Details of QM calculations

Clustering was done on **1R^{TS}**, **2R^{TS}**, **3R^{TS}**, **4R^{TS}**, **1R2R^{TS}** and **1R2S^{TS}** (Supplementary Figure 8) to narrow down the conformational space to 5 representative conformers for each ensemble. Each of these representative conformers was fully optimized to a transition state using G09 and B3LYP/LANL2DZ/6-31G* with Grimme's empirical dispersion.[1] Transition states were confirmed using harmonic frequency analysis. All 5 representatives were optimized to QM transition states for every conformer besides **1R^{TS}**, for which only 4 transition states could be located. The coordinates, energies and frequencies are found in Supplementary Tables 3-31. Energies are reported in hartrees.

[1] Grimme, S., Antony, J., Ehrlich, S. & Krieg, H. A consistent and accurate *ab initio* parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu. *J. Chem. Phys.* **132**, 154104 (2010).

Supplementary Table 3. **O1R^{TS}** representative 1

C	-1.640751	3.209351	-1.671174
C	-1.030605	3.339871	-0.274604
N	-3.022982	3.319411	-1.761739
C	-3.923325	2.823994	-0.764066
C	-4.826355	3.593614	-0.110090
C	-3.740025	1.371369	-0.475296
O	-2.684431	0.809050	-0.786945
N	-4.729091	0.643507	0.134794
C	-4.479358	-0.698638	0.487624
C	-5.373372	-1.699206	0.342571
C	-6.705778	-1.646727	-0.270777
C	-3.159907	-0.906441	1.188309
N	-0.433764	2.082521	0.127111
C	-1.176821	-2.467918	1.178259
N	-2.447754	-1.977936	0.746702
O	-2.795550	-0.140758	2.085016
C	-0.973641	-3.792670	1.330380
O	-0.944073	3.093356	-2.668768
C	-5.118866	5.019403	-0.191720
C	-1.974930	-4.860126	1.257630
C	-3.289499	-4.710684	1.741999
C	-4.206683	-5.752683	1.631014
C	-3.834503	-6.958830	1.028554
C	-2.528853	-7.127074	0.561732
C	-1.603111	-6.092460	0.689060
C	-7.698056	-2.526397	0.202043
C	-8.979343	-2.520802	-0.343839
C	-9.291832	-1.647238	-1.388793
C	-8.310487	-0.787395	-1.888810
C	-7.030583	-0.783897	-1.337405
C	-6.122643	5.518408	0.666502
C	-6.466214	6.866557	0.663879
C	-5.810372	7.748439	-0.198464
C	-4.811731	7.272045	-1.054501
C	-4.466390	5.924594	-1.057199
H	-1.777526	3.671615	0.457274
H	-0.241088	4.093374	-0.325556
H	-3.333911	3.204194	-2.723934
H	-5.427182	3.074002	0.634711
H	-5.680768	0.984610	0.174065
H	-5.099147	-2.654697	0.784324
H	-1.003583	1.259166	-0.029996
H	-2.796377	-2.426094	-0.094883
H	0.062518	-4.100988	1.442701
H	-3.572091	-3.789410	2.239825
H	-5.211409	-5.630096	2.026231
H	-4.553496	-7.767913	0.939225
H	-2.228651	-8.067291	0.108499
H	-0.583856	-6.230321	0.336335
H	-7.458492	-3.210792	1.012253
H	-9.733181	-3.200923	0.041905
H	-10.289126	-1.645317	-1.818664
H	-8.539763	-0.124741	-2.718579
H	-6.266546	-0.142836	-1.765674
H	-6.634095	4.836353	1.341727
H	-7.241615	7.229127	1.331997
H	-6.075066	8.801848	-0.204274
H	-4.300272	7.956768	-1.724727
H	-3.689923	5.566301	-1.720101

C	3.633837	2.454805	-1.099974
C	1.895231	1.221448	-2.591100
P	1.922907	-0.464951	-1.840573
P	4.266241	1.102383	-0.006033
C	4.628159	-3.133087	-4.520386
C	4.229876	-3.560218	-3.250521
C	3.425756	-2.742066	-2.458491
C	2.995091	-1.490213	-2.929411
C	3.383753	-1.079157	-4.211715
C	4.203527	-1.892660	-4.997486
H	3.158620	-3.061788	-1.455336
H	3.059438	-0.124021	-4.610771
C	-2.229145	-2.351451	-2.769321
C	-1.196954	-3.121046	-2.220093
C	0.032852	-2.533652	-1.930901
C	0.253570	-1.167842	-2.186788
C	-0.787279	-0.400809	-2.728802
C	-2.018086	-0.996163	-3.017945
H	0.818189	-3.137928	-1.493264
H	-0.669431	0.660190	-2.916997
C	8.134532	-0.030820	-2.302247
C	7.143894	-0.995527	-2.123681
C	5.987019	-0.688263	-1.403739
C	5.805651	0.589564	-0.866709
C	6.814142	1.555997	-1.041228
C	7.970142	1.245344	-1.753353
H	5.226087	-1.443571	-1.265818
H	6.705400	2.545492	-0.605350
C	5.827641	3.032163	3.898464
C	6.262439	1.764212	3.498298
C	5.794202	1.210142	2.309710
C	4.885966	1.921851	1.507251
C	4.446928	3.189775	1.913172
C	4.923513	3.739999	3.106573
H	6.136715	0.226198	2.000859
H	3.714310	3.734897	1.332052
H	-3.187019	-2.808693	-3.003846
H	5.264878	-3.764310	-5.133633
H	6.192413	3.463392	4.826360
H	9.035400	-0.269493	-2.860489
H	4.507517	-1.554107	-5.983831
H	4.555473	-4.524870	-2.871324
H	-2.816093	-0.384731	-3.427237
H	-1.349807	-4.177204	-2.013752
H	8.744615	1.996872	-1.877087
H	7.259722	-1.989992	-2.544474
H	4.578686	4.722369	3.416194
H	6.966226	1.209031	4.111618
Rh	2.656525	-0.457100	0.447539
O	1.144132	-2.019358	0.847778
C	0.013101	-1.562507	1.165154
N	-0.165198	-0.268117	1.454174
C	0.936039	0.653758	1.480728
C	1.935520	0.488154	2.477593
H	-1.074789	-0.003552	1.861294
H	3.787827	-1.498595	0.115380
H	3.256993	-0.497295	1.968358
H	2.545633	1.375222	2.629844
C	0.677032	2.006695	0.907126
O	1.406508	2.977176	1.140344
C	1.012833	-1.638901	6.104235
C	1.581046	-2.343552	5.042544

C	1.907950	-1.687127	3.853739
C	1.666193	-0.316889	3.716671
C	1.101820	0.390080	4.790385
C	0.775410	-0.268046	5.975349
H	0.761486	-2.151414	7.028430
H	1.776811	-3.408142	5.137246
H	2.348386	-2.235887	3.028742
H	0.917288	1.457203	4.692278
H	0.339545	0.291198	6.798417
C	3.228880	1.990151	-2.510763
H	1.573345	1.139904	-3.634712
H	1.110156	1.786119	-2.077241
H	3.112323	2.890136	-3.125722
H	4.041712	1.411833	-2.966069
H	2.789110	2.924219	-0.588834
H	4.437204	3.196367	-1.173770

Sum of electronic and zero-point energy: -3953.505337
Sum of electronic and thermal free energies: -3953.617148
Frequency: -643.1748

Supplementary Table 4. **O1R^{TS}** representative 2

C	-0.803055	3.700742	-2.399427
C	0.217388	2.601812	-2.087150
N	-1.656909	4.166742	-1.408976
C	-1.621972	3.823232	-0.025048
C	-0.763509	4.337356	0.885826
C	-2.543029	2.735096	0.396746
O	-2.417041	2.116880	1.467428
N	-3.539823	2.400918	-0.481611
C	-4.247638	1.179726	-0.324293
C	-5.587763	1.051773	-0.289802
C	-6.637202	2.072486	-0.331180
C	-3.330902	-0.013113	-0.363762
N	-0.049655	1.661853	-1.022317
C	-2.427269	-1.886485	0.951891
N	-3.407256	-0.877397	0.693711
O	-2.508173	-0.136331	-1.272888
C	-2.706271	-3.202302	1.084946
O	-0.819339	4.201716	-3.511490
C	0.317543	5.304752	0.755776
C	-3.959426	-3.928903	0.921905
C	-5.100467	-3.414889	0.271016
C	-6.247192	-4.191647	0.135842
C	-6.287616	-5.490868	0.652187
C	-5.164132	-6.018001	1.294004
C	-4.010939	-5.248347	1.417560
C	-7.950232	1.652322	-0.620318
C	-9.000874	2.564658	-0.675778
C	-8.762052	3.918178	-0.428401
C	-7.467527	4.349033	-0.122329
C	-6.413463	3.440940	-0.075798
C	0.602477	6.058942	-0.403235
C	1.682251	6.936595	-0.426444
C	2.501447	7.085509	0.696657
C	2.230947	6.351373	1.853896
C	1.150034	5.476577	1.882218
H	1.154033	3.110420	-1.833919
H	0.366571	2.079108	-3.037140
H	-2.143850	5.012760	-1.691572
H	-0.882142	3.918565	1.882576
H	-3.590738	2.897707	-1.363666
H	-5.955445	0.025909	-0.270534
H	-0.778964	0.970069	-1.162606
H	-4.045989	-0.630068	1.441202
H	-1.848891	-3.812322	1.357474
H	-5.073384	-2.418685	-0.152759
H	-7.114099	-3.785633	-0.377749
H	-7.187488	-6.090189	0.548339
H	-5.186313	-7.028324	1.691899
H	-3.133125	-5.662821	1.905708
H	-8.142821	0.598801	-0.809361
H	-10.004488	2.219894	-0.906847
H	-9.579473	4.632318	-0.466619
H	-7.280358	5.398574	0.086295
H	-5.419342	3.784800	0.182653
H	-0.012709	5.967900	-1.288425
H	1.885232	7.509097	-1.326866
H	3.342608	7.772336	0.669905
H	2.859292	6.463818	2.732690
H	0.945173	4.902787	2.782470

C	5.079995	-2.404658	-0.564442
C	3.254656	-3.678970	-1.872104
P	1.747991	-2.689546	-1.427062
P	4.087044	-0.946327	-0.011322
C	-1.307298	-6.119874	-0.696003
C	-1.465074	-5.291519	-1.806618
C	-0.554516	-4.261006	-2.053644
C	0.519092	-4.041575	-1.179711
C	0.667714	-4.876154	-0.058712
C	-0.233439	-5.912815	0.175163
H	-0.691570	-3.632540	-2.926168
H	1.471196	-4.697619	0.649200
C	0.281331	-0.269307	-5.082061
C	1.493746	-0.955781	-5.179222
C	1.953544	-1.731586	-4.111892
C	1.202869	-1.814507	-2.931874
C	-0.016829	-1.123372	-2.840726
C	-0.481313	-0.365248	-3.912806
H	2.899683	-2.253575	-4.209084
H	-0.619357	-1.190532	-1.941864
C	6.228917	1.023990	3.573912
C	6.426739	-0.336192	3.325511
C	5.811923	-0.945274	2.230201
C	5.002416	-0.188470	1.371942
C	4.802121	1.180742	1.623301
C	5.416115	1.778617	2.723701
H	5.968153	-2.005769	2.055187
H	4.159499	1.768851	0.972664
C	4.763106	1.961356	-3.548820
C	3.466774	1.556706	-3.235403
C	3.239409	0.701182	-2.154625
C	4.313498	0.236059	-1.390558
C	5.619925	0.656674	-1.703247
C	5.841559	1.514032	-2.777616
H	2.230409	0.397506	-1.913655
H	6.460683	0.329962	-1.097103
H	-0.070503	0.333862	-5.914000
H	-2.019914	-6.916983	-0.506037
H	4.936835	2.629039	-4.387893
H	6.706844	1.493989	4.428592
H	-0.102987	-6.551365	1.044629
H	-2.297722	-5.444013	-2.487072
H	-1.433589	0.148812	-3.821658
H	2.086524	-0.888456	-6.086790
H	5.258669	2.836246	2.914715
H	7.059841	-0.924712	3.983257
H	6.851994	1.836800	-3.011158
H	2.627276	1.902960	-3.829236
Rh	1.912783	-1.470667	0.637880
O	-0.075512	-2.269445	1.179549
C	-1.017747	-1.432905	1.080631
N	-0.774935	-0.118041	1.003072
C	0.549419	0.405411	0.962496
C	1.408242	0.212892	2.141536
H	-1.532164	0.551134	1.159728
H	2.647378	-2.784402	1.072018
H	2.282428	-1.142148	2.217966
H	2.260198	0.889389	2.153596
C	0.841778	1.502317	0.016448
O	1.831574	2.230984	0.147558
C	-0.479911	-0.236273	5.995835
C	0.519585	-1.134817	5.619101

C	1.125734	-1.024804	4.366478
C	0.748067	-0.013791	3.476832
C	-0.263944	0.882290	3.860155
C	-0.870391	0.771615	5.110841
H	-0.955267	-0.324416	6.968697
H	0.824876	-1.927999	6.295805
H	1.885907	-1.742968	4.069411
H	-0.587832	1.657974	3.172530
H	-1.652710	1.472109	5.389958
C	4.614805	-2.967944	-1.916960
H	3.283001	-4.477170	-1.121687
H	3.041163	-4.162897	-2.831895
H	4.616275	-2.167861	-2.665369
H	5.359306	-3.700839	-2.250474
H	6.120418	-2.069725	-0.639103
H	5.025953	-3.171855	0.214616

Sum of electronic and zero-point energy: -3953.500315
Sum of electronic and thermal free energies: -3953.611589
Frequency: -746.0648

Supplementary Table 5. **O1R^{TS}** representative 3

C	-2.593980	2.091887	-1.513973
C	-1.355695	2.936972	-1.862589
N	-3.071563	2.276642	-0.257890
C	-4.154363	1.645010	0.424625
C	-4.951045	2.359866	1.247286
C	-4.238377	0.137787	0.518705
O	-4.485905	-0.397317	1.603600
N	-4.006952	-0.583074	-0.613796
C	-4.112057	-2.009452	-0.702133
C	-4.990308	-2.622322	-1.524978
C	-6.072264	-2.084722	-2.345377
C	-3.037041	-2.845553	-0.059105
N	-0.293998	2.120647	-2.453643
C	-1.016179	-2.435667	1.318032
N	-2.381024	-2.228090	0.995634
O	-2.724680	-3.952532	-0.475577
C	-0.465565	-3.536722	1.882749
O	-3.053651	1.305719	-2.343449
C	-4.980807	3.806117	1.474821
C	-1.073992	-4.758757	2.381852
C	-0.203791	-5.800716	2.765118
C	-0.697194	-7.003804	3.260184
C	-2.076080	-7.184819	3.394241
C	-2.952465	-6.156591	3.031018
C	-2.462850	-4.957647	2.524685
C	-6.618480	-2.937234	-3.327592
C	-7.650285	-2.511678	-4.159209
C	-8.173817	-1.224646	-4.016626
C	-7.658940	-0.372105	-3.035487
C	-6.619634	-0.790848	-2.209813
C	-5.399789	4.260298	2.740999
C	-5.386333	5.616430	3.057794
C	-4.979193	6.553646	2.104240
C	-4.601503	6.122938	0.829056
C	-4.600406	4.765560	0.515205
H	-0.987085	3.504826	-1.006976
H	-1.657795	3.665272	-2.621152
H	-2.585508	2.958714	0.317596
H	-5.592227	1.763900	1.891203
H	-3.899198	-0.058551	-1.488201
H	-4.834756	-3.696091	-1.605536
H	-0.350828	2.060187	-3.465535
H	-2.881348	-1.476324	1.466414
H	0.618449	-3.502639	1.951423
H	0.868564	-5.657634	2.660482
H	-0.011027	-7.796232	3.544780
H	-2.467153	-8.121364	3.781725
H	-4.024396	-6.294118	3.139479
H	-3.150165	-4.169680	2.248963
H	-6.218724	-3.942259	-3.436495
H	-8.049929	-3.184357	-4.912481
H	-8.982930	-0.890161	-4.659604
H	-8.073436	0.624280	-2.910471
H	-6.251209	-0.119398	-1.444895
H	-5.721641	3.534937	3.483879
H	-5.702848	5.943729	4.043931
H	-4.975475	7.612483	2.346164
H	-4.317650	6.849424	0.072624
H	-4.334478	4.448879	-0.487319

