623764	1.404761	0.054480
C	-1.250650	1.178807	0.006728
C	-0.753985	-0.140757	-0.098592
C	-1.681598	-1.207284	-0.134207
C	-3.047785	-0.951083	-0.090563
C	-3.546617	0.355014	0.000781
C	0.666092	-0.458335	-0.104227
O	0.762224	-1.023059	1.811978
O	1.824314	-1.664940	2.190480
O	-3.906339	-2.038593	-0.137561
O	-3.139912	2.686234	0.154239
C	1.721364	0.515684	-0.079504
O	1.644580	1.744504	0.011739
S	3.365489	-0.323275	-0.097307
C	4.452377	1.143275	-0.060761
H	0.941330	-1.459476	-0.424624
H	-0.544491	2.006073	0.053418
H	-1.332358	-2.237320	-0.176579
H	-4.617005	0.563108	0.038663
H	-4.810472	-1.714001	-0.057044
H	-2.394340	3.296689	0.207514
H	5.110905	1.145097	-0.938321
H	5.052780	1.144314	0.857466
H	3.791993	2.021533	-0.074850

24

r(C-O) = 2.10

C	-2.628280	1.402295	0.053607
C	-1.255103	1.181718	0.011264
C	-0.751499	-0.137261	-0.092838
C	-1.677330	-1.206825	-0.133323
C	-3.044397	-0.954746	-0.093268
C	-3.548439	0.349244	-0.003280
C	0.665371	-0.444296	-0.105714
O	0.768990	-1.014322	1.912784
O	1.883902	-1.476228	2.356328
O	-3.899239	-2.045376	-0.144245
O	-3.150008	2.681840	0.152079
C	1.717393	0.522066	-0.077615
O	1.652873	1.750963	0.022910
S	3.360670	-0.329786	-0.108198
C	4.457717	1.127887	-0.064697
H	0.946212	-1.458091	-0.376637
H	-0.552005	2.011556	0.062107
H	-1.325654	-2.235971	-0.179734
H	-4.619565	0.553883	0.030833
H	-4.804681	-1.723081	-0.069477
H	-2.406826	3.295067	0.206966
H	5.097284	1.146723	-0.956034
H	5.077171	1.105658	0.840389
H	3.800738	2.008902	-0.045754

24

r(C-O) = 2.20

C	-2.630791	1.400957	0.053064
C	-1.257575	1.183185	0.014663
C	-0.749678	-0.135713	-0.088121
C	-1.675565	-1.206834	-0.132645
C	-3.042734	-0.956627	-0.095673
C	-3.549744	0.346453	-0.006410
C	0.664758	-0.436451	-0.106886
O	0.804048	-1.009052	2.012720
O	1.940912	-1.370296	2.468779
O	-3.896038	-2.048612	-0.149902
O	-3.155132	2.679602	0.150408
C	1.715129	0.524654	-0.076019
O	1.658448	1.753449	0.032187
S	3.360791	-0.333648	-0.117099
C	4.461633	1.120457	-0.067837
H	0.948517	-1.459656	-0.336381
H	-0.556192	2.014462	0.068118
H	-1.323014	-2.235680	-0.181944
H	-4.621265	0.549187	0.024888
H	-4.802098	-1.726994	-0.079935
H	-2.413052	3.294047	0.206670
H	5.088675	1.153086	-0.967724
H	5.093369	1.083516	0.828150
H	3.805554	2.001583	-0.026526

24

r(C-O) = 2.30

C	-2.631974	1.400268	0.052634
C	-1.258841	1.183951	0.017268
C	-0.748268	-0.135236	-0.084119
C	-1.674889	-1.207024	-0.132142
C	-3.041969	-0.957528	-0.097779
C	-3.550581	0.345144	-0.008811
C	0.664507	-0.431998	-0.107912
O	0.863320	-1.014498	2.108203
O	2.020813	-1.303936	2.545261
O	-3.894625	-2.050068	-0.154714
O	-3.157705	2.678427	0.149138
C	1.713570	0.525686	-0.074620
O	1.661942	1.754458	0.040246
S	3.361864	-0.335805	-0.124689
C	4.463879	1.116820	-0.070384
H	0.950105	-1.461462	-0.306032
H	-0.558215	2.015865	0.072494
H	-1.322343	-2.235884	-0.183832
H	-4.622263	0.547125	0.020446
H	-4.801010	-1.728488	-0.088985
H	-2.416167	3.293415	0.206742
H	5.082587	1.160028	-0.975630
H	5.103797	1.070041	0.819280
H	3.807597	1.997082	-0.013407

24

r(C-O) = 2.40

C	-2.632380	1.399930	0.052319
C	-1.259309	1.184273	0.019337
C	-0.747087	-0.135273	-0.080895
C	-1.674772	-1.207311	-0.131703
C	-3.041598	-0.957913	-0.099564
C	-3.551057	0.344695	-0.010713
C	0.664533	-0.429462	-0.108732
O	0.949646	-1.018946	2.200212
O	2.131033	-1.246949	2.593394
O	-3.894230	-2.050512	-0.158755
O	-3.158623	2.677905	0.148239
C	1.712233	0.526018	-0.073497
O	1.664098	1.754896	0.046724
S	3.362986	-0.337007	-0.130785
C	4.464871	1.115126	-0.072415
H	0.951349	-1.463211	-0.283179
H	-0.558953	2.016408	0.075965
H	-1.322538	-2.236290	-0.185476
H	-4.622804	0.546406	0.016871
H	-4.800741	-1.728542	-0.096834
H	-2.417250	3.293094	0.205978
H	5.078507	1.165940	-0.980766
H	5.109718	1.061900	0.813310
H	3.807877	1.994273	-0.005132

24

r(C-O) = 2.50

C	-2.632290	1.399778	0.051989
C	-1.259319	1.184304	0.020735
C	-0.746038	-0.135644	-0.078381
C	-1.674901	-1.207621	-0.131490
C	-3.041425	-0.957977	-0.100867
C	-3.551316	0.344703	-0.011955
C	0.664831	-0.428050	-0.109450
O	1.059746	-1.030342	2.284559
O	2.266819	-1.204966	2.609402
O	-3.894297	-2.050461	-0.161690
O	-3.158558	2.677797	0.147318
C	1.710808	0.526252	-0.072550
O	1.665392	1.755306	0.052017
S	3.363866	-0.337695	-0.135658
C	4.465085	1.114336	-0.073896
H	0.953009	-1.464586	-0.266232
H	-0.558927	2.016438	0.078225
H	-1.323266	-2.236804	-0.187127
H	-4.623055	0.546432	0.014536
H	-4.800819	-1.727922	-0.103068
H	-2.417094	3.292916	0.204825
H	5.076190	1.169932	-0.983701
H	5.112235	1.057131	0.809893
H	3.807260	1.992497	-0.000605