C	3.636646	1.430277	-2.590396
C	3.456155	-1.155749	-2.705169
P	3.126068	-1.549135	-0.928503
P	3.602826	1.773039	-0.769401
C	7.112085	-2.912759	1.013812
C	5.967697	-2.698006	1.788911
C	4.778258	-2.298395	1.182025
C	4.713184	-2.120265	-0.212123
C	5.857716	-2.362752	-0.982696
C	7.053269	-2.747783	-0.370199
H	3.896923	-2.111633	1.789559
H	5.835112	-2.251169	-2.061391
C	0.365548	-5.275874	-1.039373
C	0.018325	-4.111743	-1.726837
C	0.860274	-3.001231	-1.703130
C	2.072668	-3.049572	-0.992473
C	2.427081	-4.228829	-0.317403
C	1.575137	-5.334943	-0.346574
H	0.563276	-2.092321	-2.213123
H	3.362942	-4.294063	0.226082
C	8.133260	2.111160	0.130433
C	7.501393	3.032972	-0.711127
C	6.132459	2.935834	-0.949347
C	5.378816	1.913421	-0.343193
C	6.015913	1.002148	0.506325
C	7.389777	1.099781	0.737983
H	5.648864	3.664731	-1.594660
H	5.446330	0.215791	0.983188
C	1.852155	6.023668	-0.183947
C	2.564049	5.388922	0.840364
C	3.121454	4.130171	0.626998
C	2.977917	3.491573	-0.616816
C	2.269505	4.134286	-1.641689
C	1.708655	5.396555	-1.422499
H	3.663893	3.636176	1.428422
H	2.129151	3.655245	-2.603221
H	-0.313245	-6.122673	-1.031352
H	8.042286	-3.213116	1.487577
H	1.418586	7.005609	-0.017009
H	9.201337	2.187809	0.313026
H	7.936612	-2.919571	-0.978390
H	6.003724	-2.834035	2.866032
H	1.856334	-6.241048	0.182661
H	-0.931321	-4.057483	-2.246709
H	7.870461	0.378957	1.392454
H	8.074921	3.828484	-1.177988
H	1.165610	5.888856	-2.224459
H	2.682918	5.874567	1.804435
Rh	2.258303	0.298521	0.333885
O	1.036427	-1.182501	1.357029
C	-0.121426	-1.341928	0.881916
N	-0.609986	-0.475002	-0.037207
C	0.103860	0.680500	-0.473910
C	0.367384	1.750744	0.439187
H	-1.523992	-0.667402	-0.432113
H	3.448707	0.140095	1.340546
H	1.768238	1.509984	1.331993
H	0.755520	2.628201	-0.064863
C	0.079728	0.875171	-1.959981
O	0.372959	-0.014959	-2.756515
C	-2.235308	3.047424	3.598875
C	-1.631159	3.957454	2.728432

C	-0.729697	3.503726	1.764999
C	-0.441697	2.129135	1.631185
C	-1.013336	1.234877	2.548916
C	-1.907914	1.693085	3.516621
H	-2.948663	3.396023	4.338395
H	-1.870946	5.014743	2.791647
H	-0.243939	4.219133	1.104567
H	-0.740992	0.189811	2.541723
H	-2.356551	0.981755	4.203264
C	4.313272	0.097319	-2.963612
H	3.908683	-2.036122	-3.174361
H	2.466579	-1.023058	-3.152953
H	4.525650	0.129880	-4.038752
H	5.286146	0.022686	-2.463925
H	2.604571	1.436991	-2.954884
H	4.171441	2.261589	-3.063371

Sum of electronic and zero-point energy: -3953.491184
Sum of electronic and thermal free energies: -3953.599166
Frequency: -673.3802

Supplementary Table 6. **O1R^{TS}** representative 4

C	-1.228150	-1.496995	-3.487653
C	-0.606387	-0.112826	-3.677418
N	-2.601316	-1.668730	-3.334817
C	-3.647360	-0.915314	-2.774434
C	-4.678879	-1.506859	-2.118361
C	-3.746389	0.541463	-3.096312
O	-3.402329	1.005318	-4.174735
N	-4.369738	1.366403	-2.159267
C	-4.359614	1.318469	-0.738075
C	-5.453907	1.527165	0.031168
C	-6.863327	1.666749	-0.323725
C	-3.022076	1.041587	-0.127467
N	-0.172156	0.433513	-2.400574
C	-1.499020	1.495162	1.776737
N	-2.641596	1.779056	0.967598
O	-2.266138	0.213936	-0.634538
C	-1.599029	1.330543	3.113783
O	-0.523287	-2.500131	-3.519375
C	-4.886676	-2.911128	-1.754734
C	-2.829179	1.269507	3.906671
C	-4.004627	0.651568	3.431517
C	-5.153352	0.613683	4.218300
C	-5.153587	1.194249	5.490942
C	-3.988965	1.788923	5.982951
C	-2.833453	1.814760	5.203537
C	-7.384572	1.504518	-1.625842
C	-8.753728	1.609966	-1.855501
C	-9.631250	1.890214	-0.803817
C	-9.131742	2.055295	0.490607
C	-7.765423	1.939531	0.726815
C	-3.855607	-3.855076	-1.548751
C	-4.151386	-5.167233	-1.181598
C	-5.475555	-5.575444	-1.012203
C	-6.508478	-4.651697	-1.195864
C	-6.216398	-3.339316	-1.554351
H	-1.295343	0.565433	-4.183426
H	0.279659	-0.258553	-4.296839
H	-2.804360	-2.662706	-3.363967
H	-5.513344	-0.856491	-1.875560
H	-4.570676	2.279041	-2.559100
H	-5.275862	1.561671	1.104351
H	-0.823747	0.372387	-1.625211
H	-3.323832	2.410070	1.370410
H	-0.657825	1.274975	3.653198
H	-3.992168	0.150189	2.470618
H	-6.044640	0.116514	3.845047
H	-6.050925	1.167152	6.102111
H	-3.978646	2.225849	6.977060
H	-1.927179	2.271637	5.592740
H	-6.721315	1.284423	-2.452620
H	-9.138039	1.477468	-2.862672
H	-10.697123	1.978806	-0.992409
H	-9.806788	2.270895	1.313558
H	-7.382343	2.059949	1.737930
H	-2.813120	-3.564599	-1.624638
H	-3.339252	-5.870420	-1.020665
H	-5.700783	-6.599946	-0.730999
H	-7.542377	-4.955064	-1.057810
H	-7.025633	-2.626453	-1.693443
C	3.815402	-1.189756	-2.206173

C	1.729722	-2.389424	-1.209635
P	1.816417	-1.715225	0.505315
P	4.375007	-0.127682	-0.798165
C	4.362516	-4.831811	2.833694
C	4.448898	-3.478179	3.157436
C	3.693729	-2.539099	2.452768
C	2.843412	-2.941536	1.415779
C	2.747908	-4.310478	1.109551
C	3.506681	-5.246762	1.809695
H	3.777824	-1.486767	2.698747
H	2.080223	-4.655221	0.326033
C	-2.308520	-2.251060	2.541512
C	-1.154398	-2.016326	3.297939
C	0.073679	-1.864540	2.662860
C	0.165906	-1.950643	1.261597
C	-0.992654	-2.172506	0.509780
C	-2.226720	-2.322002	1.153132
H	0.967414	-1.687712	3.253655
H	-0.948776	-2.223260	-0.573322
C	7.793052	-2.393671	1.382315
C	7.178482	-1.294222	1.985855
C	6.134833	-0.634326	1.340306
C	5.703838	-1.049345	0.070290
C	6.340397	-2.142664	-0.537029
C	7.370417	-2.816306	0.121860
H	5.636821	0.193081	1.835697
H	6.044190	-2.482181	-1.523234
C	6.445403	3.571956	-2.681014
C	6.672039	3.228791	-1.344693
C	6.068863	2.096841	-0.802130
C	5.232153	1.289556	-1.591209
C	5.004518	1.639548	-2.931000
C	5.613909	2.776431	-3.468977
H	6.253619	1.844183	0.236672
H	4.329775	1.065092	-3.551444
H	-3.266722	-2.372718	3.038435
H	4.956275	-5.562095	3.376061
H	6.914802	4.455939	-3.103092
H	8.596560	-2.917675	1.891731
H	3.428264	-6.300335	1.556897
H	5.113312	-3.146100	3.949671
H	-3.119511	-2.490824	0.561491
H	-1.214775	-1.954970	4.380865
H	7.843193	-3.669653	-0.355485
H	7.502288	-0.957016	2.966465
H	5.428767	3.038229	-4.506699
H	7.318993	3.842525	-0.724666
Rh	2.611032	0.542332	0.497073
O	0.838102	1.029247	1.766740
C	-0.157042	1.468852	1.139475
N	-0.032564	1.913776	-0.123826
C	1.168248	1.740454	-0.893369
C	2.267007	2.609926	-0.661922
H	-0.840351	2.325037	-0.573199
H	3.533765	0.212735	1.717421
H	3.303265	2.026279	0.576056
H	2.998467	2.574458	-1.463916
C	1.010326	1.085211	-2.228020
O	1.885696	1.149815	-3.098857
C	1.897291	6.547244	1.012053
C	1.608059	5.442710	1.817566
C	1.737580	4.148914	1.313477

C	2.155839	3.946397	-0.008858
C	2.472646	5.058379	-0.804844
C	2.334308	6.351297	-0.299602
H	1.798823	7.553417	1.409387
H	1.293500	5.588383	2.847463
H	1.560148	3.292814	1.954597
H	2.824318	4.907271	-1.822465
H	2.578655	7.203280	-0.927619
C	3.116308	-2.520829	-1.868683
H	1.224315	-3.360045	-1.208295
H	1.099760	-1.719192	-1.798548
H	2.966706	-3.044308	-2.820020
H	3.763497	-3.159934	-1.258410
H	3.130670	-0.557407	-2.778889
H	4.689497	-1.373403	-2.841137

Sum of electronic and zero-point energy: -3953.485542
Sum of electronic and thermal free energies: -3953.596915
Frequency: -616.6241

Supplementary Table 7. **O2R^{TS}** representative 1

C	4.008790	-1.145722	2.279532
C	2.752575	1.139745	2.372174
P	2.703394	1.509706	0.556421
P	4.105894	-1.434366	0.454150
C	6.607020	3.865652	-0.310458
C	6.034922	3.063175	-1.297945
C	4.873111	2.339269	-1.027307
C	4.270456	2.407420	0.235189
C	4.840774	3.236497	1.216809
C	6.005307	3.954128	0.947426
H	4.437258	1.710457	-1.795653
H	4.378791	3.332783	2.194378
C	-0.638453	4.593970	-0.295489
C	-0.934113	3.394498	0.356963
C	0.087438	2.498271	0.665041
C	1.412463	2.782070	0.303947
C	1.704383	3.987343	-0.353312
C	0.680359	4.892109	-0.641874
H	-0.155837	1.562356	1.154657
H	2.722162	4.221079	-0.645416
C	8.284249	0.011045	-0.969046
C	8.027402	-0.133417	0.394508
C	6.773371	-0.563594	0.832444
C	5.751267	-0.829383	-0.091080
C	6.018709	-0.674874	-1.461086
C	7.279081	-0.271000	-1.896852
H	6.607988	-0.687922	1.896867
H	5.231750	-0.855495	-2.186770
C	4.312030	-6.047878	-0.044630
C	4.973310	-5.208817	-0.944319
C	4.927082	-3.825467	-0.778319
C	4.215410	-3.261974	0.293568
C	3.548395	-4.110266	1.194397
C	3.602808	-5.494977	1.022165
H	5.459915	-3.192432	-1.478944
H	2.958568	-3.704554	2.006154
H	-1.439310	5.283339	-0.546804
H	7.515712	4.422998	-0.519142
H	4.349689	-7.125454	-0.175475
H	9.262198	0.341149	-1.307245
H	6.439752	4.584705	1.717836
H	6.496605	2.989184	-2.277918
H	0.917456	5.825152	-1.145899
H	-1.960233	3.135307	0.582883
H	7.470939	-0.163547	-2.960693
H	8.803769	0.082921	1.122568
H	3.082937	-6.139168	1.725462
H	5.531378	-5.629864	-1.775594
Rh	2.322991	-0.486344	-0.637115
O	0.662069	0.528468	-1.690524
C	-0.493998	0.214797	-1.308000
N	-0.699457	-0.622972	-0.274036
C	0.352281	-1.375665	0.320685
C	0.984855	-2.380613	-0.535810
H	-1.632289	-0.992962	-0.153025
H	3.335134	-0.004096	-1.714783
H	2.167287	-1.887727	-1.518730
H	1.534251	-3.144460	0.004939
C	-1.866146	-3.562031	-3.542744
C	-1.894604	-4.111456	-2.256334

C	-0.904037	-3.777329	-1.332657
C	0.112079	-2.869744	-1.672578
C	0.148818	-2.345469	-2.968754
C	-0.833710	-2.692691	-3.900738
H	-2.638688	-3.819869	-4.262167
H	-2.702606	-4.772925	-1.959584
H	-0.955885	-4.171989	-0.324815
H	0.924092	-1.634712	-3.237790
H	-0.794133	-2.271758	-4.901672
C	3.986598	0.309961	2.782616
H	2.722445	2.080005	2.933193
H	1.829173	0.597655	2.599463
H	3.999880	0.261073	3.878497
H	4.899137	0.838820	2.489630
H	3.081502	-1.637436	2.582359
H	4.836508	-1.694559	2.742062
C	-4.910219	-2.862273	-0.270080
C	-4.878153	-2.853019	1.266028
N	-4.907809	-1.664205	-0.970924
C	-5.026176	-0.331886	-0.480924
C	-6.066029	0.144676	0.238680
C	-3.873474	0.599890	-0.741075
O	-3.795926	1.713148	-0.232108
N	-2.922515	0.110692	-1.617040
C	-1.710620	0.792100	-1.919885
C	-1.602858	1.971003	-2.572500
C	-2.608528	2.826951	-3.184159
N	-4.110938	-1.800506	1.909207
C	-2.762309	-1.763212	1.753618
C	-1.974771	-0.633757	2.354672
N	-0.594339	-0.922500	2.596114
C	0.328564	-1.594771	1.776805
O	1.168793	-2.301377	2.342786
C	-2.554121	0.549062	2.665452
O	-2.192951	-2.634992	1.086148
O	-4.990250	-3.920290	-0.868297
C	-7.308345	-0.497463	0.662366
C	-2.008058	1.769227	3.249801
C	-3.927038	2.427484	-3.482645
C	-4.818476	3.317096	-4.072492
C	-4.422139	4.625704	-4.368619
C	-3.117678	5.036429	-4.085137
C	-2.219255	4.142953	-3.508408
C	-7.886482	-1.615248	0.023169
C	-9.071214	-2.167795	0.501237
C	-9.703717	-1.626004	1.625464
C	-9.152594	-0.511617	2.261490
C	-7.974276	0.051955	1.777328
C	-2.796291	2.934389	3.147869
C	-2.341686	4.155470	3.636122
C	-1.091502	4.237219	4.253571
C	-0.306588	3.087951	4.382995
C	-0.756470	1.866124	3.891657
H	-4.480620	-3.832496	1.540758
H	-5.911608	-2.783238	1.616096
H	-5.016705	-1.823629	-1.969004
H	-5.919173	1.162680	0.594635
H	-2.992549	-0.862720	-1.896016
H	-0.588900	2.361831	-2.596697
H	-4.587308	-1.138362	2.501168
H	-0.404556	-1.205799	3.554713
H	-3.600909	0.644051	2.388208

H	-4.244365	1.413917	-3.271932
H	-5.828704	2.991319	-4.303492
H	-5.125302	5.317558	-4.823412
H	-2.799831	6.048015	-4.320630
H	-1.203172	4.460518	-3.289851
H	-7.418832	-2.041720	-0.856204
H	-9.505351	-3.023628	-0.007180
H	-10.625353	-2.065262	1.995741
H	-9.644535	-0.076941	3.126660
H	-7.556232	0.929073	2.265887
H	-3.757809	2.878480	2.643597
H	-2.959494	5.042526	3.532876
H	-0.733454	5.188277	4.636797
H	0.660417	3.143542	4.875272
H	-0.134013	0.988749	4.000319

Sum of electronic and zero-point energy: -3953.496025
Sum of electronic and thermal free energies: -3953.604179
Frequency: -795.1597

Supplementary Table 8. **O2R^{TS}** representative 2

C	4.278507	-2.961796	-1.329401
C	2.066494	-4.074049	-2.096210
P	0.795895	-3.028806	-1.216345
P	3.737956	-1.358261	-0.571659
C	-1.526668	-6.519838	0.774012
C	-0.574836	-5.802953	1.504048
C	0.087870	-4.721175	0.921893
C	-0.194439	-4.348561	-0.402115
C	-1.158874	-5.067810	-1.126673
C	-1.822824	-6.145205	-0.538631
H	0.810618	-4.157623	1.500800
H	-1.399274	-4.783670	-2.146225
C	-1.956064	-1.040025	-4.352398
C	-2.437614	-1.333945	-3.074295
C	-1.616615	-1.979531	-2.153491
C	-0.302841	-2.340327	-2.499748
C	0.167912	-2.052108	-3.789566
C	-0.658067	-1.405989	-4.710272
H	-2.018247	-2.215167	-1.173435
H	1.175909	-2.325576	-4.086530
C	6.824526	-0.243137	2.695019
C	6.622575	-1.583831	2.362040
C	5.726384	-1.929727	1.348975
C	5.026293	-0.932997	0.654829
C	5.233841	0.413581	0.994583
C	6.130163	0.754952	2.007129
H	5.575529	-2.979137	1.117009
H	4.713982	1.202309	0.461564
C	4.252740	1.429288	-4.236973
C	5.357006	1.155963	-3.422450
C	5.217249	0.350925	-2.291539
C	3.963489	-0.194419	-1.968866
C	2.868348	0.061122	-2.804863
C	3.008470	0.876219	-3.928967
H	6.078192	0.158240	-1.658888
H	1.898037	-0.363000	-2.582247
H	-2.593239	-0.531116	-5.070083
H	-2.039274	-7.363474	1.228130
H	4.368003	2.063801	-5.111158
H	7.521205	0.022014	3.484988
H	-2.568934	-6.691815	-1.107998
H	-0.350085	-6.081025	2.529844
H	-0.284535	-1.191479	-5.707826
H	-3.445435	-1.062434	-2.776248
H	6.283483	1.802347	2.247464
H	7.161351	-2.364648	2.890865
H	2.139786	1.071424	-4.551076
H	6.330083	1.572162	-3.668657
Rh	1.663957	-1.447548	0.356228
O	-0.211986	-1.735024	1.410335
C	-1.146648	-0.954409	1.086892
N	-0.883370	0.178639	0.395369
C	0.431444	0.606661	0.056157
C	1.408708	0.872480	1.059552
H	-1.659502	0.666584	-0.034160
H	2.352867	-2.657349	1.095012
H	2.226049	-0.500486	1.564768
H	2.300902	1.325328	0.636830
C	0.917906	2.428368	5.043153
C	2.187714	2.212720	4.497072