24

r(C-O) = 2.60

C	-2.631979	1.399689	0.051697
C	-1.259057	1.184188	0.021760
C	-0.745104	-0.136080	-0.076465
C	-1.675011	-1.207912	-0.131355
C	-3.041234	-0.957945	-0.101855
C	-3.551373	0.344874	-0.012830
C	0.665368	-0.427053	-0.110016
O	1.192108	-1.043823	2.360235
O	2.423288	-1.168223	2.595339
O	-3.894482	-2.050232	-0.163888
O	-3.158021	2.677843	0.146582
C	1.709126	0.526688	-0.071785
O	1.666231	1.756067	0.056109
S	3.364187	-0.338226	-0.139415
C	4.464698	1.113633	-0.075015
H	0.954962	-1.465433	-0.253430
H	-0.558505	2.016231	0.079832
H	-1.323902	-2.237271	-0.188553
H	-4.623100	0.546657	0.012804
H	-4.800952	-1.727067	-0.108053
H	-2.416336	3.292776	0.203376
H	5.076663	1.170323	-0.984189
H	5.110803	1.055168	0.809465
H	3.805979	1.991180	-0.001036

24

r(C-O) = 2.70

C	-2.631737	1.399548	0.051494
C	-1.258826	1.184098	0.022510
C	-0.744291	-0.136348	-0.075061
C	-1.674896	-1.208076	-0.131230
C	-3.040938	-0.957986	-0.102634
C	-3.551366	0.344880	-0.013471
C	0.666125	-0.426025	-0.110403
O	1.337425	-1.040668	2.431560
O	2.586116	-1.116570	2.563999
O	-3.894356	-2.050218	-0.165602
O	-3.157656	2.677775	0.146132
C	1.707102	0.527558	-0.071185
O	1.667269	1.757313	0.059025
S	3.364231	-0.338839	-0.142162
C	4.464262	1.112433	-0.075884
H	0.957044	-1.465748	-0.243072
H	-0.558198	2.016127	0.081029
H	-1.324153	-2.237561	-0.189709
H	-4.623093	0.546680	0.011504
H	-4.800818	-1.726643	-0.112076
H	-2.415827	3.292599	0.202362
H	5.081477	1.165606	-0.981700
H	5.104833	1.056025	0.812774
H	3.804692	1.989964	-0.007897

24

r(C-O) = 2.80

C	-2.631737	1.399548	0.051494
C	-1.258826	1.184098	0.022510
C	-0.744291	-0.136348	-0.075061
C	-1.674896	-1.208076	-0.131230
C	-3.040938	-0.957986	-0.102634
C	-3.551366	0.344880	-0.013471
C	0.666125	-0.426025	-0.110403
O	1.337516	-1.032139	2.538091
O	2.586207	-1.108041	2.670530
O	-3.894356	-2.050218	-0.165602
O	-3.157656	2.677775	0.146132
C	1.707102	0.527558	-0.071185
O	1.667269	1.757313	0.059025
S	3.364231	-0.338839	-0.142162
C	4.464262	1.112433	-0.075884
H	0.957044	-1.465748	-0.243072
H	-0.558198	2.016127	0.081029
H	-1.324153	-2.237561	-0.189709
H	-4.623093	0.546680	0.011504
H	-4.800818	-1.726643	-0.112076
H	-2.415827	3.292599	0.202362
H	5.081477	1.165606	-0.981700
H	5.104833	1.056025	0.812774
H	3.804692	1.989964	-0.007897

24

r(C-O) = 2.90

C	-2.631737	1.399548	0.051494
C	-1.258826	1.184098	0.022510
C	-0.744291	-0.136348	-0.075061
C	-1.674896	-1.208076	-0.131230
C	-3.040938	-0.957986	-0.102634
C	-3.551366	0.344880	-0.013471
C	0.666125	-0.426025	-0.110403
O	1.352180	-1.023413	2.644594
O	2.600871	-1.099315	2.777033
O	-3.894356	-2.050218	-0.165602
O	-3.157656	2.677775	0.146132
C	1.707102	0.527558	-0.071185
O	1.667269	1.757313	0.059025
S	3.364231	-0.338839	-0.142162
C	4.464262	1.112433	-0.075884
H	0.957044	-1.465748	-0.243072
H	-0.558198	2.016127	0.081029
H	-1.324153	-2.237561	-0.189709
H	-4.623093	0.546680	0.011504
H	-4.800818	-1.726643	-0.112076
H	-2.415827	3.292599	0.202362
H	5.081477	1.165606	-0.981700
H	5.104833	1.056025	0.812774
H	3.804692	1.989964	-0.007897

24

r(C-O) = 3.00

C	-2.631737	1.399548	0.051494
C	-1.258826	1.184098	0.022510
C	-0.744291	-0.136348	-0.075061
C	-1.674896	-1.208076	-0.131230
C	-3.040938	-0.957986	-0.102634
C	-3.551366	0.344880	-0.013471
C	0.666125	-0.426025	-0.110403
O	1.366840	-1.015076	2.746255
O	2.615531	-1.090978	2.878694
O	-3.894356	-2.050218	-0.165602
O	-3.157656	2.677775	0.146132
C	1.707102	0.527558	-0.071185
O	1.667269	1.757313	0.059025
S	3.364231	-0.338839	-0.142162
C	4.464262	1.112433	-0.075884
H	0.957044	-1.465748	-0.243072
H	-0.558198	2.016127	0.081029
H	-1.324153	-2.237561	-0.189709
H	-4.623093	0.546680	0.011504
H	-4.800818	-1.726643	-0.112076
H	-2.415827	3.292599	0.202362
H	5.081477	1.165606	-0.981700
H	5.104833	1.056025	0.812774
H	3.804692	1.989964	-0.007897

24

r(C-O) = 4.00

C	-2.631737	1.399548	0.051494
C	-1.258826	1.184098	0.022510
C	-0.744291	-0.136348	-0.075061
C	-1.674896	-1.208076	-0.131230
C	-3.040938	-0.957986	-0.102634
C	-3.551366	0.344880	-0.013471
C	0.666125	-0.426025	-0.110403
O	1.567443	-0.931539	3.755664
O	2.816134	-1.007441	3.888103
O	-3.894356	-2.050218	-0.165602
O	-3.157656	2.677775	0.146132
C	1.707102	0.527558	-0.071185
O	1.667269	1.757313	0.059025
S	3.364231	-0.338839	-0.142162
C	4.464262	1.112433	-0.075884
H	0.957044	-1.465748	-0.243072
H	-0.558198	2.016127	0.081029
H	-1.324153	-2.237561	-0.189709
H	-4.623093	0.546680	0.011504
H	-4.800818	-1.726643	-0.112076
H	-2.415827	3.292599	0.202362
H	5.081477	1.165606	-0.981700
H	5.104833	1.056025	0.812774
H	3.804692	1.989964	-0.007897

24

r(C-O) = 5.00

C	-2.631737	1.399548	0.051494
C	-1.258826	1.184098	0.022510
C	-0.744291	-0.136348	-0.075061
C	-1.674896	-1.208076	-0.131230
C	-3.040938	-0.957986	-0.102634
C	-3.551366	0.344880	-0.013471
C	0.666125	-0.426025	-0.110403
O	1.846482	-0.849792	4.729364
O	3.095172	-0.925694	4.861804
O	-3.894356	-2.050218	-0.165602
O	-3.157656	2.677775	0.146132
C	1.707102	0.527558	-0.071185
O	1.667269	1.757313	0.059025
S	3.364231	-0.338839	-0.142162
C	4.464262	1.112433	-0.075884
H	0.957044	-1.465748	-0.243072
H	-0.558198	2.016127	0.081029
H	-1.324153	-2.237561	-0.189709
H	-4.623093	0.546680	0.011504
H	-4.800818	-1.726643	-0.112076
H	-2.415827	3.292599	0.202362
H	5.081477	1.165606	-0.981700
H	5.104833	1.056025	0.812774
H	3.804692	1.989964	-0.007897

r(C-O) / Å	RB3LYP Singlet	BS-B3LYP Singlet	UB3LYP Triplet	PNO-CCSD(T) Singlet	PNO-CCSD(T) Triplet	T1 Singlet	T1 Triplet
1.20	-381.0157	-381.0157	-380.9307	-380.5064		0.0172	
1.25	-381.0319	-381.0319	-380.9484	-380.5223	-380.4112	0.0172	0.0417
1.30	-381.0419	-381.0419	-380.9606	-380.5319	-380.4245	0.0172	0.0319
1.35	-381.0473	-381.0473	-380.9689	-380.5366	-380.4319	0.0173	0.0363
1.40	-381.0493	-381.0493	-380.9744	-380.5379	-380.4370	0.0174	0.0397
1.45	-381.0490	-381.0490	-380.9782	-380.5367	-380.4416	0.0177	0.0399
1.50	-381.0471	-381.0471	-380.9814	-380.5337	-380.4452	0.0182	0.0404
1.55	-381.0444	-381.0444	-380.9848	-380.5297	-380.4489	0.0190	0.0413
1.60	-381.0414	-381.0414	-380.9889	-380.5252	-380.4537	0.0201	0.0418
1.65	-381.0384	-381.0384	-380.9939	-380.5208	-380.4608	0.0216	0.0391
1.70	-381.0357	-381.0357	-380.9994	-380.5168	-380.4671	0.0230	0.0348
1.75	-381.0336	-381.0336	-381.0051	-380.5135	-380.4727	0.0245	0.0338
1.80	-381.0319	-381.0319	-381.0108	-380.5110	-380.4780	0.0254	0.0329
1.85	-381.0307	-381.0308	-381.0164	-380.5091	-380.4829	0.0256	0.0320
1.90	-381.0298	-381.0304	-381.0216	-380.5074	-380.4874	0.0249	0.0312
1.95	-381.0291	-381.0307	-381.0263	-380.5062	-380.4912	0.0240	0.0309
2.00	-381.0286	-381.0315	-381.0307	-380.5051	-380.4945	0.0230	0.0310
2.05	-381.0282	-381.0326	-381.0347	-380.5046	-380.4973	0.0223	0.0315
2.10	-381.0278	-381.0337	-381.0383	-380.5035	-380.4995	0.0218	0.0326
2.15	-381.0274	-381.0350	-381.0414	-380.5025	-380.5011	0.0216	0.0342
2.20	-381.0271	-381.0363	-381.0441	-380.5015	-380.5024	0.0216	0.0365
2.25	-381.0266	-381.0375	-381.0465	-380.5003	-380.5064	0.0219	0.0277
2.30	-381.0262	-381.0385	-381.0485	-380.4990	-380.5073	0.0222	0.0282
2.35	-381.0257	-381.0395	-381.0502	-380.4976	-380.5081	0.0224	0.0291
2.40	-381.0252	-381.0403	-381.0517	-380.4962		0.0227	
2.45	-381.0246	-381.0410	-381.0529	-380.4950	-380.5098	0.0230	0.0386
2.50	-381.0240	-381.0415	-381.0539	-380.4924	-380.5108	0.0219	0.0388
2.55	-381.0235	-381.0420	-381.0547	-380.4912	-380.5117	0.0218	0.0389
2.60	-381.0229	-381.0424	-381.0554	-380.4900	-380.5126	0.0218	0.0389
2.65	-381.0222	-381.0427	-381.0560	-380.4873	-380.5130	0.0201	0.0386
2.70	-381.0216	-381.0429	-381.0564	-380.4864	-380.5155	0.0201	0.0224
2.75	-381.0210	-381.0430	-381.0568	-380.4856	-380.5161	0.0200	0.0212
2.80	-381.0204	-381.0431	-381.0570	-380.4847	-380.5165	0.0198	0.0201
2.85	-381.0199	-381.0432	-381.0572	-380.4838	-380.5170	0.0197	0.0193
2.90	-381.0193	-381.0432	-381.0574	-380.4831	-380.5173	0.0195	0.0186
2.95	-381.0188	-381.0432	-381.0575	-380.4823	-380.5176	0.0193	0.0181
3.00	-381.0183	-381.0432	-381.0576	-380.4815	-380.5178	0.0191	0.0176
3.50	-381.0138	-381.0461	-381.0568	-380.4768	-380.5183	0.0172	0.0159
4.00		-381.0446	-381.0562	-380.4748	-380.5179	0.0169	0.0154
5.00	-381.0063	-381.0415	-381.0568	-380.4735	-380.5173	0.0170	0.0151

Table S4. Raw energies for oxobutenide anion. DFT calculations use the aug-cc-pVDZ basis set. PNO-CCSD(T) calculations use the cc-pVDZ-F12 basis set. Last two columns show the raw results for the T1 diagnosis test of CC calculations.