C	2.318899	1.661057	3.225547
C	1.185254	1.306625	2.471461
C	-0.083371	1.512327	3.035877
C	-0.215111	2.079029	4.306341
H	0.814923	2.861725	6.033720
H	3.076874	2.479661	5.061260
H	3.308328	1.502989	2.804383
H	-0.980337	1.272816	2.485137
H	-1.212693	2.242382	4.704045
C	3.399649	-3.426869	-2.506168
H	1.572325	-4.513307	-2.970304
H	2.267650	-4.898931	-1.402784
H	3.243253	-2.599405	-3.206717
H	3.967907	-4.183108	-3.061181
H	5.310035	-2.811385	-1.667711
H	4.288125	-3.725124	-0.544225
C	-3.238924	2.965802	1.507744
C	-2.408710	4.262280	1.513881
N	-3.723503	2.604351	0.289883
C	-4.610902	1.537193	-0.075767
C	-5.684506	1.767717	-0.862620
C	-4.202830	0.102155	0.150973
O	-4.521431	-0.798201	-0.618137
N	-3.409876	-0.102651	1.255350
C	-2.559633	-1.228007	1.404586
C	-2.938944	-2.496645	1.695662
C	-4.252353	-3.044215	1.993659
N	-0.997632	4.019221	1.239863
C	-0.590956	3.727225	-0.031780
C	0.873532	3.458496	-0.245966
N	1.146921	2.518528	-1.294670
C	0.461532	1.293522	-1.273188
O	-0.090236	0.848762	-2.267682
C	1.821488	4.116521	0.451914
O	-1.381542	3.675292	-0.978630
O	-3.390158	2.320073	2.551075
C	-6.259075	3.024351	-1.339098
C	3.280914	4.036831	0.381031
C	-5.405014	-2.268332	2.240389
C	-6.617342	-2.883114	2.531363
C	-6.713516	-4.278580	2.573223
C	-5.581618	-5.060860	2.333585
C	-4.363260	-4.449118	2.054248
C	-6.063886	4.275165	-0.716483
C	-6.653291	5.424914	-1.234752
C	-7.442299	5.357613	-2.386852
C	-7.657027	4.125115	-3.008366
C	-7.081604	2.971396	-2.483004
C	4.000925	3.538801	-0.724189
C	5.394902	3.547447	-0.714934
C	6.098218	4.028117	0.392678
C	5.397284	4.510018	1.501965
C	4.005324	4.522925	1.489624
H	-2.497704	4.690368	2.513344
H	-2.784446	4.979855	0.779292
H	-3.397916	3.181396	-0.484437
H	-6.160738	0.862435	-1.232627
H	-3.349254	0.661409	1.937335
H	-2.127405	-3.220849	1.684424
H	-0.417464	3.718476	2.014042
H	1.087937	2.919066	-2.228923
H	1.451948	4.814090	1.200680

H	-5.342999	-1.188500	2.219933
H	-7.494935	-2.273184	2.725267
H	-7.666089	-4.751454	2.794997
H	-5.648543	-6.144475	2.368834
H	-3.481853	-5.055515	1.868705
H	-5.481879	4.339601	0.195018
H	-6.502801	6.377566	-0.734773
H	-7.895924	6.258423	-2.789979
H	-8.279316	4.062291	-3.896262
H	-7.258775	2.012737	-2.963925
H	3.475065	3.154436	-1.588922
H	5.931324	3.171897	-1.579535
H	7.184445	4.033184	0.388681
H	5.934159	4.890151	2.366412
H	3.463139	4.909847	2.348702

Sum of electronic and zero-point energy: -3953.49836
Sum of electronic and thermal free energies: -3953.605536
Frequency: -661.2544

Supplementary Table 9. **O2R^{TS}** representative 3

C	-3.960643	-2.193496	-2.828120
C	-1.468829	-2.360277	-3.648932
P	-0.538376	-1.573354	-2.247240
P	-3.712745	-1.451835	-1.143258
C	3.028679	0.661803	-4.213940
C	1.709241	1.043608	-4.478814
C	0.646653	0.347217	-3.907788
C	0.888295	-0.757497	-3.073127
C	2.212149	-1.155318	-2.837011
C	3.277846	-0.446226	-3.401210
H	-0.370826	0.686962	-4.073550
H	2.418881	-2.022120	-2.218892
C	1.361345	-4.944348	0.299875
C	1.333795	-3.623162	0.760459
C	0.769798	-2.626124	-0.035564
C	0.225786	-2.935479	-1.294535
C	0.267337	-4.260675	-1.749119
C	0.831817	-5.260133	-0.952274
H	0.721614	-1.607739	0.340456
H	-0.141767	-4.530024	-2.716973
C	-7.389612	1.030479	0.140544
C	-6.622218	0.350861	1.090454
C	-5.549540	-0.446202	0.687743
C	-5.238469	-0.563184	-0.677887
C	-6.006370	0.124644	-1.627683
C	-7.082314	0.912899	-1.217770
H	-4.944227	-0.962612	1.426476
H	-5.765951	0.060500	-2.684787
C	-3.788496	-5.412311	1.252698
C	-4.954422	-4.908076	0.668110
C	-4.925811	-3.692484	-0.013415
C	-3.726368	-2.964458	-0.109808
C	-2.569542	-3.469632	0.489014
C	-2.597517	-4.691683	1.161805
H	-5.839457	-3.305940	-0.456903
H	-1.651746	-2.906876	0.445640
H	1.794813	-5.723633	0.920246
H	3.852444	1.227942	-4.638451
H	-3.813604	-6.361160	1.781035
H	-8.225971	1.647431	0.456516
H	4.297717	-0.770439	-3.209640
H	1.512856	1.904517	-5.110523
H	0.850085	-6.285198	-1.311328
H	1.737728	-3.363121	1.733342
H	-7.678717	1.436894	-1.959043
H	-6.859195	0.437630	2.147129
H	-1.686172	-5.069787	1.615626
H	-5.886520	-5.460585	0.743864
Rh	-1.979671	0.034582	-1.223048
O	-0.494121	1.566026	-1.527215
C	0.347973	1.676158	-0.599854
N	0.071186	1.257135	0.648459
C	-1.231505	0.724204	0.960752
C	-2.423086	1.469980	0.730221
H	0.739731	1.479024	1.386921
H	-2.550431	0.254003	-2.670488
H	-3.027132	1.203885	-0.791687
H	-3.277226	0.976663	1.184993
C	-3.235237	5.680353	0.459564
C	-4.263191	4.732498	0.486934

C	-3.956747	3.377786	0.550580
C	-2.619493	2.936678	0.589848
C	-1.597454	3.897027	0.567976
C	-1.907115	5.256207	0.504416
H	-3.469614	6.739805	0.409071
H	-5.301553	5.050334	0.460916
H	-4.758394	2.642794	0.570301
H	-0.559820	3.606988	0.649716
H	-1.101861	5.985502	0.500060
C	-2.779229	-3.085536	-3.272906
H	-1.679385	-1.536326	-4.340306
H	-0.798462	-3.047836	-4.176021
H	-2.585175	-3.844804	-2.505916
H	-3.108634	-3.633561	-4.163681
H	-4.117327	-1.382436	-3.545983
H	-4.872125	-2.800562	-2.791171
C	5.506204	0.070137	3.219895
C	4.380368	-0.808554	3.757873
N	5.274659	0.711196	2.008875
C	4.326589	0.361794	1.018121
C	4.284540	-0.833598	0.377986
C	3.231623	1.361358	0.794832
O	2.710543	2.003450	1.718071
N	2.821720	1.496783	-0.496699
C	1.688437	2.237054	-0.935666
C	1.764431	3.207098	-1.870099
C	2.935801	3.807766	-2.503674
N	3.090680	-0.140874	3.652298
C	1.948733	-0.850630	3.482053
C	0.671440	-0.069331	3.307437
N	-0.306831	-0.841876	2.645777
C	-1.387733	-0.422408	1.891144
O	-2.463150	-1.018750	1.989095
C	0.490880	1.167323	3.828521
O	1.912689	-2.084927	3.477851
O	6.547480	0.238190	3.825815
C	5.189870	-1.981052	0.422233
C	-0.723303	1.992018	3.914245
C	4.240987	3.762865	-1.972488
C	5.306804	4.328640	-2.667325
C	5.098334	4.944948	-3.904985
C	3.807770	5.014751	-4.435971
C	2.738172	4.462829	-3.736251
C	6.507497	-1.947730	0.927652
C	7.300026	-3.091608	0.901956
C	6.803449	-4.290183	0.379169
C	5.505152	-4.336910	-0.133175
C	4.712111	-3.193329	-0.118195
C	-2.007502	1.456925	4.137570
C	-3.114886	2.296625	4.227458
C	-2.967183	3.681721	4.105166
C	-1.696565	4.225693	3.913725
C	-0.584919	3.389278	3.826936
H	4.634260	-1.035172	4.796767
H	4.336839	-1.756742	3.208846
H	5.979478	1.406235	1.784802
H	3.406896	-0.994667	-0.244408
H	3.367394	1.057954	-1.231733
H	0.804856	3.543433	-2.254651
H	3.082432	0.837878	3.379507
H	-0.399509	-1.790303	2.998452
H	1.377787	1.642459	4.236386

H	4.414579	3.310937	-1.003552
H	6.304813	4.294962	-2.239788
H	5.934430	5.379920	-4.444652
H	3.634986	5.506491	-5.388759
H	1.733824	4.525636	-4.147837
H	6.918743	-1.031973	1.332556
H	8.311816	-3.047396	1.293825
H	7.427219	-5.179271	0.369082
H	5.110092	-5.261246	-0.544736
H	3.699749	-3.240001	-0.507605
H	-2.137748	0.386694	4.250949
H	-4.097537	1.866755	4.400852
H	-3.835172	4.331330	4.164408
H	-1.571591	5.300190	3.822031
H	0.403629	3.815412	3.672722

Sum of electronic and zero-point energy: -3953.493909
Sum of electronic and thermal free energies: -3953.600527
Frequency: -634.7129

Supplementary Table 10. **O2R^{TS}** representative 4

C	4.919964	1.849363	-1.878928
C	2.708568	2.895947	-2.860448
P	1.413628	2.160766	-1.752546
P	4.236072	0.868870	-0.455130
C	-2.404973	1.521469	-4.318036
C	-1.162363	1.048895	-4.753674
C	-0.018002	1.271000	-3.991532
C	-0.095342	1.994646	-2.789176
C	-1.344670	2.469089	-2.359448
C	-2.494385	2.233546	-3.121118
H	0.929782	0.853464	-4.318128
H	-1.442881	3.035970	-1.440159
C	0.151148	5.369164	1.347000
C	-0.145247	4.015582	1.533720
C	0.270628	3.082867	0.586067
C	0.968707	3.479630	-0.563196
C	1.257290	4.838060	-0.745337
C	0.855361	5.774367	0.211385
H	0.098199	2.024888	0.749773
H	1.793555	5.180784	-1.624024
C	6.860058	-2.817300	0.474027
C	6.145734	-2.173529	1.488424
C	5.405642	-1.024949	1.205210
C	5.375329	-0.515466	-0.104536
C	6.087042	-1.167127	-1.120374
C	6.831954	-2.310711	-0.828013
H	4.841212	-0.531677	1.991769
H	6.057645	-0.797340	-2.141028
C	5.077657	3.990297	2.859738
C	3.757954	3.681244	2.531495
C	3.486050	2.703819	1.573139
C	4.528530	2.038522	0.925163
C	5.858681	2.347752	1.264132
C	6.128573	3.316507	2.228690
H	2.465739	2.447717	1.344622
H	6.682538	1.824324	0.786407
H	-0.162564	6.103282	2.083184
H	-3.294971	1.325710	-4.908884
H	5.291469	4.748199	3.608045
H	7.438312	-3.709309	0.697193
H	-3.443930	2.624309	-2.764299
H	-1.091804	0.487429	-5.680533
H	1.090381	6.824439	0.064655
H	-0.688404	3.684794	2.414854
H	7.388269	-2.806824	-1.618024
H	6.165296	-2.563665	2.502110
H	7.158102	3.545377	2.488434
H	2.933360	4.194195	3.018059
Rh	2.203110	0.014935	-1.062274
O	0.480052	-0.898614	-1.952201
C	-0.514267	-1.039135	-1.195572
N	-0.388990	-0.998870	0.147295
C	0.915092	-0.910643	0.746865
C	1.923400	-1.882675	0.491727
H	-1.187727	-1.333842	0.692491
H	2.929281	-0.030852	-2.452169
H	2.821813	-1.477286	-0.856395
H	2.775929	-1.752575	1.152410
C	1.702888	-6.004075	-0.702335
C	0.525275	-5.258466	-0.642697

C	0.554912	-3.908911	-0.287924
C	1.774420	-3.283903	0.015052
C	2.955786	-4.048553	-0.041409
C	2.922782	-5.392648	-0.395659
H	1.672185	-7.053581	-0.980855
H	-0.429009	-5.727578	-0.864949
H	-0.383326	-3.378024	-0.209839
H	3.905797	-3.575614	0.196695
H	3.845830	-5.964221	-0.430902
C	4.089329	3.114541	-2.200098
H	2.801738	2.204575	-3.704702
H	2.337185	3.842402	-3.267905
H	3.981512	3.722221	-1.293224
H	4.683989	3.717381	-2.896592
H	5.940096	2.151312	-1.617094
H	4.971104	1.196096	-2.755549
C	-4.289744	2.233565	0.230238
C	-3.653424	2.314793	1.628216
N	-4.865900	1.033431	-0.135629
C	-4.664639	-0.216875	0.525563
C	-5.360161	-0.628956	1.608446
C	-3.504110	-1.026877	0.058661
O	-3.037308	-1.991318	0.681260
N	-2.953051	-0.603482	-1.120302
C	-1.860382	-1.208904	-1.793663
C	-1.954572	-1.712148	-3.044032
C	-3.122183	-1.881975	-3.904336
N	-2.522344	1.430027	1.839151
C	-2.492418	0.469479	2.820185
C	-1.196804	-0.287634	2.926590
N	-0.004386	0.436391	2.605469
C	1.120274	-0.077163	1.950157
O	2.243074	0.194885	2.375999
C	-1.264557	-1.593644	3.263806
O	-3.461029	0.207464	3.525185
O	-4.326903	3.206264	-0.510471
C	-6.473342	0.003339	2.306354
C	-0.187903	-2.579897	3.400750
C	-4.460609	-1.845098	-3.459939
C	-5.510065	-1.987343	-4.363796
C	-5.253888	-2.162646	-5.727151
C	-3.933959	-2.218515	-6.181865
C	-2.882792	-2.090864	-5.278326
C	-6.705449	-0.391075	3.639387
C	-7.734295	0.178153	4.383585
C	-8.564323	1.141273	3.804016
C	-8.355798	1.533605	2.478169
C	-7.319147	0.975920	1.734975
C	1.074429	-2.282195	3.948902
C	2.064974	-3.259993	4.005775
C	1.814980	-4.548760	3.524110
C	0.557071	-4.864153	3.006762
C	-0.438863	-3.891486	2.955617
H	-4.401587	2.063994	2.385936
H	-3.350120	3.358929	1.748138
H	-5.371167	1.073240	-1.015824
H	-4.992106	-1.552218	2.046766
H	-3.345567	0.210478	-1.578009
H	-1.004238	-1.984808	-3.494747
H	-1.688132	1.579154	1.292011
H	0.294981	1.089962	3.326048
H	-2.276925	-1.976555	3.356761

H	-4.678096	-1.734448	-2.405226
H	-6.534552	-1.968266	-4.002943
H	-6.077332	-2.267276	-6.427553
H	-3.725363	-2.369453	-7.236949
H	-1.856887	-2.142245	-5.634322
H	-6.048179	-1.126848	4.093030
H	-7.890978	-0.129851	5.413119
H	-9.372635	1.582051	4.380537
H	-9.005526	2.274824	2.021770
H	-7.175270	1.282933	0.706448
H	1.280333	-1.289540	4.331943
H	3.033968	-3.014771	4.431423
H	2.593773	-5.304923	3.559227
H	0.357097	-5.861816	2.628676
H	-1.413869	-4.130388	2.538810

Sum of electronic and zero-point energy: -3953.49619
Sum of electronic and thermal free energies: -3953.60424
Frequency: -628.5372

Supplementary Table 11. **O2R^{TS}** representative 5

C	4.497012	0.218116	-2.323972
C	2.895959	-1.719616	-2.946023
P	2.142774	-2.134618	-1.308022
P	4.287496	0.345899	-0.486393
C	4.258454	-5.911351	0.348842
C	4.480983	-5.541015	-0.977998
C	3.837772	-4.421690	-1.512827
C	2.978769	-3.652709	-0.716884
C	2.754311	-4.035552	0.618570
C	3.385542	-5.161709	1.144072
H	4.020337	-4.157401	-2.549106
H	2.095263	-3.439852	1.244625
C	-2.221021	-3.385421	-2.260526
C	-1.341706	-4.319829	-1.713943
C	-0.016666	-3.970661	-1.449325
C	0.444755	-2.676504	-1.737632
C	-0.442816	-1.748840	-2.308276
C	-1.766265	-2.101511	-2.567727
H	0.652363	-4.704516	-1.013018
H	-0.113957	-0.738696	-2.533164
C	8.205288	-1.818386	0.747218
C	6.984362	-2.484979	0.854871
C	5.794439	-1.827054	0.537426
C	5.816116	-0.496548	0.098262
C	7.050219	0.167778	-0.012369
C	8.235443	-0.489369	0.315537
H	4.853823	-2.353648	0.635556
H	7.086680	1.201715	-0.343841
C	5.084364	4.773063	0.645266
C	4.880746	3.802698	1.631013
C	4.642441	2.478920	1.267460
C	4.589595	2.110647	-0.088035
C	4.779201	3.090735	-1.071463
C	5.038887	4.413389	-0.702036
H	4.491783	1.727868	2.038097
H	4.727979	2.838077	-2.124120
H	-3.262305	-3.643029	-2.416062
H	4.760279	-6.781478	0.762331
H	5.280648	5.803471	0.927883
H	9.130165	-2.328381	1.001396
H	3.204800	-5.448098	2.176218
H	5.154685	-6.121970	-1.601242
H	-2.448004	-1.357039	-2.963654
H	-1.692464	-5.318331	-1.469952
H	9.182158	0.037518	0.236953
H	6.947916	-3.517916	1.188964
H	5.204991	5.161298	-1.472781
H	4.913240	4.074349	2.681998
Rh	2.285923	-0.406394	0.320124
O	0.488912	-1.242556	1.189267
C	-0.615702	-0.806705	0.759598
N	-0.682957	0.352991	0.056952
C	0.515117	1.079055	-0.247457
C	1.280985	1.707959	0.785628
H	-1.482954	0.444053	-0.585771
H	3.197156	-1.293979	1.224809
H	2.375098	0.724633	1.505045
H	2.006297	2.405173	0.376049
C	-0.314596	3.250756	4.468008
C	0.366881	4.067882	3.564366

C	0.898522	3.526525	2.395055
C	0.738127	2.163256	2.100225
C	0.082102	1.340668	3.028568
C	-0.443226	1.885573	4.200195
H	-0.725778	3.669421	5.382172
H	0.490334	5.128019	3.766599
H	1.430942	4.166772	1.698774
H	0.037518	0.271606	2.869332
H	-0.941779	1.235684	4.914182
C	4.346897	-1.207082	-2.885322
H	2.820755	-2.600281	-3.593335
H	2.247548	-0.950261	-3.380822
H	4.736157	-1.196469	-3.910468
H	4.983137	-1.905725	-2.328320
H	3.764223	0.884272	-2.782742
H	5.504452	0.590447	-2.542644
C	-5.123487	2.128401	0.127512
C	-5.234263	2.123902	-1.406211
N	-5.197526	0.925976	0.788488
C	-5.363555	-0.370923	0.216568
C	-6.492975	-0.787855	-0.396982
C	-4.190127	-1.309434	0.246728
O	-4.245642	-2.434449	-0.227259
N	-3.073216	-0.828008	0.916277
C	-1.864002	-1.536964	1.070392
C	-1.734126	-2.836112	1.449440
C	-2.697754	-3.814132	1.926582
N	-4.004279	2.715580	-1.924309
C	-2.853863	2.006559	-1.780245
C	-1.573426	2.764149	-1.656266
N	-0.441713	2.141396	-2.259994
C	0.685050	1.660867	-1.610400
O	1.782223	1.756879	-2.163279
C	-1.539661	3.870827	-0.872230
O	-2.865142	0.768414	-1.685576
O	-4.907736	3.176063	0.723427
C	-7.769182	-0.106479	-0.607183
C	-0.462717	4.789338	-0.515859
C	-3.937326	-3.486058	2.510523
C	-4.781097	-4.482465	2.989003
C	-4.417809	-5.828589	2.880736
C	-3.189135	-6.172297	2.310996
C	-2.333923	-5.174222	1.853769
C	-8.225821	0.992749	0.151537
C	-9.455663	1.582376	-0.126524
C	-10.255378	1.097586	-1.166575
C	-9.824775	0.002641	-1.918805
C	-8.600526	-0.597580	-1.634584
C	0.812116	4.819230	-1.119791
C	1.756929	5.758101	-0.715425
C	1.459828	6.683539	0.290000
C	0.197772	6.674912	0.888174
C	-0.750789	5.739015	0.486922
H	-6.084201	2.745689	-1.693230
H	-5.357655	1.131574	-1.832143
H	-5.121711	1.014778	1.798275
H	-6.405094	-1.774606	-0.846182
H	-3.041912	0.170089	1.080158
H	-0.717238	-3.205987	1.371158
H	-3.940877	3.724386	-1.897240
H	-0.249772	2.384454	-3.227593
H	-2.484411	4.107862	-0.383426

H	-4.223772	-2.446010	2.613372
H	-5.729022	-4.211154	3.444985
H	-5.085610	-6.603824	3.245500
H	-2.896031	-7.215346	2.232968
H	-1.372324	-5.440417	1.421528
H	-7.631794	1.370866	0.974383
H	-9.795314	2.421127	0.474362
H	-11.212156	1.564816	-1.381162
H	-10.445057	-0.388209	-2.720039
H	-8.272492	-1.455480	-2.216112
H	1.074638	4.122808	-1.905135
H	2.733605	5.762601	-1.185388
H	2.206339	7.409507	0.599342
H	-0.046697	7.393511	1.664812
H	-1.728219	5.728390	0.961966

Sum of electronic and zero-point energy: -3953.499481
Sum of electronic and thermal free energies: -3953.607416
Frequency: -703.0665

Supplementary Table 12. **O3R^{TS}** representative 1

C	-2.297469	-2.583110	-1.953973
C	-1.157600	-0.480731	-2.959362
P	-1.866677	0.812378	-1.840001
P	-3.285862	-1.928381	-0.536517
C	-5.356319	2.328685	-4.503580
C	-5.633689	1.806017	-3.241166
C	-4.591274	1.376667	-2.415884
C	-3.264231	1.454421	-2.850345
C	-2.991047	1.995936	-4.119931
C	-4.030571	2.429111	-4.939512
H	-4.813334	0.977567	-1.435934
H	-1.964265	2.092204	-4.462611
C	0.993157	4.459739	-1.894866
C	-0.331107	4.582489	-1.453108
C	-1.168151	3.471991	-1.447664
C	-0.694037	2.219838	-1.882727
C	0.632183	2.097598	-2.315561
C	1.468077	3.221352	-2.325758
H	-2.193091	3.569950	-1.103307
H	1.030867	1.148034	-2.657405
C	-7.691532	-1.601278	-1.979680
C	-7.287258	-0.978626	-0.795794
C	-5.961253	-1.067503	-0.375633
C	-5.020694	-1.792129	-1.126239
C	-5.439971	-2.428389	-2.304351
C	-6.765606	-2.325240	-2.730946
H	-5.649197	-0.545745	0.523652
H	-4.744026	-3.003186	-2.905203
C	-3.330602	-5.254701	2.696836
C	-2.427686	-5.342660	1.637829
C	-2.419249	-4.372603	0.631982
C	-3.324936	-3.302372	0.682243
C	-4.231499	-3.219515	1.752881
C	-4.235450	-4.189968	2.751330
H	-1.679372	-4.442516	-0.153861
H	-4.931893	-2.393107	1.813920
H	1.641568	5.332210	-1.911964
H	-6.165812	2.662537	-5.146632
H	-3.329934	-6.008689	3.478781
H	-8.722118	-1.522325	-2.313434
H	-3.807991	2.846515	-5.917456
H	-6.658762	1.723551	-2.891584
H	2.493227	3.106107	-2.658413
H	-0.702384	5.543397	-1.109358
H	-7.070925	-2.812502	-3.652334
H	-8.001727	-0.414780	-0.202811
H	-4.941577	-4.113534	3.572979
H	-1.716188	-6.161958	1.591711
Rh	-2.369010	-0.019520	0.351471
O	-1.492362	1.871922	1.144110
C	-0.261653	1.788980	1.400663
N	0.363259	0.605503	1.450359
C	-0.308564	-0.621211	1.144449
C	-1.223816	-1.173428	2.083178
H	1.283422	0.580427	1.906412
H	-3.815052	0.583463	0.261019
H	-2.802831	-0.582206	1.836199
H	-1.438066	-2.219163	1.886839
C	-0.981721	-0.320220	6.281200

C	-0.651107	-1.577327	5.769836
C	-0.777019	-1.832712	4.404552
C	-1.216485	-0.823447	3.533263
C	-1.564108	0.429464	4.052717
C	-1.445233	0.677533	5.420409
H	-0.891580	-0.123499	7.345694
H	-0.303769	-2.363708	6.434324
H	-0.515307	-2.808700	4.005600
H	-1.954846	1.192760	3.389171
H	-1.723557	1.650728	5.815223
C	-2.128471	-1.656732	-3.173132
H	-0.936545	-0.009179	-3.922857
H	-0.203543	-0.836259	-2.557520
H	-1.719538	-2.270865	-3.983802
H	-3.098132	-1.286921	-3.527352
H	-1.314542	-2.816282	-1.534464
H	-2.752671	-3.533255	-2.254751
C	2.950184	2.192233	1.608803
C	4.340455	2.494921	1.027142
N	1.939858	2.993047	1.178829
C	0.566063	3.014370	1.587898
C	-0.065631	4.175266	1.868155
C	0.417131	-1.521410	0.218043
N	4.968598	1.329613	0.427198
C	4.421499	0.821255	-0.717288
C	5.127825	-0.277246	-1.453592
N	4.349514	-0.882696	-2.477088
C	2.990624	-1.122067	-2.336940
C	2.582066	-1.566768	-0.965391
N	1.453183	-0.904380	-0.456883
O	0.146055	-2.712430	0.082918
C	3.245799	-2.540351	-0.307605
O	2.202403	-1.021961	-3.267544
C	6.447086	-0.533085	-1.280569
O	3.364791	1.299113	-1.148309
O	2.816349	1.286312	2.435576
C	0.453971	5.537008	1.949925
C	2.948869	-2.984517	1.066286
C	7.303754	-1.542891	-1.895781
C	2.731605	-4.338860	1.355287
C	2.399416	-4.739968	2.649693
C	2.292523	-3.794932	3.673120
C	2.535543	-2.445287	3.400401
C	2.865059	-2.043860	2.107322
C	1.807653	5.863942	2.173417
C	2.217656	7.193868	2.210598
C	1.293545	8.225311	2.017919
C	-0.053809	7.919482	1.810082
C	-0.469518	6.590976	1.789554
C	6.831038	-2.625834	-2.669006
C	7.718471	-3.565535	-3.185146
C	9.092686	-3.446349	-2.955915
C	9.577566	-2.381740	-2.192396
C	8.692404	-1.446258	-1.665106
H	4.968599	2.828468	1.857885
H	4.297223	3.295700	0.282830
H	2.134286	3.592107	0.381249
H	-1.143232	4.081299	1.975736
H	5.613989	0.780254	0.975246
H	4.616645	-0.656037	-3.431739
H	1.502306	0.108791	-0.445622
H	4.044121	-3.049250	-0.843869

H	6.972794	0.133605	-0.600555
H	2.795157	-5.073007	0.556775
H	2.222901	-5.791455	2.859035
H	2.034169	-4.109076	4.680851
H	2.466607	-1.704129	4.191423
H	3.073826	-0.998227	1.906589
H	2.529894	5.076336	2.350121
H	3.261720	7.428939	2.396843
H	1.620166	9.260834	2.041949
H	-0.779953	8.715443	1.673993
H	-1.520417	6.356702	1.638361
H	5.769336	-2.733989	-2.852289
H	7.336447	-4.395782	-3.772273
H	9.779882	-4.179567	-3.368018
H	10.642837	-2.283372	-2.005471
H	9.075706	-0.624035	-1.065244

Sum of electronic and zero-point energy: -3953.508181
Sum of electronic and thermal free energies: -3953.616242
Frequency: -678.9292

Supplementary Table 13. **O3R^{TS}** representative 2

C	1.078007	-5.158115	-0.412853
C	3.140035	-3.953886	0.666114
P	3.062184	-2.199845	0.068565
P	-0.059593	-3.671519	-0.295579
C	6.064237	-1.974399	-3.476774
C	4.931613	-1.157856	-3.451352
C	4.013706	-1.257239	-2.403648
C	4.225592	-2.171685	-1.357760
C	5.366642	-2.990786	-1.394342
C	6.277593	-2.893834	-2.447670
H	3.139425	-0.617818	-2.394322
H	5.562896	-3.704035	-0.599981
C	4.866790	0.821205	3.071266
C	3.544949	0.390614	3.194917
C	3.037342	-0.559128	2.309802
C	3.846500	-1.093816	1.296192
C	5.179682	-0.661771	1.181929
C	5.682715	0.290119	2.069123
H	1.992593	-0.834509	2.395003
H	5.818408	-1.046763	0.394158
C	-3.449841	-4.111806	-3.418748
C	-2.155384	-4.534014	-3.731415
C	-1.140700	-4.455961	-2.776712
C	-1.415087	-3.963352	-1.493066
C	-2.714911	-3.529389	-1.189437
C	-3.727233	-3.608275	-2.146129
H	-0.134473	-4.760850	-3.050986
H	-2.950490	-3.136996	-0.206841
C	-1.811188	-4.309248	3.953030
C	-2.291444	-5.075401	2.884678
C	-1.796318	-4.875890	1.596385
C	-0.804110	-3.906552	1.366376
C	-0.304566	-3.170474	2.446467
C	-0.814134	-3.358139	3.733128
H	-2.190514	-5.462916	0.772346
H	0.472565	-2.434002	2.288496
H	5.255038	1.581909	3.742129
H	6.774573	-1.898504	-4.295057
H	-2.209300	-4.462233	4.952055
H	-4.236328	-4.173376	-4.165323
H	7.154098	-3.535362	-2.460927
H	4.754613	-0.444575	-4.251495
H	6.708682	0.630911	1.962858
H	2.889461	0.821131	3.943476
H	-4.728680	-3.278637	-1.885355
H	-1.932038	-4.920990	-4.721353
H	-0.431349	-2.749964	4.546650
H	-3.055320	-5.828959	3.055931
Rh	0.845643	-1.607262	-0.594822
O	1.704026	0.349983	-0.973596
C	1.618581	1.242557	-0.086121
N	0.651040	1.198146	0.858655
C	-0.367730	0.220344	0.899544
C	-1.202029	-0.116856	-0.199660
H	0.855408	1.680088	1.737209
H	1.201835	-2.183350	-1.995862
H	-0.583029	-1.182818	-1.255316
H	-1.967576	-0.824476	0.105586
C	-2.886700	2.365866	-3.276074

C	-3.493291	1.168183	-2.885705
C	-2.891593	0.364755	-1.920607
C	-1.675703	0.745611	-1.316774
C	-1.073573	1.945283	-1.725258
C	-1.680067	2.749918	-2.689591
H	-3.362442	3.000465	-4.016756
H	-4.439610	0.866340	-3.325147
H	-3.369453	-0.562938	-1.616763
H	-0.167752	2.301882	-1.261123
H	-1.214962	3.695971	-2.947223
C	2.596716	-4.907400	-0.426606
H	4.169163	-4.211990	0.933026
H	2.551182	-4.018435	1.588278
H	3.079777	-5.884710	-0.310679
H	2.897285	-4.542423	-1.415048
H	0.798896	-5.720538	-1.309291
H	0.810488	-5.784442	0.444653
C	1.746807	3.830645	1.757299
C	0.894155	5.073977	2.023463
N	2.075762	3.633932	0.442273
C	2.561836	2.383734	-0.059132
C	3.808787	2.174366	-0.541253
C	-0.785638	-0.084396	2.299639
N	-0.499997	4.721211	1.773585
C	-0.991321	4.698222	0.512677
C	-2.418431	4.209525	0.330100
N	-2.802073	2.901064	0.736479
C	-2.519292	2.185935	1.860711
C	-3.033841	0.764707	1.862332
N	-2.163671	-0.167215	2.501448
O	0.005604	-0.224827	3.226612
C	-4.238229	0.443945	1.342644
O	-1.856257	2.601185	2.816422
C	-3.225037	4.914997	-0.488492
O	-0.345571	5.094085	-0.466921
O	1.991435	3.014853	2.642459
C	4.984582	3.027643	-0.606598
C	-4.891509	-0.852370	1.167893
C	-4.580656	4.558858	-0.925467
C	-4.459560	-2.065446	1.744382
C	-5.142424	-3.251970	1.481748
C	-6.259379	-3.263080	0.642054
C	-6.698684	-2.069454	0.061885
C	-6.025405	-0.880337	0.327119
C	5.041485	4.360660	-0.148988
C	6.227438	5.083120	-0.233269
C	7.377890	4.497988	-0.772914
C	7.338142	3.178715	-1.231648
C	6.154291	2.452384	-1.148667
C	-5.504038	3.878360	-0.106357
C	-6.758531	3.516657	-0.594652
C	-7.120522	3.829097	-1.908418
C	-6.228435	4.532928	-2.721249
C	-4.977173	4.902804	-2.231207
H	1.166187	5.916896	1.383657
H	1.006900	5.349130	3.072431
H	1.627526	4.261656	-0.225666
H	3.969394	1.170484	-0.922913
H	-0.992454	4.160600	2.473852
H	-3.288222	2.392856	0.005815
H	-2.380908	-0.381681	3.471459
H	-4.817589	1.275573	0.947205