r(C-O) / Å	RB3LYP Singlet	BS-B3LYP Singlet	UB3LYP Triplet	PNO-CCSD(T) Singlet	PNO-CCSD(T) Triplet	T1 Singlet	T1 Triplet
1.20	-818.5647	-818.5647	-818.4644	-817.5352		0.0174	
1.25	-818.5803	-818.5803	-818.4826	-817.5507		0.0175	
1.30	-818.5897	-818.5897	-818.4955	-817.5599		0.0175	
1.35	-818.5945	-818.5945	-818.5043	-817.5643		0.0175	
1.40	-818.5958	-818.5958	-818.5104	-817.5651	-817.4607	0.0176	0.0333
1.45	-818.5947	-818.5947	-818.5149	-817.5633	-817.4654	0.0177	0.0349
1.50	-818.5920	-818.5920	-818.5193	-817.5598	-817.4697	0.0180	0.0373
1.55	-818.5883	-818.5883	-818.5243	-817.5550	-817.4721	0.0184	0.0347
1.60	-818.5843	-818.5843	-818.5307	-817.5494	-817.4786	0.0191	0.0353
1.65	-818.5805	-818.5805	-818.5383	-817.5436	-817.4869	0.0204	0.0351
1.70	-818.5774	-818.5774	-818.5459	-817.5387	-817.4950	0.0221	0.0325
1.75	-818.5752	-818.5752	-818.5527	-817.5351	-817.5016	0.0237	0.0303
1.80	-818.5738	-818.5739	-818.5585	-817.5328	-817.5068	0.0244	0.0293
1.85	-818.5730	-818.5736	-818.5638	-817.5311	-817.5111	0.0239	0.0287
1.90	-818.5726	-818.5743	-818.5687	-817.5301	-817.5151	0.0229	0.0283
1.95	-818.5728	-818.5758	-818.5738	-817.5295	-817.5186	0.0218	0.0280
2.00	-818.5729	-818.5774	-818.5782	-817.5290	-817.5222	0.0208	0.0273
2.10	-818.5731	-818.5809	-818.5858	-817.5278	-817.5284	0.0196	0.0311
2.20	-818.5731	-818.5842	-818.5919	-817.5265	-817.5333	0.0192	0.0328
2.30	-818.5727	-818.5867	-818.5965	-817.5250	-817.5379	0.0192	0.0335
2.40	-818.5719	-818.5888	-818.5998	-817.5221	-817.5415	0.0184	0.0338
2.50	-818.5709	-818.5901	-818.6021	-817.5203	-817.5443	0.0180	0.0338
2.60	-818.5697	-818.5910	-818.6036	-817.5186	-817.5482	0.0177	0.0189
2.70	-818.5684	-818.5914	-818.6044	-817.5166	-817.5496	0.0171	0.0174
2.80	-818.5671	-818.5915	-818.6048	-817.5155	-817.5504	0.0169	0.0165
2.90	-818.5659	-818.5913	-818.6048	-817.5144	-817.5509	0.0167	0.0158
3.00	-818.5647	-818.5913	-818.6050	-817.5132	-817.5514	0.0165	0.0155
3.50	-818.5603	-818.5904	-818.6047	-817.5096	-817.5516	0.0162	0.0150
4.00	-818.5460	-818.5918	-818.6044	-817.5077	-817.5509	0.0162	0.0149
5.00	-818.5570	-818.5931	-818.6038	-817.5060	-817.5501	0.0162	0.0147

Table S5. Raw energies for S-methyl-butenthioate anion. DFT calculations use the aug-cc-pVDZ basis set. PNO-CCSD(T) calculations use the cc-pVDZ-F12 basis set. Last two columns show the raw results for the T1 diagnosis test of CC calculations.

r(C-O) / Å	RB3LYP Singlet	BS-B3LYP Singlet	UB3LYP Triplet	PNO-CCSD(T) Singlet	PNO-CCSD(T) Triplet	T1 Singlet	T1 Triplet
1.30	-1122.7426	-1122.7426	-1122.6501	-1121.2976		0.0162	
1.35	-1122.7475	-1122.7475	-1122.6590	-1121.3020		0.0163	
1.40	-1122.7489	-1122.7489	-1122.6653	-1121.3027		0.0163	
1.45	-1122.7479	-1122.7479	-1122.6751	-1121.3009		0.0165	
1.50	-1122.7453	-1122.7453	-1122.6813	-1121.2971		0.0166	
1.55	-1122.7418	-1122.7418	-1122.6886	-1121.2923	-1121.2145	0.0170	0.0280
1.60	-1122.7381	-1122.7381	-1122.6960	-1121.2871	-1121.2221	0.0178	0.0287
1.65	-1122.7348	-1122.7348	-1122.7030	-1121.2822		0.0190	
1.70	-1122.7323	-1122.7323	-1122.7092	-1121.2781	-1121.2382	0.0201	0.0263
1.75	-1122.7305	-1122.7305	-1122.7150	-1121.2755	-1121.2444	0.0211	0.0249
1.80	-1122.7293	-1122.7294	-1122.7208	-1121.2737	-1121.2496	0.0214	0.0244
1.85	-1122.7287	-1122.7294	-1122.7255	-1121.2718	-1121.2539	0.0209	0.0241
1.90	-1122.7283	-1122.7301	-1122.7304	-1121.2715	-1121.2585	0.0200	0.0238
1.95	-1122.7286	-1122.7318	-1122.7345	-1121.2712		0.0191	
2.00	-1122.7288	-1122.7335	-1122.7421	-1121.2711	-1121.2657	0.0182	0.0242
2.10	-1122.7294	-1122.7373	-1122.7483	-1121.2704	-1121.2722	0.0173	0.0265
2.20	-1122.7296	-1122.7408	-1122.7528	-1121.2698	-1121.2779	0.0170	0.0275
2.30	-1122.7294	-1122.7435	-1122.7559	-1121.2679	-1121.2828	0.0165	0.0279
2.40	-1122.7288	-1122.7454	-1122.7578	-1121.2668	-1121.2865	0.0164	0.0281
2.50	-1122.7279	-1122.7466	-1122.7587	-1121.2657	-1121.2890	0.0162	0.0282
2.60	-1122.7270	-1122.7470	-1122.7587	-1121.2646	-1121.2924	0.0160	0.0156
2.70	-1122.7260	-1122.7468	-1122.7604	-1121.2633	-1121.2926	0.0158	0.0149
2.80	-1122.7250	-1122.7478	-1122.7614	-1121.2621	-1121.2946	0.0157	0.0147
2.90	-1122.7237	-1122.7483	-1122.7619	-1121.2610	-1121.2960	0.0156	0.0146
3.00	-1122.7225	-1122.7485	-1122.7614	-1121.2600	-1121.2968	0.0155	0.0146
4.00	-1122.7143		-1122.7614	-1121.2543	-1121.2974	0.0153	0.0144

Table S6. Raw energies for DpA anion. DFT calculations use the aug-cc-pVDZ basis set. PNO-CCSD(T) calculations use the cc-pVDZ-F12 basis set. Last two columns show the raw results for the T1 diagnosis test of CC calculations.

r(C-O) / Å	vHCISCF	vSHCI (ε1=5e-3)	SHCI (ε1=5e-3)	vSHCI (ε1=1e-3)	SHCI (ε1=1e-3)	vSHCI (ε1=5e-4)	SHCI (ε1=5e-4)	FCI extrap.
1.20	-0.241734	-0.207020	-0.259114	-0.241764	-0.260240	-0.248294	-0.260890	-0.261219
1.25	-0.265596	-0.236203	-0.277645	-0.265660	-0.279429	-0.270318	-0.279877	-0.280452
1.30	-0.277263	-0.248545	-0.289299	-0.277279	-0.291104	-0.282173	-0.291575	-0.292165
1.35	-0.283903	-0.255810	-0.296345	-0.283916	-0.297864	-0.288954	-0.298314	-0.298808
1.40	-0.286278	-0.258349	-0.298696	-0.286320	-0.300395	-0.291488	-0.300873	-0.301443
1.45	-0.285652	-0.257641	-0.297704	-0.285695	-0.299831	-0.291006	-0.300378	-0.301114
1.50	-0.282763	-0.254146	-0.295489	-0.282780	-0.297385	-0.288248	-0.297910	-0.298559
1.55	-0.278266	-0.249204	-0.291350	-0.278281	-0.293280	-0.283907	-0.293828	-0.294495
1.60	-0.272650	-0.243198	-0.285892	-0.272654	-0.287975	-0.278459	-0.288621	-0.289344
1.65	-0.266473	-0.236233	-0.280112	-0.266523	-0.282276	-0.272411	-0.282954	-0.283710
1.70	-0.260274	-0.228774	-0.272909	-0.260286	-0.276222	-0.266319	-0.277018	-0.278239
1.75	-0.255412	-0.225957	-0.268631	-0.255436	-0.271321	-0.261548	-0.272043	-0.273064
1.80	-0.250650	-0.220305	-0.264248	-0.250713	-0.267051	-0.256982	-0.267743	-0.268813
1.85	-0.246597	-0.215006	-0.260282	-0.246632	-0.263340	-0.253160	-0.264128	-0.265270
1.90	-0.243491	-0.211213	-0.257515	-0.243535	-0.260710	-0.250213	-0.261496	-0.262707
1.95	-0.241134	-0.207810	-0.255577	-0.241206	-0.258736	-0.248132	-0.259559	-0.260717
2.00	-0.239341	-0.206106	-0.254185	-0.239421	-0.257248	-0.246515	-0.258084	-0.259218
2.05	-0.237791	-0.204584	-0.252899	-0.237903	-0.255935	-0.245186	-0.256806	-0.257930
2.10	-0.236572	-0.203320	-0.251416	-0.236679	-0.254750	-0.243996	-0.255663	-0.256923
2.15	-0.235422	-0.201903	-0.250365	-0.235558	-0.253736	-0.242943	-0.254672	-0.255939
2.20	-0.234687	-0.201051	-0.249421	-0.234787	-0.252856	-0.242018	-0.253766	-0.255063
2.25	-0.234711	-0.202171	-0.249604	-0.234862	-0.252330	-0.241636	-0.253108	-0.254108
2.30	-0.233853	-0.201257	-0.248852	-0.234048	-0.251438	-0.240746	-0.252206	-0.253137
2.35	-0.232939	-0.199743	-0.247988	-0.233119	-0.250505	-0.239775	-0.251264	-0.252146
2.40	-0.231991	-0.198542	-0.247356	-0.232196	-0.249645	-0.238812	-0.250368	-0.251153
2.45	-0.230968	-0.197427	-0.246071	-0.231206	-0.248580	-0.237824	-0.249334	-0.250201
2.50	-0.230048	-0.196143	-0.245157	-0.230325	-0.247618	-0.236848	-0.248364	-0.249196
2.55	-0.229106	-0.195394	-0.244167	-0.229445	-0.246612	-0.235888	-0.247368	-0.248190
2.60	-0.228218	-0.194438	-0.243656	-0.228576	-0.245802	-0.235000	-0.246515	-0.247217
2.65	-0.227320	-0.193534	-0.242539	-0.227706	-0.244782	-0.234130	-0.245527	-0.246254
2.70	-0.226534	-0.192716	-0.241405	-0.226981	-0.243840	-0.233294	-0.244600	-0.245392
2.75	-0.225806	-0.191713	-0.241061	-0.226289	-0.243156	-0.232537	-0.243871	-0.244523
2.80	-0.225112	-0.190902	-0.239741	-0.225618	-0.242191	-0.231820	-0.242955	-0.243722
2.85	-0.224541	-0.190194	-0.239467	-0.225032	-0.241631	-0.231172	-0.242335	-0.242996
2.90	-0.223929	-0.189636	-0.238461	-0.224466	-0.240837	-0.230591	-0.241590	-0.242313
2.95	-0.223401	-0.189224	-0.238377	-0.223971	-0.240426	-0.230097	-0.241139	-0.241745
3.00	-0.222933	-0.188735	-0.237235	-0.223541	-0.239710	-0.229641	-0.240482	-0.241227
3.50	-0.217466	-0.183992	-0.231911	-0.218219	-0.234076	-0.224149	-0.234762	-0.235401
4.00	-0.213720	-0.180836	-0.227566	-0.214476	-0.230007	-0.220316	-0.230718	-0.231460
5.00	-0.209538	-0.176785	-0.223374	-0.210351	-0.225763	-0.216122	-0.226469	-0.227187

Table S7. Raw SHCI extrapolated absolute energies for oxobutenide anion, singlet state. vHCISCF stands for orbital optimization, vSHCI for CI with no perturbation, SHCI includes full perturbation and FCI is the final extrapolated value, following the reference method in text. ε_1 parameters are in parenthesis. Energies are given in E_h and shifted 379 E_h.