H	-2.779574	5.792367	-0.949418
H	-3.590803	-2.087825	2.389725
H	-4.793097	-4.172999	1.936857
H	-6.787048	-4.192260	0.447187
H	-7.568880	-2.064722	-0.588251
H	-6.370930	0.046615	-0.125264
H	4.158126	4.819957	0.275316
H	6.257879	6.108408	0.124081
H	8.300000	5.068775	-0.835199
H	8.227828	2.719493	-1.652673
H	6.122101	1.425372	-1.505301
H	-5.248548	3.668066	0.927175
H	-7.462955	3.008226	0.058487
H	-8.098404	3.546670	-2.287566
H	-6.510617	4.800699	-3.735530
H	-4.287531	5.452212	-2.866866

Sum of electronic and zero-point energy: -3953.492664
Sum of electronic and thermal free energies: -3953.600379
Frequency: -616.2573

Supplementary Table 14. **O3R^{TS}** representative 3

C	4.801468	-2.873569	-0.469041
C	5.533082	-0.593255	0.515108
P	3.940155	0.303131	0.889676
P	2.950573	-2.715735	-0.456035
C	5.464694	4.544856	-0.253755
C	5.125519	3.616444	-1.242991
C	4.619174	2.366859	-0.886488
C	4.461233	2.023346	0.467525
C	4.786437	2.966357	1.452896
C	5.283575	4.221113	1.091548
H	4.337816	1.661182	-1.662065
H	4.661892	2.724341	2.502898
C	3.489360	0.380589	5.514328
C	4.735592	0.078997	4.960265
C	4.896080	0.036984	3.574733
C	3.805993	0.291119	2.723717
C	2.556437	0.585435	3.291176
C	2.401522	0.633561	4.677440
H	5.878058	-0.187827	3.171543
H	1.691810	0.742756	2.656563
C	1.471032	-5.125795	-4.146842
C	2.609348	-4.321183	-4.241334
C	3.068246	-3.619763	-3.126289
C	2.403858	-3.727157	-1.893413
C	1.258817	-4.534724	-1.809612
C	0.795103	-5.226613	-2.930547
H	3.939133	-2.979961	-3.231238
H	0.725976	-4.634058	-0.869379
C	1.922330	-5.168077	3.349011
C	1.672218	-3.796885	3.312s
C	1.957167	-3.060387	2.158370
C	2.490057	-3.695389	1.028891
C	2.744494	-5.079596	1.074719
C	2.460496	-5.808779	2.227741
H	1.758708	-1.995431	2.150967
H	3.154560	-5.591509	0.208594
H	3.368295	0.413924	6.593518
H	5.867693	5.514814	-0.532247
H	1.704035	-5.739384	4.247022
H	1.112880	-5.667095	-5.017766
H	5.535794	4.940509	1.865519
H	5.251905	3.866104	-2.292840
H	1.425304	0.858479	5.096756
H	5.586493	-0.121001	5.605513
H	-0.096982	-5.840529	-2.846454
H	3.140431	-4.235163	-5.185037
H	2.661650	-6.876130	2.252870
H	1.258926	-3.286897	4.177379
Rh	2.199875	-0.550029	-0.595351
O	1.576086	1.493811	-1.029708
C	0.490660	1.936750	-0.565104
N	-0.378431	1.133936	0.079888
C	-0.339663	-0.280854	0.060052
C	-0.298874	-0.991015	-1.157089
H	-1.165604	1.549114	0.571422
H	3.285966	-0.502048	-1.714807
H	1.199153	-1.096029	-1.742302
H	-0.393597	-2.068737	-1.027331
C	-1.916165	0.247007	-4.964331
C	-0.835883	-0.638789	-4.915773

C	-0.284447	-1.007144	-3.690781
C	-0.800841	-0.496322	-2.488565
C	-1.893197	0.379273	-2.548127
C	-2.444889	0.749918	-3.775919
H	-2.341396	0.537802	-5.920887
H	-0.418886	-1.041666	-5.834603
H	0.562159	-1.688341	-3.667272
H	-2.340798	0.769771	-1.644175
H	-3.291807	1.429750	-3.785346
C	5.517651	-2.123272	0.667760
H	5.781241	-0.322246	-0.517887
H	6.322232	-0.157634	1.136604
H	5.096907	-2.412985	1.638301
H	6.558707	-2.469293	0.676637
H	5.027644	-3.944361	-0.409407
H	5.167043	-2.515240	-1.437247
C	-1.767562	4.510806	0.479280
C	-3.299940	4.730609	0.413027
N	-1.283051	3.647015	-0.486913
C	0.094414	3.361307	-0.701195
C	1.052652	4.278172	-0.980712
C	-0.725015	-0.905604	1.369511
N	-4.125063	3.600909	0.835553
C	-4.339403	2.524347	0.040250
C	-5.276700	1.472840	0.585586
N	-4.806596	0.146877	0.475532
C	-3.516933	-0.162795	0.823168
C	-2.989525	-1.552983	0.607392
N	-1.780951	-1.828937	1.325432
O	-0.157193	-0.675738	2.429043
C	-3.625617	-2.470591	-0.159699
O	-2.797482	0.711068	1.319861
C	-6.529296	1.796427	0.974252
O	-3.842177	2.418323	-1.086416
O	-1.074963	5.096910	1.289088
C	0.950013	5.710498	-1.247859
C	-3.303501	-3.863433	-0.464995
C	-7.608578	0.912694	1.436334
C	-2.284110	-4.612787	0.162252
C	-2.071957	-5.945153	-0.184334
C	-2.861897	-6.561391	-1.160324
C	-3.873745	-5.834064	-1.791951
C	-4.093279	-4.504949	-1.443107
C	-0.210034	6.337543	-1.745082
C	-0.214977	7.700200	-2.025075
C	0.929677	8.472053	-1.802761
C	2.089390	7.865493	-1.316535
C	2.102645	6.497585	-1.056314
C	-7.384326	-0.282178	2.150276
C	-8.454242	-1.071604	2.569231
C	-9.767208	-0.690053	2.284212
C	-10.006327	0.499835	1.592044
C	-8.939879	1.295585	1.181675
H	-3.587896	4.993296	-0.610285
H	-3.516313	5.573912	1.069478
H	-1.988254	3.167236	-1.048406
H	2.063197	3.877352	-0.998165
H	-4.376094	3.526013	1.811974
H	-5.487359	-0.582807	0.309411
H	-1.931361	-2.202712	2.261640
H	-4.523825	-2.122938	-0.665934
H	-6.801729	2.843281	0.860567

H	-1.664596	-4.152422	0.920731
H	-1.292810	-6.509855	0.320370
H	-2.697573	-7.604052	-1.417392
H	-4.495564	-6.304173	-2.548024
H	-4.887030	-3.946578	-1.933369
H	-1.097953	5.747234	-1.940877
H	-1.113920	8.164792	-2.420725
H	0.918199	9.537365	-2.015190
H	2.984966	8.457019	-1.148565
H	3.008323	6.023811	-0.687942
H	-6.373588	-0.569259	2.423201
H	-8.262233	-1.981294	3.131343
H	-10.598322	-1.308056	2.611116
H	-11.024650	0.810986	1.377776
H	-9.132310	2.222938	0.648017

Sum of electronic and zero-point energy: -3953.487473
Sum of electronic and thermal free energies: -3953.603549
Frequency: -600.0306

Supplementary Table 15. **O3R^{TS}** representative 4

C	1.616949	-3.758152	1.532280
C	3.335749	-2.004879	2.405008
P	3.373517	-0.827610	0.977706
P	1.393854	-3.263042	-0.238705
C	7.237397	-1.641309	-1.452768
C	6.248227	-0.779247	-1.937160
C	5.102389	-0.536243	-1.181560
C	4.939842	-1.139241	0.079441
C	5.943849	-1.987456	0.564529
C	7.082905	-2.242942	-0.203287
H	4.319967	0.108677	-1.572370
H	5.848083	-2.465535	1.533601
C	3.948228	3.338620	2.988474
C	4.691407	2.998994	1.855032
C	4.533889	1.747174	1.259105
C	3.612539	0.820304	1.774980
C	2.840931	1.182002	2.892817
C	3.025207	2.424120	3.505247
H	5.139192	1.497664	0.395273
H	2.085054	0.510227	3.280275
C	4.430250	-6.120293	-2.258631
C	3.270881	-6.619009	-1.655447
C	2.351932	-5.744440	-1.079662
C	2.582312	-4.356756	-1.106313
C	3.739909	-3.864679	-1.719304
C	4.661990	-4.745287	-2.289767
H	1.447808	-6.140875	-0.624840
H	3.923508	-2.798991	-1.752158
C	-2.770887	-4.602039	-1.745247
C	-1.749209	-4.263831	-2.639206
C	-0.493320	-3.907186	-2.156624
C	-0.242120	-3.888414	-0.772737
C	-1.269169	-4.226655	0.117960
C	-2.530182	-4.585260	-0.372010
H	0.295096	-3.635405	-2.852844
H	-1.106778	-4.205732	1.191357
H	4.084471	4.305765	3.464391
H	8.124494	-1.840535	-2.047131
H	-3.752368	-4.879584	-2.119037
H	5.145709	-6.804436	-2.705937
H	7.848267	-2.912561	0.178226
H	6.363994	-0.305596	-2.907811
H	2.436870	2.679294	4.382646
H	5.405372	3.703753	1.438915
H	5.558771	-4.347355	-2.755211
H	3.081497	-7.688409	-1.637792
H	-3.319981	-4.848120	0.321201
H	-1.931805	-4.275212	-3.709718
Rh	1.512166	-1.012575	-0.505047
O	1.752570	1.134321	-0.872647
C	1.138865	1.852970	-0.035878
N	0.211304	1.321706	0.777047
C	-0.192727	-0.043494	0.700569
C	-0.829141	-0.594990	-0.465350
H	-0.259602	1.928941	1.442249
H	2.452422	-1.384993	-1.710603
H	0.251431	-1.129672	-1.554305
H	-1.253987	-1.570386	-0.243913
C	-3.390714	1.281002	-3.356048

C	-3.666283	0.009812	-2.846587
C	-2.780400	-0.587319	-1.949541
C	-1.618948	0.088736	-1.528424
C	-1.335597	1.348788	-2.074344
C	-2.219779	1.939918	-2.977044
H	-4.083387	1.755788	-4.044303
H	-4.571491	-0.513348	-3.141154
H	-2.996087	-1.577886	-1.556621
H	-0.429822	1.872996	-1.810309
H	-2.010001	2.935067	-3.354417
C	3.042042	-3.477567	2.058900
H	4.282985	-1.921872	2.948622
H	2.549895	-1.627229	3.061347
H	3.166355	-4.053799	2.983271
H	3.785344	-3.871177	1.355286
H	0.880362	-3.219025	2.137191
H	1.403554	-4.831009	1.601510
C	0.110240	4.970928	1.479295
C	-0.984253	5.140536	0.432784
N	0.979108	3.898705	1.305773
C	1.382007	3.305585	0.077806
C	1.963922	3.952638	-0.959720
C	-0.481338	-0.619571	2.065211
N	-1.878193	3.988575	0.487438
C	-2.907180	3.906692	-0.394777
C	-3.928113	2.802959	-0.180708
N	-3.614441	1.524166	0.373821
C	-2.897826	1.117094	1.448791
C	-2.943339	-0.372170	1.718396
N	-1.798915	-0.911692	2.353246
O	0.379303	-0.828955	2.917197
C	-4.081435	-1.080878	1.531059
O	-2.234157	1.854423	2.195069
C	-5.128847	2.955346	-0.775859
O	-3.033826	4.687915	-1.334764
O	0.187565	5.672669	2.471073
C	2.340916	5.356337	-1.092311
C	-4.416017	-2.478881	1.807401
C	-6.225153	1.975116	-0.784914
C	-3.689432	-3.351950	2.643141
C	-4.124291	-4.657901	2.860820
C	-5.282339	-5.133591	2.238979
C	-6.011793	-4.285351	1.401081
C	-5.590422	-2.973844	1.199973
C	2.614361	6.207249	0.000175
C	2.973578	7.534474	-0.214566
C	3.063225	8.043191	-1.514084
C	2.809887	7.209755	-2.606286
C	2.463730	5.877888	-2.396838
C	-6.630459	1.287917	0.374831
C	-7.645259	0.332074	0.319114
C	-8.272168	0.043610	-0.896881
C	-7.896568	0.737289	-2.050811
C	-6.891711	1.702282	-1.992990
H	-0.571294	5.225824	-0.576382
H	-1.511645	6.071393	0.661082
H	1.628876	3.788138	2.081088
H	2.141251	3.334735	-1.837521
H	-1.959297	3.454485	1.352658
H	-3.993304	0.771140	-0.189691
H	-1.910490	-1.242673	3.305991
H	-4.916952	-0.525139	1.115282

H	-5.245284	3.852424	-1.377190
H	-2.785302	-3.022965	3.136097
H	-3.555952	-5.307556	3.520284
H	-5.616209	-6.152395	2.411889
H	-6.916175	-4.641904	0.916726
H	-6.173983	-2.312761	0.563304
H	2.565627	5.830556	1.013861
H	3.183713	8.175521	0.636438
H	3.336429	9.082191	-1.673848
H	2.886854	7.596048	-3.618302
H	2.272412	5.229423	-3.248318
H	-6.164959	1.530683	1.325405
H	-7.957335	-0.175073	1.228234
H	-9.063847	-0.698898	-0.940138
H	-8.393862	0.532989	-2.994748
H	-6.605003	2.243393	-2.890795

Sum of electronic and zero-point energy: -3953.499257
Sum of electronic and thermal free energies: -3953.607378
Frequency: -735.6902

Supplementary Table 16. **O3R^{TS}** representative 5

C	1.672789	2.540219	1.627398
C	-0.857513	2.056497	2.100036
P	-1.494817	2.194706	0.368122
P	1.697208	2.659549	-0.219069
C	-2.563805	6.682102	-0.159887
C	-2.171009	5.920505	-1.260790
C	-1.825762	4.578224	-1.097629
C	-1.868294	3.980853	0.168404
C	-2.289743	4.749364	1.267601
C	-2.626668	6.092387	1.105166
H	-1.511555	3.993687	-1.955386
H	-2.365852	4.303600	2.254426
C	-5.662148	0.161564	0.255705
C	-5.538438	1.500280	-0.123487
C	-4.295376	2.134832	-0.077564
C	-3.159567	1.429324	0.351482
C	-3.291919	0.085691	0.717594
C	-4.533777	-0.544634	0.677935
H	-4.216403	3.174744	-0.374610
H	-2.427384	-0.485989	1.024442
C	1.452949	7.135501	-1.408593
C	1.242243	6.138209	-2.363399
C	1.278466	4.795764	-1.992108
C	1.553718	4.430663	-0.664893
C	1.778496	5.437949	0.285351
C	1.715710	6.782499	-0.084551
H	1.068244	4.028491	-2.730563
H	2.003798	5.189543	1.316680
C	5.913795	1.300326	-1.595708
C	5.093135	2.051670	-2.442407
C	3.850084	2.495573	-1.997675
C	3.414012	2.202230	-0.694526
C	4.246794	1.456788	0.154963
C	5.489460	1.007647	-0.300046
H	3.220699	3.067436	-2.670992
H	3.923415	1.171660	1.146810
H	-6.628132	-0.332978	0.209561
H	-2.824512	7.729040	-0.286011
H	6.877238	0.942289	-1.947313
H	1.410113	8.182427	-1.694613
H	-2.942497	6.676307	1.965003
H	-2.121360	6.371233	-2.247458
H	-4.599390	-1.591453	0.953457
H	-6.410499	2.057055	-0.455164
H	1.878280	7.552322	0.664144
H	1.033890	6.404827	-3.395657
H	6.110577	0.408584	0.357676
H	5.417464	2.286712	-3.451954
Rh	0.135008	1.250665	-1.126808
O	-1.500213	-0.130550	-1.841450
C	-1.408331	-1.317870	-1.437465
N	-0.322003	-1.750553	-0.772654
C	0.745278	-0.884458	-0.386395
C	1.712673	-0.519809	-1.363015
H	-0.109142	-2.750751	-0.794987
H	-0.223328	2.412042	-2.117164
H	1.220612	0.905742	-2.290614
H	2.618433	-0.116694	-0.924851
C	2.612042	-2.844949	-4.853392