r(C-O) / Å	vHCISCF	vSHCI (ε1=5e-3)	SHCI (ε1=5e-3)	vSHCI (ε1=1e-3)	SHCI (ε1=1e-3)	vSHCI (ε1=5e-4)	SHCI (ε1=5e-4)	FCI extrap.
1.20	-0.141518	-0.130984	-0.146643	-0.136789	-0.147232	-0.144374	-0.148044	-0.148468
1.30	-0.162828	-0.170181	-0.185325	-0.175976	-0.186019	-0.183220	-0.186845	-0.187329
1.40	-0.186945	-0.186680	-0.201995	-0.192523	-0.202624	-0.199800	-0.203381	-0.203808
1.50	-0.144484	-0.169486	-0.191412	-0.178149	-0.192882	-0.189060	-0.194604	-0.195703
1.60	-0.151372	-0.141881	-0.164044	-0.149561	-0.164989	-0.160578	-0.166341	-0.167149
1.70	-0.131823	-0.165215	-0.184796	-0.172249	-0.185661	-0.181845	-0.186785	-0.187463
1.80	-0.144407	-0.177997	-0.197833	-0.185089	-0.198789	-0.195006	-0.200052	-0.200817
1.90	-0.188159	-0.185089	-0.206311	-0.192863	-0.207676	-0.203989	-0.209367	-0.210434
2.00	-0.191390	-0.190922	-0.210132	-0.197885	-0.211340	-0.207766	-0.212766	-0.213725
2.10	-0.202929	-0.203673	-0.221593	-0.210192	-0.222578	-0.219343	-0.223792	-0.224537
2.20	-0.214936	-0.215428	-0.232648	-0.221737	-0.233523	-0.230566	-0.234625	-0.235249
2.30	-0.224723	-0.225212	-0.241850	-0.231297	-0.242625	-0.239699	-0.243635	-0.244195
2.40	-0.232585	-0.232628	-0.249053	-0.238615	-0.249801	-0.246951	-0.250794	-0.251331
2.50	-0.238525	-0.238598	-0.254652	-0.244466	-0.255366	-0.252634	-0.256314	-0.256814
2.60	-0.243216	-0.243166	-0.258946	-0.248919	-0.259619	-0.256939	-0.260529	-0.260998
2.70	-0.246609	-0.246535	-0.262172	-0.252251	-0.262825	-0.260191	-0.263714	-0.264165
2.80	-0.249105	-0.249101	-0.264594	-0.254792	-0.265241	-0.262638	-0.266104	-0.266543
2.90	-0.251138	-0.251037	-0.266442	-0.256704	-0.267070	-0.264489	-0.267915	-0.268338
3.00	-0.252555	-0.252031	-0.267698	-0.257752	-0.268344	-0.265711	-0.269234	-0.269681

Table S8. Raw SHCI extrapolated absolute energies for oxobutenide anion, triplet state. vHCISCF stands for orbital optimization, vSHCI for CI with no perturbation, SHCI includes full perturbation and FCI is the final extrapolated value, following the reference method in text. ε_1 parameters are in parenthesis. Energies are given in E_h and shifted 379 E_h.

r(C-O) / Å	vHCISCF	vSHCI (ε1=5e-3)	SHCI (ε1=5e-3)	vSHCI (ε1=1e-3)	SHCI (ε1=1e-3)	vSHCI (ε1=5e-4)	SHCI (ε1=5e-4)	FCI extrap.
1.20	-0.897990	-0.850143	-0.914997	-0.898085	-0.925886	-0.909255	-0.929053	-0.934795
1.25	-0.926677	-0.884868	-0.937633	-0.926727	-0.947509	-0.935047	-0.949689	-0.954168
1.30	-0.937511	-0.895130	-0.948526	-0.937636	-0.958517	-0.946073	-0.960769	-0.965231
1.35	-0.942712	-0.899974	-0.954358	-0.942857	-0.964286	-0.951379	-0.966541	-0.971054
1.40	-0.944686	-0.902623	-0.959710	-0.944985	-0.967695	-0.953652	-0.969657	-0.973316
1.45	-0.944743	-0.904739	-0.963915	-0.944961	-0.969010	-0.953574	-0.970404	-0.972799
1.50	-0.941606	-0.900674	-0.960544	-0.941773	-0.965940	-0.950491	-0.967382	-0.969889
1.55	-0.935933	-0.894519	-0.955763	-0.936120	-0.961258	-0.945036	-0.962693	-0.965343
1.60	-0.931265	-0.890018	-0.949968	-0.931399	-0.955768	-0.940245	-0.957298	-0.960034
1.65	-0.923864	-0.881794	-0.943230	-0.923958	-0.949182	-0.933095	-0.950768	-0.953630
1.70	-0.916321	-0.873864	-0.936183	-0.916421	-0.942273	-0.925735	-0.943928	-0.946923
1.75	-0.909421	-0.865751	-0.929744	-0.909519	-0.936014	-0.919101	-0.937771	-0.940841
1.80	-0.903885	-0.858915	-0.924404	-0.903972	-0.931078	-0.913871	-0.932952	-0.936213
1.85	-0.899764	-0.853743	-0.920721	-0.899863	-0.927606	-0.910083	-0.929577	-0.932937
1.90	-0.896922	-0.850142	-0.918181	-0.897052	-0.925218	-0.907430	-0.927215	-0.930646
1.95	-0.892139	-0.844030	-0.914461	-0.892266	-0.921855	-0.903043	-0.923933	-0.927661
2.00	-0.890938	-0.843270	-0.913013	-0.891084	-0.920206	-0.901836	-0.922328	-0.925890
2.10	-0.889153	-0.841786	-0.911668	-0.889293	-0.918704	-0.900207	-0.920830	-0.924353
2.20	-0.887732	-0.840978	-0.911217	-0.887882	-0.917609	-0.898865	-0.919607	-0.922820
2.30	-0.886228	-0.840112	-0.909870	-0.886392	-0.915791	-0.897273	-0.917729	-0.920665
2.40	-0.884827	-0.839689	-0.908479	-0.884950	-0.913897	-0.895677	-0.915722	-0.918381
2.50	-0.883402	-0.839557	-0.906705	-0.883539	-0.911845	-0.894065	-0.913600	-0.916123
2.60	-0.883952	-0.842938	-0.905158	-0.884039	-0.910113	-0.893775	-0.911713	-0.914118
2.70	-0.884510	-0.845965	-0.904122	-0.884613	-0.908851	-0.893856	-0.910346	-0.912598
2.80	-0.884568	-0.847412	-0.903175	-0.884644	-0.907845	-0.893585	-0.909240	-0.911450
2.90	-0.884478	-0.848226	-0.902438	-0.884574	-0.907045	-0.893198	-0.908336	-0.910507
3.00	-0.884805	-0.848802	-0.902159	-0.884904	-0.906752	-0.893314	-0.908004	-0.910119
3.50	-0.884862	-0.849182	-0.901201	-0.884965	-0.905674	-0.892974	-0.906814	-0.908769
4.00	-0.884438	-0.849139	-0.900298	-0.884554	-0.904768	-0.892448	-0.905865	-0.907786
5.00	-0.883565	-0.848483	-0.899182	-0.883685	-0.903676	-0.891546	-0.904765	-0.906685