C	3.589510	-2.543532	-3.902997
C	3.272211	-1.748146	-2.802145
C	1.965003	-1.266907	-2.624645
C	0.997155	-1.543113	-3.601006
C	1.320956	-2.330480	-4.704897
H	2.858893	-3.457845	-5.715489
H	4.603900	-2.913989	-4.024121
H	4.036172	-1.505855	-2.069100
H	0.012146	-1.097862	-3.522315
H	0.565598	-2.532681	-5.459184
C	0.379363	2.936827	2.366213
H	-1.648573	2.295715	2.815874
H	-0.614493	1.001198	2.252454
H	0.598239	2.857610	3.438122
H	0.136963	3.987551	2.177522
H	1.902906	1.492376	1.840894
H	2.513914	3.133794	2.004053
C	-2.160460	-3.761469	0.365706
C	-1.538823	-5.082602	0.861729
N	-2.275488	-3.600072	-0.988144
C	-2.504476	-2.310992	-1.586001
C	-3.664700	-1.920530	-2.157870
C	1.160165	-0.994824	1.033784
N	-0.199931	-4.814784	1.375834
C	0.772236	-4.424048	0.511439
C	2.051638	-3.913403	1.072153
N	2.209815	-3.860007	2.486313
C	1.872072	-2.879963	3.428651
C	0.694148	-1.963405	3.204975
N	0.285587	-1.648094	1.880215
O	2.246759	-0.580757	1.450863
C	0.121007	-1.478043	4.323951
O	2.495355	-2.865705	4.480627
C	3.055702	-3.651200	0.200151
O	0.548269	-4.437788	-0.715676
O	-2.456595	-2.886659	1.177530
C	-4.947322	-2.592136	-2.299447
C	-1.024391	-0.571286	4.472047
C	4.409580	-3.162802	0.445516
C	-2.244508	-0.770194	3.808327
C	-3.310274	0.107782	4.017179
C	-3.170368	1.196258	4.879803
C	-1.959906	1.398620	5.551984
C	-0.901718	0.512658	5.362559
C	-5.186722	-3.946846	-1.986145
C	-6.460732	-4.488142	-2.124500
C	-7.522324	-3.695356	-2.573775
C	-7.302534	-2.352586	-2.890741
C	-6.027940	-1.809607	-2.759622
C	4.818064	-2.464817	1.602584
C	6.141284	-2.052269	1.744160
C	7.082135	-2.316192	0.744141
C	6.688460	-2.987013	-0.417297
C	5.367834	-3.400240	-0.564262
H	-1.484152	-5.841088	0.076171
H	-2.156299	-5.455023	1.680716
H	-1.807863	-4.299262	-1.556769
H	-3.638945	-0.897824	-2.527139
H	-0.039747	-4.736579	2.370983
H	3.050281	-4.328930	2.816726
H	-0.644254	-1.903686	1.563177
H	0.610393	-1.781684	5.246592

H	2.821522	-3.877052	-0.837357
H	-2.372576	-1.628733	3.157989
H	-4.248137	-0.058796	3.497829
H	-4.003478	1.874992	5.039846
H	-1.847787	2.235238	6.236091
H	0.032511	0.657485	5.899130
H	-4.373800	-4.570754	-1.637752
H	-6.629596	-5.533624	-1.883240
H	-8.514555	-4.124528	-2.679101
H	-8.121759	-1.732796	-3.242963
H	-5.858475	-0.763204	-2.999179
H	4.104981	-2.202593	2.371028
H	6.437697	-1.518400	2.642693
H	8.113367	-1.996974	0.866928
H	7.410272	-3.191049	-1.202886
H	5.062635	-3.922172	-1.467454

Sum of electronic and zero-point energy: -3953.514967
Sum of electronic and thermal free energies: -3953.619657
Frequency: -557.7065

Supplementary Table 17. **O4R^{TS}** representative 1

C	-4.317272	0.890639	2.530207
C	-3.753831	-1.633699	2.377980
P	-3.458669	-1.844896	0.564269
P	-4.246868	1.414034	0.753340
C	-7.328771	-3.479198	-1.396012
C	-6.236064	-3.073785	-2.169936
C	-5.081615	-2.596517	-1.552856
C	-5.003220	-2.523322	-0.150317
C	-6.090162	-2.959141	0.618182
C	-7.251320	-3.426256	-0.004155
H	-4.238914	-2.269121	-2.155811
H	-6.048706	-2.938717	1.702011
C	-0.452488	-5.360896	0.181204
C	-0.006959	-4.088628	0.549231
C	-0.919808	-3.045482	0.700590
C	-2.287190	-3.255652	0.463048
C	-2.727588	-4.540092	0.107299
C	-1.813342	-5.587452	-0.023959
H	-0.557568	-2.058966	0.966386
H	-3.779233	-4.726012	-0.080616
C	-8.803374	1.458604	-0.135981
C	-7.989566	0.539695	-0.797341
C	-6.609633	0.538770	-0.580619
C	-6.031254	1.451258	0.309201
C	-6.859434	2.376378	0.973013
C	-8.234114	2.381559	0.747084
H	-5.991011	-0.176897	-1.105434
H	-6.428533	3.105176	1.653842
C	-2.857408	5.828662	0.720204
C	-3.728146	5.350516	-0.263264
C	-4.176918	4.031717	-0.218823
C	-3.763493	3.178686	0.817519
C	-2.883928	3.660761	1.800162
C	-2.437348	4.983343	1.748439
H	-4.851738	3.666098	-0.987453
H	-2.507978	3.005015	2.577248
H	0.264462	-6.165118	0.044214
H	-8.232618	-3.841457	-1.877446
H	-2.505068	6.855403	0.681331
H	-9.875952	1.461934	-0.308232
H	-8.092761	-3.748711	0.602283
H	-6.285746	-3.124731	-3.253850
H	-2.168324	-6.575160	-0.304468
H	1.053123	-3.903911	0.667512
H	-8.860652	3.106839	1.258258
H	-8.419106	-0.183157	-1.484626
H	-1.752491	5.345481	2.509530
H	-4.055474	6.003364	-1.067166
Rh	-2.820225	0.172220	-0.553177
O	-1.658304	-1.197370	-1.858646
C	-0.413995	-1.114078	-1.720499
N	0.179998	-0.305828	-0.826550
C	-0.573324	0.571075	0.021896
C	-1.154617	1.781127	-0.548994
H	1.175935	-0.131007	-0.949349
H	-4.080190	0.026813	-1.455419
H	-2.485865	1.542854	-1.432881
H	-1.476436	2.499161	0.194527
C	1.026205	3.559892	-3.807697

C	1.034315	4.131406	-2.533486
C	0.286718	3.564146	-1.501555
C	-0.470764	2.407538	-1.734706
C	-0.497128	1.853524	-3.020459
C	0.251793	2.423668	-4.050043
H	1.606509	4.006034	-4.610442
H	1.618350	5.028175	-2.343122
H	0.311274	3.994238	-0.505729
H	-1.129053	0.992296	-3.218582
H	0.219383	1.987087	-5.044607
C	-4.785455	-0.553920	2.760378
H	-2.773317	-1.373686	2.793638
H	-4.037876	-2.606333	2.795083
H	-4.990923	-0.663090	3.832167
H	-5.739793	-0.725876	2.249548
H	-3.323016	1.033249	2.951754
H	-5.010420	1.585726	3.016808
C	0.466372	-2.001472	-2.596048
C	-0.361242	0.525744	1.487465
O	-1.237765	0.800715	2.306666
N	0.877670	0.071856	1.953187
C	2.147932	0.531556	1.515637
C	3.283182	-0.175819	1.748287
C	3.502444	-1.546429	2.193733
C	2.204281	1.968480	1.066601
N	1.879505	-1.703816	-2.519001
C	2.730041	-2.459344	-1.766103
C	4.132338	-1.919945	-1.513946
N	4.422687	-0.573169	-1.151695
C	3.706270	0.581510	-1.183221
C	4.276596	1.702085	-0.358552
N	3.320569	2.423172	0.380726
O	1.305438	2.750654	1.358090
C	5.577152	2.062517	-0.465127
O	2.636393	0.754865	-1.780868
C	5.114393	-2.843615	-1.406285
O	2.430593	-3.570685	-1.339189
C	6.305057	3.137362	0.211033
C	6.525201	-2.622194	-1.068230
C	5.889651	3.725190	1.424597
C	6.651673	4.725444	2.023321
C	7.835839	5.167406	1.426808
C	8.265636	4.588626	0.229928
C	7.512633	3.580405	-0.365347
C	2.484755	-2.482913	2.470681
C	2.804420	-3.789285	2.830011
C	4.138699	-4.194248	2.927775
C	5.160080	-3.280294	2.656853
C	4.844140	-1.975060	2.294769
C	7.271561	-1.521101	-1.534544
C	8.599539	-1.344240	-1.145982
C	9.209603	-2.262457	-0.288608
C	8.490291	-3.374647	0.159649
C	7.166968	-3.558202	-0.233666
H	0.103164	-1.910363	-3.624331
H	0.308656	-3.034043	-2.271193
H	0.828374	-0.059033	2.961307
H	4.206951	0.367971	1.581504
H	2.171628	-0.757739	-2.749142
H	5.260960	-0.513379	-0.582281
H	3.316356	3.432136	0.267576
H	6.161123	1.512517	-1.201145

H	4.786902	-3.874897	-1.490286
H	4.987872	3.377509	1.915584
H	6.321517	5.159671	2.962695
H	8.422786	5.951988	1.895250
H	9.188786	4.920132	-0.236441
H	7.854423	3.130143	-1.294450
H	1.446025	-2.194224	2.383014
H	2.004358	-4.496627	3.028048
H	4.379333	-5.214316	3.212829
H	6.200857	-3.582246	2.721045
H	5.646624	-1.273250	2.078639
H	6.822905	-0.829377	-2.242163
H	9.162299	-0.495685	-1.524778
H	10.243128	-2.122925	0.014301
H	8.965567	-4.103356	0.810279
H	6.608403	-4.420928	0.118430

Sum of electronic and zero-point energy: -3953.488855
Sum of electronic and thermal free energies: -3953.597503
Frequency: -767.4746

Supplementary Table 18. **O4R^{TS}** representative 2

C	-3.190394	0.896842	2.409059
C	-1.659182	-1.188554	2.611287
P	-1.938026	-1.973080	0.963155
P	-4.036357	0.638771	0.784027
C	-4.975646	-5.440633	1.574996
C	-4.647845	-4.991598	0.292586
C	-3.742166	-3.944484	0.129059
C	-3.137663	-3.340746	1.244826
C	-3.459078	-3.810082	2.525831
C	-4.380428	-4.847368	2.688658
H	-3.528919	-3.572282	-0.868929
H	-3.003646	-3.373424	3.408154
C	1.899938	-4.463215	0.097504
C	1.895799	-3.546351	1.146530
C	0.763789	-2.769591	1.411923
C	-0.382952	-2.904370	0.617667
C	-0.369815	-3.820003	-0.451729
C	0.759470	-4.596466	-0.706125
H	0.805962	-2.057953	2.228721
H	-1.243648	-3.933066	-1.081835
C	-8.015078	-1.250867	2.234688
C	-7.663148	0.054256	2.594697
C	-6.477598	0.613268	2.123609
C	-5.627987	-0.128636	1.281571
C	-5.996112	-1.426341	0.913648
C	-7.182145	-1.987151	1.393148
H	-6.222745	1.633816	2.396466
H	-5.359301	-2.003137	0.257427
C	-5.296083	4.784574	-0.837592
C	-4.311422	4.712933	0.147710
C	-3.923693	3.476250	0.671453
C	-4.532121	2.302039	0.206140
C	-5.521921	2.378105	-0.788681
C	-5.902107	3.613770	-1.305725
H	-3.129255	3.437157	1.405532
H	-5.994846	1.470819	-1.154776
H	2.779326	-5.072125	-0.094461
H	-5.690353	-6.248341	1.704106
H	-5.591207	5.748046	-1.243331
H	-8.938849	-1.685689	2.605777
H	-4.629321	-5.191059	3.688545
H	-5.106209	-5.447897	-0.580291
H	0.744330	-5.316736	-1.520281
H	2.778121	-3.419600	1.765551
H	-7.444414	-3.001248	1.106359
H	-8.314789	0.637539	3.238906
H	-6.669633	3.664530	-2.072511
H	-3.833512	5.618534	0.509909
Rh	-2.690105	-0.433353	-0.721924
O	-1.401796	-1.538873	-2.175252
C	-0.260217	-1.036801	-2.304231
N	0.086055	0.120155	-1.730364
C	-0.867000	0.925030	-1.019653
C	-1.907937	1.545209	-1.759149
H	1.012838	0.493716	-1.964820
H	-3.955125	-1.325826	-0.994623
H	-3.324190	0.555531	-1.863269
H	-2.389475	2.358698	-1.223333
C	-1.377390	2.307559	-5.955229

C	-1.070585	3.268284	-4.987955
C	-1.283226	2.996249	-3.637038
C	-1.795645	1.751295	-3.238738
C	-2.111567	0.795880	-4.209909
C	-1.901772	1.074972	-5.562743
H	-1.217498	2.522823	-7.007880
H	-0.670701	4.234114	-5.284569
H	-1.034354	3.739914	-2.885232
H	-2.528488	-0.157932	-3.904760
H	-2.157542	0.328396	-6.309623
C	-2.863657	-0.403250	3.165135
H	-0.798519	-0.518614	2.510671
H	-1.356198	-1.964169	3.322718
H	-2.612894	-0.124286	4.195055
H	-3.754156	-1.040169	3.228006
H	-2.280199	1.473291	2.222360
H	-3.863406	1.515518	3.013261
C	0.808878	-1.723304	-3.155358
C	-0.402626	1.531435	0.255205
O	-0.952177	2.502054	0.771359
N	0.704623	0.908312	0.780645
C	1.668669	1.493749	1.621229
C	2.140632	2.746999	1.481346
C	1.817209	3.641183	0.353432
C	2.183347	0.557676	2.674406
N	2.065866	-1.989120	-2.465562
C	2.977146	-1.013332	-2.197551
C	4.275177	-1.488540	-1.603830
N	4.772973	-0.684739	-0.556047
C	3.942482	-0.366760	0.487998
C	4.405383	0.526933	1.593668
N	3.570493	0.478856	2.754746
O	1.453179	-0.071053	3.430302
C	5.501665	1.314548	1.489860
O	2.797087	-0.830401	0.495832
C	4.953168	-2.525271	-2.139936
O	2.780253	0.179983	-2.453455
C	6.055351	2.311060	2.399004
C	6.239141	-3.083962	-1.703783
C	7.220291	2.988622	1.978902
C	7.804429	3.974430	2.767926
C	7.233071	4.310260	3.997755
C	6.076943	3.652398	4.429367
C	5.493045	2.661044	3.646605
C	2.024892	3.191270	-0.962546
C	1.720471	4.012847	-2.046615
C	1.206724	5.295523	-1.831359
C	1.013548	5.755255	-0.526103
C	1.322560	4.935760	0.560079
C	6.640435	-3.118145	-0.352604
C	7.865834	-3.674019	0.009903
C	8.716108	-4.202707	-0.964892
C	8.324157	-4.190679	-2.306106
C	7.094798	-3.646024	-2.669861
H	1.013434	-1.086021	-4.022673
H	0.395284	-2.669850	-3.503877
H	0.998817	0.029273	0.368769
H	2.827531	3.113769	2.241556
H	2.132516	-2.850710	-1.934990
H	5.774870	-0.568253	-0.479640
H	3.870259	-0.160467	3.487214
H	6.051132	1.236858	0.553889

H	4.527529	-2.958919	-3.041956
H	7.665832	2.736684	1.019414
H	8.701076	4.481594	2.424411
H	7.685462	5.079545	4.616835
H	5.629855	3.911785	5.384681
H	4.598865	2.158898	3.991146
H	2.451721	2.207331	-1.134320
H	1.887883	3.651255	-3.057326
H	0.971115	5.937988	-2.675685
H	0.623084	6.754365	-0.353374
H	1.159143	5.289917	1.574139
H	5.972060	-2.747068	0.418050
H	8.153983	-3.703695	1.056963
H	9.672064	-4.631999	-0.679766
H	8.974549	-4.610578	-3.067854
H	6.792708	-3.642540	-3.714194

Sum of electronic and zero-point energy: -3953.50958
Sum of electronic and thermal free energies: -3953.617792
Frequency: -634.1374

Supplementary Table 19. **O4R^{TS}** representative 3

C	3.776901	0.916468	-2.130749
C	3.725353	-1.683489	-2.374259
P	3.320098	-2.171653	-0.635783
P	3.681359	1.147690	-0.295034
C	7.241265	-3.524196	1.437049
C	6.055346	-3.374613	2.163505
C	4.885445	-2.979991	1.516797
C	4.882261	-2.744935	0.129498
C	6.070021	-2.917098	-0.593128
C	7.245225	-3.296413	0.060643
H	3.971585	-2.839817	2.087774
H	6.097567	-2.752304	-1.664914
C	0.569770	-5.904630	-0.944054
C	0.275627	-4.743906	-1.663707
C	1.121767	-3.637813	-1.594325
C	2.283733	-3.681352	-0.801972
C	2.579182	-4.854172	-0.088863
C	1.725878	-5.957604	-0.163906
H	0.862831	-2.734387	-2.132249
H	3.470884	-4.917357	0.524293
C	8.181062	1.489306	0.757611
C	7.565519	2.428464	-0.076864
C	6.206200	2.323547	-0.361484
C	5.445270	1.275000	0.188271
C	6.065136	0.348055	1.032721
C	7.429706	0.453879	1.312341
H	5.734312	3.068459	-0.997123
H	5.489357	-0.456791	1.469557
C	1.925915	5.313827	0.690410
C	2.583137	4.552044	1.662766
C	3.134720	3.320151	1.324151
C	3.037804	2.835222	0.007336
C	2.376923	3.600270	-0.961479
C	1.825986	4.839838	-0.616826
H	3.636280	2.725866	2.082829
H	2.271209	3.240766	-1.980266
H	-0.110820	-6.749254	-0.978495
H	8.155746	-3.820992	1.942612
H	1.493847	6.275592	0.951970
H	9.241824	1.571812	0.976685
H	8.162211	-3.414364	-0.509394
H	6.043671	-3.556881	3.234274
H	1.967308	-6.857297	0.395109
H	-0.635528	-4.690142	-2.250512
H	7.896969	-0.280425	1.961473
H	8.144012	3.244063	-0.501059
H	1.319153	5.429156	-1.371065
H	2.663830	4.916907	2.682505
Rh	2.334409	-0.411740	0.658573
O	1.170819	-1.975811	1.638165
C	0.059783	-2.193454	1.100705
N	-0.435443	-1.388372	0.148159
C	0.219983	-0.184075	-0.265687
C	0.349354	0.924382	0.634935
H	-1.342319	-1.606840	-0.258545
H	3.482351	-0.522885	1.723404
H	1.706366	0.763598	1.623240
H	0.691603	1.817105	0.120841
C	-2.478939	2.124817	3.624369

C	-1.903808	3.048651	2.746974
C	-0.931988	2.632770	1.837142
C	-0.538567	1.281149	1.774077
C	-1.084055	0.377290	2.696165
C	-2.055873	0.795102	3.605356
H	-3.246307	2.444268	4.322085
H	-2.218409	4.088296	2.767315
H	-0.489216	3.351064	1.151780
H	-0.735517	-0.644878	2.730389
H	-2.496778	0.072156	4.283307
C	4.521612	-0.373476	-2.541515
H	2.758099	-1.588351	-2.872609
H	4.257059	-2.513852	-2.851626
H	4.764867	-0.281050	-3.606626
H	5.481788	-0.428335	-2.015282
H	2.757157	0.902506	-2.528633
H	4.296105	1.787003	-2.547429
C	-0.781085	-3.381055	1.544061
C	0.173704	0.057327	-1.752014
O	0.701916	-0.664213	-2.591880
N	-0.495360	1.201112	-2.172726
C	-1.624761	1.750774	-1.515765
C	-1.958147	3.061092	-1.565674
C	-1.300595	4.207686	-2.193120
C	-2.577325	0.730813	-0.938192
N	-2.184299	-3.152086	1.316281
C	-2.925388	-3.877265	0.413502
C	-4.271763	-3.277850	0.093153
N	-4.394497	-1.847942	0.082566
C	-4.278972	-1.018039	1.146004
C	-4.333851	0.475400	0.862468
N	-3.315962	1.137556	0.126497
O	-2.649978	-0.393452	-1.453386
C	-5.242192	1.206049	1.541305
O	-4.183815	-1.407293	2.313917
C	-5.235588	-4.086182	-0.393732
O	-2.510123	-4.894399	-0.132096
C	-5.396959	2.668278	1.498349
C	-6.590519	-3.799875	-0.859397
C	-5.284077	3.408430	0.305294
C	-5.375622	4.800087	0.316965
C	-5.588607	5.480151	1.519516
C	-5.739923	4.755734	2.705325
C	-5.656264	3.364146	2.692934
C	-0.342499	4.132905	-3.224181
C	0.187607	5.291150	-3.789399
C	-0.210194	6.550316	-3.330477
C	-1.154164	6.643742	-2.303647
C	-1.700599	5.487537	-1.753616
C	-7.282824	-4.845872	-1.504163
C	-8.576688	-4.665688	-1.985548
C	-9.215601	-3.434891	-1.821168
C	-8.550518	-2.390508	-1.171220
C	-7.253834	-2.564709	-0.696728
H	-0.554295	-3.567165	2.598800
H	-0.466200	-4.259973	0.971569
H	-0.491944	1.261626	-3.186420
H	-2.889833	3.327048	-1.073713
H	-2.689513	-2.524581	1.938878
H	-4.280194	-1.414146	-0.830003
H	-3.059070	2.032979	0.529604
H	-5.854525	0.664910	2.257673

H	-4.932245	-5.128406	-0.468852
H	-5.159001	2.883686	-0.637154
H	-5.301557	5.351638	-0.616678
H	-5.660597	6.563818	1.529230
H	-5.930042	5.275435	3.640033
H	-5.776093	2.805285	3.617344
H	-0.014183	3.175146	-3.604052
H	0.913096	5.210489	-4.593731
H	0.205971	7.449762	-3.774404
H	-1.474047	7.617027	-1.943197
H	-2.449251	5.566089	-0.968280
H	-6.791659	-5.807655	-1.628774
H	-9.087347	-5.485062	-2.482996
H	-10.226884	-3.291077	-2.190841
H	-9.048621	-1.435203	-1.030489
H	-6.759377	-1.749052	-0.184919

Sum of electronic and zero-point energy: -3953.497272
Sum of electronic and thermal free energies: -3953.604566
Frequency: -691.1566

Supplementary Table 20. **O4R^{TS}** representative 4

C	-2.678186	0.643153	2.155603
C	-2.465234	-1.926461	1.735110
P	-2.603069	-1.929846	-0.111548
P	-3.132114	1.251643	0.467322
C	-7.005758	-2.816735	-1.280592
C	-6.041237	-2.528608	-2.251076
C	-4.730420	-2.250560	-1.871224
C	-4.360583	-2.268987	-0.515238
C	-5.326330	-2.589008	0.447537
C	-6.645520	-2.848193	0.066337
H	-3.987528	-2.016894	-2.629099
H	-5.065274	-2.643911	1.498453
C	-0.469383	-5.883691	-1.286796
C	-1.859298	-5.862885	-1.150587
C	-2.515864	-4.678891	-0.809775
C	-1.782929	-3.500554	-0.594502
C	-0.390325	-3.534873	-0.720821
C	0.265419	-4.716281	-1.066467
H	-3.596378	-4.677891	-0.716298
H	0.197237	-2.649220	-0.526445
C	-7.761743	1.009079	0.287559
C	-7.013754	0.764149	-0.863926
C	-5.620175	0.820445	-0.821144
C	-4.958929	1.121900	0.375644
C	-5.720546	1.385775	1.528519
C	-7.112114	1.323619	1.483853
H	-5.046168	0.608866	-1.715352
H	-5.236536	1.646498	2.464516
C	-2.206459	5.780523	0.283185
C	-3.153490	5.209212	-0.572674
C	-3.455198	3.852513	-0.474591
C	-2.816253	3.055567	0.489387
C	-1.874194	3.633882	1.354617
C	-1.570888	4.993586	1.244383
H	-4.186926	3.413453	-1.146973
H	-1.332036	3.029884	2.071154
H	0.037541	-6.805386	-1.558527
H	-8.030977	-3.021974	-1.575086
H	-1.963851	6.835939	0.197374
H	-8.846246	0.957702	0.254940
H	-7.387748	-3.078746	0.825044
H	-6.311766	-2.515884	-3.303155
H	1.347759	-4.713867	-1.140308
H	-2.437707	-6.767721	-1.314273
H	-7.688128	1.524160	2.382597
H	-7.509655	0.515006	-1.796883
H	-0.821341	5.425563	1.900122
H	-3.653491	5.818974	-1.319535
Rh	-1.885427	0.149986	-1.109144
O	-0.639078	-1.067485	-2.594060
C	0.594195	-0.976048	-2.406708
N	1.130792	-0.150503	-1.508205
C	0.354856	0.652621	-0.616944
C	-0.205341	1.854232	-1.122912
H	2.115417	0.112608	-1.617337
H	-3.203870	0.064595	-1.944277
H	-1.763449	1.573871	-1.881659
H	-0.524503	2.531562	-0.339882
C	1.380250	4.009552	-4.476562

C	1.316164	4.579809	-3.203586
C	0.754644	3.866329	-2.144852
C	0.274718	2.561698	-2.342092
C	0.309511	2.008297	-3.629458
C	0.862567	2.728628	-4.687448
H	1.809450	4.567149	-5.303940
H	1.688810	5.586662	-3.035550
H	0.694633	4.316491	-1.158174
H	-0.145154	1.040328	-3.809306
H	0.876138	2.294692	-5.683441
C	-3.158065	-0.779013	2.491715
H	-1.388019	-1.898270	1.928570
H	-2.814634	-2.891644	2.114875
H	-2.955119	-0.942953	3.557176
H	-4.244484	-0.836554	2.372509
H	-1.589064	0.716096	2.227226
H	-3.090932	1.352910	2.881130
C	1.575166	-1.893004	-3.155036
C	0.736509	0.579692	0.818519
O	0.380717	1.429949	1.641471
N	1.572466	-0.452147	1.185579
C	2.111952	-0.485947	2.502884
C	1.763437	-1.381313	3.447459
C	0.823283	-2.505630	3.383040
C	3.107257	0.557411	2.945146
N	2.963819	-1.785373	-2.708447
C	3.324554	-2.075773	-1.427324
C	4.687188	-1.604008	-0.960957
N	4.590417	-0.535295	-0.024205
C	3.996261	0.634307	-0.398031
C	3.629445	1.612596	0.655623
N	3.871443	1.275604	2.015477
O	3.334671	0.755524	4.130745
C	3.192949	2.831336	0.251002
O	3.712560	0.826592	-1.596665
C	5.817569	-2.257348	-1.280455
O	2.556501	-2.624024	-0.630009
C	2.741489	3.975517	1.037319
C	7.192010	-2.017343	-0.828834
C	2.774381	5.240740	0.411236
C	2.360074	6.387686	1.081867
C	1.889657	6.293908	2.394995
C	1.827268	5.045238	3.021597
C	2.246403	3.895084	2.356612
C	0.819217	-3.448636	2.342709
C	-0.060943	-4.532796	2.382464
C	-0.956459	-4.679005	3.442329
C	-0.963802	-3.742572	4.481362
C	-0.068180	-2.676607	4.461114
C	8.113903	-3.076770	-0.932176
C	9.433699	-2.922101	-0.515156
C	9.864217	-1.696909	-0.001098
C	8.967119	-0.628453	0.086419
C	7.644201	-0.783015	-0.319967
H	1.530325	-1.682857	-4.226280
H	1.206786	-2.910332	-2.998985
H	1.780096	-1.210138	0.540951
H	2.229600	-1.213018	4.415651
H	3.567389	-1.127930	-3.188060
H	4.916938	-0.650659	0.929113
H	4.392717	1.984677	2.525827
H	3.208859	2.981576	-0.825707

H	5.690139	-3.122073	-1.930132
H	3.137268	5.313881	-0.610846
H	2.405182	7.352130	0.584345
H	1.568925	7.186753	2.924499
H	1.447882	4.964195	4.036250
H	2.140338	2.938235	2.847486
H	1.527805	-3.357642	1.525902
H	-0.049283	-5.260133	1.578245
H	-1.637449	-5.525257	3.465369
H	-1.650500	-3.855701	5.315697
H	-0.053170	-1.962629	5.280669
H	7.785362	-4.031376	-1.336003
H	10.126576	-3.754482	-0.596182
H	10.894020	-1.571727	0.320517
H	9.302203	0.332166	0.467183
H	6.968865	0.063090	-0.272883

Sum of electronic and zero-point energy: -3953.506884
Sum of electronic and thermal free energies: -3953.612281
Frequency: -538.4606

Supplementary Table 21. **O4R^{TS}** representative 5

C	5.298189	0.368703	1.990182
C	5.504874	-2.054833	1.030929
P	3.934119	-2.260414	0.055274
P	3.672499	0.864384	1.254908
C	3.006559	-6.753467	0.742850
C	3.416744	-6.325752	-0.520501
C	3.701517	-4.977356	-0.749129
C	3.571092	-4.044263	0.289261
C	3.148739	-4.479666	1.556983
C	2.876287	-5.827483	1.782225
H	4.024362	-4.658457	-1.734524
H	3.011330	-3.761384	2.359117
C	4.980248	-1.744672	-4.425492
C	3.661471	-1.929476	-4.003331
C	3.380273	-2.102624	-2.648809
C	4.414347	-2.090745	-1.700104
C	5.738868	-1.917451	-2.132393
C	6.016726	-1.742134	-3.488830
H	2.349192	-2.196400	-2.330183
H	6.562209	-1.919191	-1.426561
C	1.665570	3.972600	4.032053
C	2.172303	2.778174	4.556208
C	2.816609	1.864230	3.724931
C	2.981116	2.148952	2.359190
C	2.472339	3.346929	1.840433
C	1.813696	4.254207	2.674065
H	3.164588	0.920426	4.135123
H	2.576310	3.578967	0.788816
C	5.016373	2.983057	-2.639599
C	5.423855	3.480760	-1.395822
C	5.005372	2.858317	-0.220752
C	4.172434	1.726178	-0.280438
C	3.776269	1.230822	-1.527662
C	4.194086	1.857601	-2.703867
H	5.312006	3.264497	0.739328
H	3.152467	0.351979	-1.593162
H	5.200877	-1.602910	-5.479791
H	2.789179	-7.803300	0.918512
H	5.347003	3.470834	-3.552240
H	1.153237	4.675207	4.683033
H	2.554453	-6.153894	2.767296
H	3.521287	-7.040450	-1.331930
H	7.044590	-1.605105	-3.812573
H	2.845139	-1.922175	-4.719013
H	1.419905	5.173387	2.249476
H	2.053493	2.553217	5.612103
H	3.882425	1.447386	-3.659688
H	6.068960	4.353370	-1.342659
Rh	2.236464	-0.890729	1.076492
O	0.903147	-2.610608	1.130824
C	-0.041577	-2.616894	0.297189
N	-0.317134	-1.561734	-0.465934
C	0.337462	-0.304094	-0.317434
C	0.245547	0.456272	0.885842
H	-1.038619	-1.648580	-1.187691
H	2.950867	-1.339757	2.409063
H	1.288223	-0.080270	2.097874
H	0.663206	1.452605	0.764007
C	-2.985651	0.587332	3.717932

C	-2.590099	1.721821	3.007002
C	-1.513774	1.651260	2.123820
C	-0.838603	0.439008	1.916685
C	-1.208206	-0.681019	2.670840
C	-2.278648	-0.606573	3.559075
H	-3.820054	0.640495	4.411553
H	-3.107583	2.666432	3.153981
H	-1.190098	2.539932	1.588752
H	-0.639043	-1.598226	2.583756
H	-2.557073	-1.482923	4.138372
C	6.089696	-0.631707	1.125504
H	5.263937	-2.429595	2.032066
H	6.251598	-2.739505	0.614011
H	6.234966	-0.208736	0.124639
H	7.090546	-0.717917	1.565804
H	5.888166	1.282234	2.126406
H	5.096463	-0.049441	2.981795
C	-0.873017	-3.890681	0.124289
C	0.627073	0.325881	-1.640487
O	1.091131	-0.293760	-2.587317
N	0.387759	1.703500	-1.750595
C	-0.829134	2.304792	-1.337846
C	-0.931103	3.623862	-1.048453
C	0.089410	4.665293	-0.932381
C	-2.034174	1.397526	-1.433197
N	-2.315478	-3.711679	0.218369
C	-2.990405	-3.114348	-0.812785
C	-4.453304	-2.824672	-0.581944
N	-4.798777	-1.478192	-0.837913
C	-3.982081	-0.488756	-0.359043
C	-4.309134	0.933974	-0.701710
N	-3.182152	1.779530	-0.786265
O	-1.980165	0.359539	-2.085571
C	-5.574884	1.404406	-0.679695
O	-3.030320	-0.755895	0.366364
C	-5.338985	-3.800122	-0.303058
O	-2.447147	-2.829308	-1.877349
C	-6.040863	2.783872	-0.855935
C	-6.793783	-3.688645	-0.133361
C	-5.332594	3.757401	-1.591300
C	-5.835137	5.049726	-1.723678
C	-7.047651	5.403146	-1.124388
C	-7.767425	4.446227	-0.405045
C	-7.273132	3.149865	-0.280750
C	1.446764	4.525309	-1.293830
C	2.340445	5.580257	-1.116019
C	1.912715	6.794836	-0.574543
C	0.570762	6.954654	-0.217451
C	-0.326065	5.906598	-0.402168
C	-7.429108	-2.520553	0.334573
C	-8.813074	-2.477853	0.486914
C	-9.593877	-3.593748	0.172447
C	-8.977034	-4.762984	-0.278250
C	-7.591745	-4.811872	-0.420080
H	-0.539159	-4.599538	0.883236
H	-0.648288	-4.305727	-0.863593
H	0.728836	2.032889	-2.650574
H	-1.938280	3.997323	-0.876628
H	-2.713081	-3.588400	1.140699
H	-5.547733	-1.268223	-1.485667
H	-3.168968	2.581110	-0.170700
H	-6.351387	0.685098	-0.425402

H	-4.934811	-4.809517	-0.258961
H	-4.408968	3.487253	-2.091012
H	-5.283936	5.781871	-2.307401
H	-7.434339	6.412763	-1.228408
H	-8.716884	4.707969	0.052974
H	-7.841344	2.407835	0.275169
H	1.820026	3.592103	-1.692770
H	3.378946	5.441907	-1.399834
H	2.615331	7.612099	-0.440068
H	0.222927	7.896459	0.197036
H	-1.369447	6.042328	-0.126682
H	-6.830544	-1.660146	0.614206
H	-9.284955	-1.572994	0.860293
H	-10.673168	-3.555144	0.287964
H	-9.574484	-5.638793	-0.514539
H	-7.117007	-5.726219	-0.767513

Sum of electronic and zero-point energy: -3953.487388
Sum of electronic and thermal free energies: -3953.597388
Frequency: -578.561