Table S9. Raw SHCI extrapolated absolute energies for S-methyl-butenthioate anion, singlet state. vHCISCF stands for orbital optimization, vSHCI for CI with no perturbation, SHCI includes full perturbation and FCI is the final extrapolated value, following the reference method in text. ε_1 parameters are in parenthesis. Energies are given in E_h and shifted 815 E_h.

r(C-O) / Å	vHCISCF	vSHCI (ε1=5e-3)	SHCI (ε1=5e-3)	vSHCI (ε1=1e-3)	SHCI (ε1=1e-3)	vSHCI (ε1=5e-4)	SHCI (ε1=5e-4)	FCI extrap.
1.65	-0.820915	-0.821285	-0.849348	-0.829701	-0.850346	-0.844329	-0.852968	-0.854509
1.75	-0.835759	-0.835900	-0.863860	-0.845335	-0.865270	-0.859167	-0.867226	-0.868600
1.85	-0.847203	-0.872102	-0.855796	-0.873353	-0.868041	-0.874954	-0.876069	-0.873408
1.90	-0.848394	-0.851509	-0.877685	-0.860592	-0.879061	-0.873565	-0.880934	-0.882217
1.95	-0.856273	-0.856455	-0.881843	-0.865209	-0.883165	-0.877829	-0.884931	-0.886145
2.00	-0.861500	-0.822699	-0.882124	-0.862322	-0.886895	-0.870794	-0.888119	-0.890464
2.10	-0.868121	-0.819590	-0.890731	-0.868169	-0.897160	-0.878369	-0.898729	-0.901802
2.30	-0.891513	-0.894255	-0.916204	-0.902038	-0.917478	-0.913540	-0.919398	-0.920557
2.40	-0.901159	-0.901658	-0.923326	-0.909373	-0.924577	-0.920723	-0.926434	-0.927544
2.50	-0.906762	-0.907253	-0.928634	-0.914885	-0.929849	-0.926086	-0.931655	-0.932717
2.60	-0.911252	-0.911390	-0.932533	-0.918909	-0.933709	-0.929979	-0.935469	-0.936495
2.70	-0.914014	-0.914065	-0.935267	-0.921564	-0.936433	-0.932689	-0.938212	-0.939244
2.80	-0.916444	-0.730710	-0.754054	-0.923907	-0.938468	-0.934800	-0.940165	-0.940165
2.90	-0.917640	-0.729315	-0.751575	-0.925040	-0.939537	-0.935896	-0.941216	-0.941216
3.00	-0.919254	-0.728840	-0.750496	-0.926587	-0.940995	-0.937372	-0.942639	-0.942639
3.50	-0.921509	-0.713650	-0.741706	-0.929055	-0.943862	-0.940033	-0.945447	-0.945447
5.00	-0.720250	-0.631211	-0.652187	-0.913950	-0.928101	-0.924051	-0.929296	-0.946566

Table S10. Raw SHCI extrapolated absolute energies for S-methyl-butenthioate anion, triplet state. vHCISCF stands for orbital optimization, vSHCI for CI with no perturbation, SHCI includes full perturbation and FCI is the final extrapolated value, following the reference method in text. ε_1 parameters are in parenthesis. Energies are given in E_h and shifted 815 E_h.

r(C-O) / Å	vSHCI (ε1=5e-3)	SHCI (ε1=5e-3)	vSHCI (ε1=1e-3)	SHCI (ε1=1e-3)	vSHCI (ε1=5e-4)	SHCI (ε1=5e-4)	FCI extrap.
1.30	-0.532912	-0.677809	-0.627215	-0.697204	-0.647215	-0.702357	-0.716648
1.35	-0.538301	-0.683159	-0.632359	-0.702667	-0.652564	-0.707852	-0.722340
1.40	-0.538695	-0.684669	-0.633619	-0.704296	-0.653887	-0.709501	-0.724015
1.45	-0.537855	-0.684203	-0.632261	-0.703460	-0.652653	-0.708631	-0.723000
1.50	-0.538724	-0.682696	-0.629989	-0.701152	-0.650599	-0.706222	-0.720362
1.55	-0.536425	-0.679267	-0.626449	-0.697318	-0.647113	-0.702298	-0.716180
1.60	-0.529802	-0.673135	-0.619829	-0.691180	-0.640731	-0.696272	-0.710245
1.65	-0.522137	-0.666051	-0.612232	-0.684158	-0.633386	-0.689397	-0.703545
1.70	-0.514223	-0.658914	-0.604721	-0.677368	-0.626161	-0.682763	-0.697330
1.75	-0.507002	-0.652923	-0.598099	-0.671651	-0.619930	-0.677217	-0.692120
1.80	-0.500630	-0.648343	-0.592783	-0.667214	-0.614927	-0.672898	-0.687909
1.85	-0.491070	-0.641945	-0.584872	-0.661239	-0.607399	-0.667098	-0.682654
1.90	-0.494619	-0.643766	-0.586567	-0.662305	-0.609036	-0.668077	-0.683090
1.95	-0.490895	-0.640475	-0.582761	-0.658947	-0.605386	-0.664774	-0.679832
2.00	-0.491373	-0.640367	-0.582630	-0.658370	-0.605306	-0.664223	-0.678819
2.10	-0.489953	-0.639176	-0.581336	-0.657097	-0.604072	-0.662955	-0.677435
2.20	-0.489634	-0.638684	-0.581113	-0.656388	-0.603779	-0.662161	-0.676275
2.30	-0.492345	-0.638530	-0.581823	-0.655681	-0.604259	-0.661379	-0.675029
2.40	-0.499052	-0.638671	-0.584806	-0.655384	-0.606650	-0.660791	-0.673985
2.50	-0.501493	-0.637827	-0.585759	-0.654489	-0.607126	-0.659697	-0.672724
2.60	-0.503125	-0.637041	-0.586206	-0.653523	-0.607183	-0.658643	-0.671444
2.70	-0.503762	-0.636155	-0.586193	-0.652573	-0.606816	-0.657550	-0.670223
2.80	-0.505701	-0.636808	-0.587724	-0.653133	-0.608025	-0.657966	-0.670422
2.90	-0.507232	-0.637121	-0.588712	-0.653335	-0.608866	-0.658120	-0.670398
3.00	-0.507952	-0.637246	-0.589361	-0.653421	-0.609447	-0.658199	-0.670324
4.00	-0.508705	-0.636138	-0.589822	-0.652274	-0.609514	-0.656936	-0.668735
5.00	-0.508377	-0.635168	-0.589249	-0.651299	-0.608896	-0.655947	-0.667692

Table S11. Raw SHCI extrapolated absolute energies for DPA anion, singlet state. vHCISCF stands for orbital optimization, vSHCI for CI with no perturbation, SHCI includes full perturbation and FCI is the final extrapolated value, following the reference method in text. ε_1 parameters are in parenthesis. Energies are given in E_h and shifted 1118 E_h.

r(C-O) / Å	vSHCI (ε1=5e-3)	SHCI (ε1=5e-3)	vSHCI (ε1=1e-3)	SHCI (ε1=1e-3)	vSHCI (ε1=5e-4)	SHCI (ε1=5e-4)	FCI extrap.
1.75	-0.543244	-0.615605	-0.564915	-0.621397	-0.601799	-0.630794	-0.640978
1.80	-0.548344	-0.621088	-0.570164	-0.626911	-0.607223	-0.636389	-0.646655
1.85	-0.552368	-0.625010	-0.574027	-0.630827	-0.611099	-0.640288	-0.650581
1.90	-0.558275	-0.630881	-0.580079	-0.636666	-0.617043	-0.646123	-0.656328
2.10	-0.572365	-0.642960	-0.593486	-0.648269	-0.629479	-0.657438	-0.666923
2.20	-0.581747	-0.650693	-0.602609	-0.655858	-0.637789	-0.664627	-0.673505
2.30	-0.590010	-0.657426	-0.610331	-0.662353	-0.644838	-0.670793	-0.679156
2.40	-0.596144	-0.662744	-0.616372	-0.667580	-0.650353	-0.675726	-0.683714
2.50	-0.600858	-0.666782	-0.620689	-0.671436	-0.654377	-0.679459	-0.687236
2.70	-0.612826	-0.679767	-0.633169	-0.684505	-0.667453	-0.692658	-0.700430
3.00	-0.619650	-0.687789	-0.640418	-0.692654	-0.675040	-0.700858	-0.708824
4.00	-0.621053	-0.691471	-0.641846	-0.696430	-0.677812	-0.705126	-0.713772
5.00	-0.619731	-0.690577	-0.640265	-0.695548	-0.676592	-0.704354	-0.713230

Table S12. Raw SHCI extrapolated absolute energies for DPA anion, triplet state. vHCISCF stands for orbital optimization, vSHCI for CI with no perturbation, SHCI includes full perturbation and FCI is the final extrapolated value, following the reference method in text. ε_1 parameters are in parenthesis. Energies are given in E_h and shifted 1118 E_h.

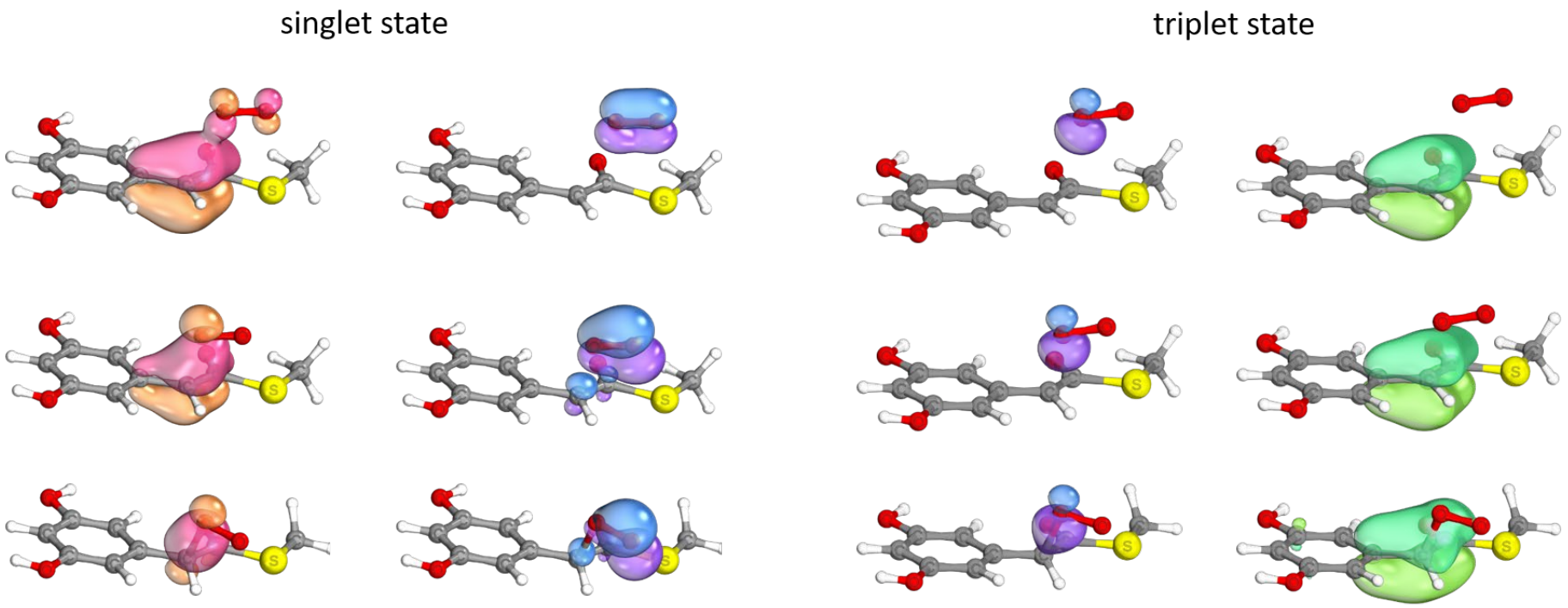

Fig S1: IBO/IAO orbitals whose nature change the most along the addition of O_2 to DPA^- for the singlet and triplet states. Top panel: large rCαO distances. Middle panels: Crossing region. Bottom panels: short rCαO distance, where the peroxide is formed.