Supplementary Table 22. **O1R2R^{TS}** representative 1

C	-4.217111	0.309705	1.897625
C	-2.216309	-0.944309	2.963380
P	-1.484059	-1.801786	1.493534
P	-4.187131	-0.332883	0.165410
C	-2.806778	-6.241442	1.577198
C	-2.168610	-5.697252	0.458009
C	-1.767284	-4.362190	0.463669
C	-1.983655	-3.559685	1.598646
C	-2.606359	-4.117716	2.722726
C	-3.023442	-5.450996	2.706774
H	-1.302941	-3.927243	-0.417556
H	-2.782195	-3.522864	3.613056
C	3.068166	-1.714833	2.439115
C	2.464668	-2.912934	2.050858
C	1.096275	-2.957766	1.776814
C	0.312872	-1.797724	1.883196
C	0.929781	-0.594525	2.263867
C	2.293183	-0.560156	2.551057
H	0.643431	-3.899600	1.487248
H	0.350007	0.319972	2.330028
C	-7.464124	-3.593716	0.536525
C	-6.136262	-3.976311	0.347026
C	-5.142527	-3.008011	0.186656
C	-5.468710	-1.647459	0.226290
C	-6.809458	-1.267720	0.417627
C	-7.799920	-2.236485	0.567136
H	-4.116924	-3.314533	0.030145
H	-7.082431	-0.215916	0.433891
C	-6.042275	2.882046	-2.599480
C	-5.873381	1.563667	-3.036316
C	-5.333874	0.610384	-2.177725
C	-4.953802	0.965458	-0.871168
C	-5.109451	2.289322	-0.441298
C	-5.662195	3.239493	-1.306675
H	-5.203007	-0.412905	-2.518980
H	-4.792783	2.599181	0.548809
H	4.133181	-1.660642	2.645003
H	-3.132447	-7.277694	1.567777
H	-6.468551	3.625553	-3.266860
H	-8.237828	-4.346983	0.655338
H	-3.517972	-5.869614	3.578561
H	-1.996482	-6.308782	-0.423181
H	2.771153	0.371029	2.828320
H	3.057705	-3.818086	1.956338
H	-8.833899	-1.932998	0.704057
H	-5.863323	-5.027293	0.321302
H	-5.794874	4.260525	-0.964195
H	-6.163518	1.280219	-4.043754
Rh	-2.100493	-0.851273	-0.581935
O	-0.184897	-1.583700	-1.373515
C	0.784307	-0.783550	-1.283304
N	0.583953	0.528522	-1.074218
C	-0.708657	1.036695	-0.721096
C	-1.713418	1.229952	-1.722712
H	1.392472	0.983741	-0.624023
H	-2.840846	-2.126471	-1.112175
H	-2.507475	-0.062173	-1.978673
H	-2.524949	1.869059	-1.379737
C	-0.700553	2.003777	-5.827084

C	-1.327140	2.974746	-5.042636
C	-1.669905	2.689901	-3.720733
C	-1.377484	1.434891	-3.167894
C	-0.766206	0.457877	-3.963331
C	-0.427463	0.745109	-5.285631
H	-0.438548	2.222357	-6.858324
H	-1.556738	3.950757	-5.460829
H	-2.166214	3.442394	-3.111845
H	-0.593321	-0.532392	-3.554923
H	0.041080	-0.020259	-5.898225
C	-3.740478	-0.727330	2.932641
H	-4.269070	-1.677565	2.789881
H	-4.035502	-0.362094	3.923567
H	-1.921534	-1.497750	3.861780
H	-1.720423	0.029400	3.002015
H	-3.583481	1.199367	1.929888
H	-5.252475	0.598580	2.111492
C	5.001935	1.989616	1.923274
C	4.488644	3.256483	2.633216
N	5.140830	2.132886	0.550347
C	5.057112	0.953753	-0.251604
C	6.120191	0.205381	-0.627972
C	3.641196	0.535145	-0.444729
O	2.774072	1.094499	0.242335
N	3.318911	-0.433197	-1.363717
C	2.181618	-1.299539	-1.369615
C	2.353002	-2.630636	-1.548440
C	3.622919	-3.364153	-1.578308
N	3.024790	3.300641	2.618751
C	2.338803	3.680333	1.512143
C	0.803469	3.641546	1.582362
N	0.357654	2.864965	0.433172
C	-0.671893	1.969311	0.466161
O	-1.471232	1.920923	1.402313
C	0.268289	5.096952	1.557445
O	2.893204	4.081582	0.486746
O	5.226786	0.957402	2.531675
C	7.550887	0.388266	-0.422266
C	-1.235174	5.161943	1.445957
C	4.685117	-3.063917	-0.700320
C	5.874739	-3.788659	-0.750645
C	6.028610	-4.823942	-1.677677
C	4.975132	-5.147161	-2.537525
C	3.779598	-4.432985	-2.480436
C	8.136817	1.520284	0.181756
C	9.517377	1.600560	0.329747
C	10.341684	0.559191	-0.110343
C	9.777021	-0.569077	-0.709726
C	8.396746	-0.650714	-0.866370
C	-2.046164	5.026675	2.578895
C	-3.435962	5.059267	2.469485
C	-4.034040	5.230112	1.218274
C	-3.234622	5.359483	0.080270
C	-1.844495	5.323089	0.195643
H	4.861196	4.166614	2.155229
H	4.825766	3.224018	3.669814
H	4.607250	2.925827	0.189215
H	5.892373	-0.719084	-1.152611
H	4.087909	-0.794149	-1.914170
H	1.446996	-3.203666	-1.719855
H	2.530612	2.838333	3.369073
H	0.930421	2.966799	-0.395470

H	4.555078	-2.293215	0.051306
H	6.676428	-3.550627	-0.056831
H	6.956864	-5.386342	-1.718413
H	5.083669	-5.960125	-3.249468
H	2.961572	-4.690626	-3.148336
H	7.504415	2.329177	0.522593
H	9.956197	2.479294	0.793429
H	11.418610	0.628443	0.013500
H	10.411144	-1.379954	-1.055908
H	7.958819	-1.529493	-1.334898
H	-1.584662	4.899426	3.555727
H	-4.051707	4.965778	3.359892
H	-5.116971	5.276394	1.136408
H	-3.690314	5.499948	-0.895663
H	-1.224522	5.433969	-0.690864
H	0.741390	5.603865	0.709729
H	0.614197	5.599926	2.469443
H	0.435711	3.131027	2.477641

Sum of electronic and zero-point energy: -3954.700451
Sum of electronic and thermal free energies: -3954.809088
Frequency: -789.401

Supplementary Table 23. **O1R2R^{TS}** representative 2

C	4.923432	-1.960661	-2.024701
C	2.720851	-2.538692	-3.326574
P	1.437026	-1.635168	-2.336260
P	4.258575	-0.847332	-0.696795
C	-2.308444	-4.382391	-2.302662
C	-1.077801	-4.840031	-1.821850
C	0.043519	-4.014661	-1.865168
C	-0.043913	-2.723744	-2.412583
C	-1.278473	-2.273527	-2.902335
C	-2.404669	-3.099573	-2.842508
H	0.979879	-4.360877	-1.437974
H	-1.368966	-1.282099	-3.332150
C	0.346202	2.216750	-4.659435
C	-0.213609	1.948858	-3.406944
C	0.111535	0.770624	-2.737990
C	0.991346	-0.159270	-3.318013
C	1.527290	0.105888	-4.586384
C	1.208001	1.292226	-5.250241
H	-0.316114	0.576543	-1.759416
H	2.199590	-0.595983	-5.066689
C	7.181130	-0.940965	2.880718
C	7.099394	-2.047386	2.031941
C	6.242402	-2.024388	0.930929
C	5.468565	-0.884816	0.667897
C	5.549160	0.227036	1.524294
C	6.404874	0.192199	2.625811
H	6.182816	-2.897205	0.287868
H	4.936637	1.103769	1.337109
C	4.826698	3.243218	-2.793067
C	5.935577	2.490431	-2.391747
C	5.756735	1.277325	-1.728831
C	4.459455	0.806526	-1.458852
C	3.359194	1.573451	-1.851247
C	3.537336	2.784422	-2.521980
H	6.624947	0.707185	-1.409282
H	2.359347	1.234332	-1.630638
H	0.111152	3.147246	-5.167851
H	-3.185547	-5.020520	-2.251116
H	4.971773	4.186785	-3.311548
H	7.847639	-0.962902	3.738150
H	-3.353330	-2.741539	-3.234447
H	-0.993387	-5.838196	-1.400594
H	1.639816	1.492592	-6.226643
H	-0.875576	2.663897	-2.937058
H	6.464808	1.053977	3.284427
H	7.702892	-2.929609	2.225428
H	2.665502	3.357782	-2.824472
H	6.940616	2.850204	-2.592692
Rh	2.185913	-1.542786	-0.047573
O	0.240247	-2.312651	0.522098
C	-0.612660	-1.416380	0.754785
N	-0.247815	-0.132779	0.933620
C	1.152084	0.192117	1.078895
C	1.925437	-0.527348	2.037495
H	-0.970347	0.489319	1.317184
H	2.762861	-2.977344	-0.407005
H	2.837467	-1.911788	1.380707
H	2.869665	-0.043731	2.275194
C	0.085131	-2.565642	5.355732

C	1.097775	-3.207478	4.638898
C	1.690588	-2.579792	3.543506
C	1.283207	-1.299697	3.149567
C	0.265182	-0.660047	3.877037
C	-0.327103	-1.288159	4.972613
H	-0.379011	-3.058309	6.205372
H	1.424267	-4.202443	4.928049
H	2.457599	-3.094530	2.972265
H	-0.056878	0.337432	3.595249
H	-1.112713	-0.777022	5.522197
C	4.128405	-1.904150	-3.345288
H	4.715020	-2.446142	-4.096888
H	4.077693	-0.866000	-3.692536
H	2.769389	-3.541105	-2.888036
H	2.350659	-2.660011	-4.350300
H	5.958776	-1.655343	-2.214772
H	4.937185	-2.982441	-1.632567
C	-2.954999	2.855212	-0.541966
C	-2.669040	4.361006	-0.483064
N	-4.192553	2.422285	-0.169399
C	-4.442750	1.053775	0.065284
C	-5.630888	0.450408	-0.154489
C	-3.309959	0.354904	0.770925
O	-2.688618	0.900480	1.687381
N	-3.034622	-0.893871	0.310865
C	-2.051125	-1.801871	0.802362
C	-2.365793	-3.082478	1.090380
C	-3.698792	-3.686651	1.143264
N	-1.371419	4.533376	0.135647
C	-0.229082	4.444201	-0.629862
C	0.992743	3.874083	0.104914
N	0.680765	2.453383	0.313117
C	1.605708	1.586080	0.797548
O	2.754224	1.947768	1.081231
C	1.410131	4.631191	1.407452
O	-0.198877	4.725497	-1.819015
O	-2.070125	2.060055	-0.861537
C	-6.847232	1.003129	-0.756554
C	0.573973	4.381272	2.646132
C	-4.848582	-2.978789	1.546938
C	-6.093609	-3.603019	1.569759
C	-6.218077	-4.942280	1.187421
C	-5.082410	-5.663553	0.810396
C	-3.833561	-5.045520	0.802298
C	-6.843092	2.060089	-1.689930
C	-8.037148	2.530877	-2.231428
C	-9.257004	1.963576	-1.852577
C	-9.275692	0.905339	-0.940356
C	-8.082925	0.424680	-0.406505
C	-0.446733	5.266080	3.028897
C	-1.228263	5.018191	4.161135
C	-0.992580	3.884486	4.939760
C	0.039118	3.010505	4.587296
C	0.814002	3.256910	3.453329
H	-3.437097	4.909677	0.071171
H	-2.611827	4.760461	-1.499903
H	-4.924459	3.090454	0.041959
H	-5.725636	-0.566636	0.221170
H	-3.566434	-1.227428	-0.484677
H	-1.522648	-3.747223	1.253206
H	-1.298907	4.205553	1.093288
H	-0.215721	2.118012	-0.027688

H	-4.753244	-1.953542	1.886791
H	-6.967415	-3.049013	1.902037
H	-7.190634	-5.425459	1.202106
H	-5.168969	-6.710140	0.533069
H	-2.950022	-5.608917	0.515481
H	-5.901775	2.483629	-2.023729
H	-8.015570	3.337312	-2.958846
H	-10.185694	2.336528	-2.274275
H	-10.218859	0.451649	-0.650399
H	-8.101306	-0.403472	0.298017
H	-0.626500	6.159967	2.436139
H	-2.009599	5.719900	4.440433
H	-1.594406	3.693225	5.823683
H	0.250895	2.140535	5.203230
H	1.634010	2.591344	3.202673
H	1.418955	5.700015	1.163159
H	2.441311	4.332912	1.606563
H	1.829007	3.956966	-0.593673

Sum of electronic and zero-point energy: -3954.706203
Sum of electronic and thermal free energies: -3954.813851
Frequency: -518.4731

Supplementary Table 24. **O1R2R^{TS}** representative 3

C	-4.873373	-1.889190	1.761058
C	-2.875401	-1.605072	3.420813
P	-1.597345	-0.828286	2.314521
P	-4.135922	-1.385392	0.132884
C	2.505811	-2.093200	4.070526
C	2.318856	-0.798538	3.588054
C	1.079217	-0.410473	3.076653
C	0.007197	-1.314810	3.053117
C	0.211733	-2.626941	3.509029
C	1.451326	-3.009768	4.019978
H	0.957747	0.598675	2.701416
H	-0.588403	-3.358683	3.456591
C	-2.301175	3.598477	3.491535
C	-1.677640	2.728551	4.391860
C	-1.433630	1.405216	4.029314
C	-1.793459	0.942057	2.749966
C	-2.411948	1.821880	1.853905
C	-2.677120	3.141389	2.228869
H	-0.949783	0.735798	4.734609
H	-2.682191	1.478212	0.864924
C	-6.487563	-4.108281	-2.797526
C	-6.864478	-2.774072	-2.640059
C	-6.156160	-1.940210	-1.772018
C	-5.054312	-2.437382	-1.059582
C	-4.678816	-3.781669	-1.223841
C	-5.396532	-4.611696	-2.083639
H	-6.461568	-0.905242	-1.658708
H	-3.820623	-4.173942	-0.687324
C	-5.563333	2.939233	-0.743467
C	-4.651896	2.296624	-1.585044
C	-4.245670	0.992105	-1.306937
C	-4.741018	0.313728	-0.183130
C	-5.665274	0.962885	0.651844
C	-6.068724	2.269664	0.373043
H	-3.521063	0.525719	-1.961430
H	-6.077082	0.466966	1.523215
H	-2.491189	4.630676	3.771156
H	3.471520	-2.397309	4.462484
H	-5.881399	3.955697	-0.957092
H	-7.039064	-4.753539	-3.475195
H	1.596207	-4.025692	4.376322
H	3.135042	-0.081921	3.600079
H	-3.164024	3.814570	1.533087
H	-1.384410	3.079886	5.377060
H	-5.098725	-5.649642	-2.202220
H	-7.710436	-2.376746	-3.193462
H	-6.779201	2.762575	1.030103
H	-4.240690	2.805636	-2.450962
Rh	-1.871830	-1.755649	0.114710
O	0.146069	-2.535124	0.332065
C	1.068842	-1.819288	-0.136367
N	0.799779	-0.806034	-0.970080
C	-0.532202	-0.479922	-1.383113
C	-1.226299	-1.393724	-2.206298
H	1.562507	-0.312252	-1.437292
H	-2.406469	-3.040736	0.848879
H	-2.096506	-2.565824	-1.264318
H	-2.121643	-0.993635	-2.675752
C	0.815982	-4.298060	-4.641757

C	1.286612	-2.988200	-4.532663
C	0.630349	-2.069925	-3.712812
C	-0.510784	-2.455380	-2.988801
C	-0.981790	-3.768022	-3.112337
C	-0.323430	-4.683936	-3.932048
H	1.330962	-5.012792	-5.277382
H	2.166663	-2.675036	-5.087401
H	0.999174	-1.050426	-3.649707
H	-1.862254	-4.075302	-2.554640
H	-0.699269	-5.699940	-4.013228
C	-4.318489	-1.227986	3.039095
H	-4.970052	-1.538374	3.865043
H	-4.407112	-0.137068	2.979441
H	-2.744591	-2.691448	3.377510
H	-2.669864	-1.280356	4.446669
H	-5.955022	-1.726401	1.692115
H	-4.725062	-2.973871	1.803173
C	3.052297	1.813551	-2.429115
C	2.445566	3.040079	-3.115114
N	4.039842	2.044915	-1.521705
C	4.492516	1.021741	-0.650112
C	5.781341	0.825746	-0.306310
C	3.376450	0.255137	0.011618
O	2.455356	0.837870	0.578330
N	3.456436	-1.105619	-0.129108
C	2.477774	-2.057283	0.262708
C	2.795300	-3.220901	0.873201
C	4.093588	-3.657469	1.381347
N	1.145015	3.269794	-2.495514
C	1.129980	3.606212	-1.163580
C	-0.148383	3.199779	-0.407703
N	-0.237692	1.730813	-0.454509
C	-0.801302	0.993844	-1.450517
O	-1.455289	1.487129	-2.379875
C	-1.421039	3.933537	-0.875400
O	2.099071	4.109813	-0.605922
O	2.591563	0.684862	-2.636804
C	6.996656	1.509725	-0.754471
C	-1.622979	5.306665	-0.257545
C	4.338738	-5.040390	1.485227
C	5.553616	-5.517484	1.972054
C	6.540011	-4.620797	2.389998
C	6.300261	-3.244438	2.323249
C	5.093806	-2.765004	1.821059
C	7.080020	2.275376	-1.935418
C	8.277771	2.884465	-2.299989
C	9.414354	2.750115	-1.497306
C	9.350431	1.986978	-0.329253
C	8.156726	1.367989	0.032203
C	-2.918686	5.847936	-0.270113
C	-3.184690	7.097733	0.286623
C	-2.151020	7.836869	0.868618
C	-0.858339	7.314156	0.879441
C	-0.592943	6.060231	0.319731
H	2.303264	2.817387	-4.173853
H	3.063540	3.934357	-3.010606
H	4.225776	3.009992	-1.266809
H	5.947290	0.069719	0.460495
H	4.258812	-1.459778	-0.636477
H	1.976336	-3.926862	0.973301
H	0.368452	2.716897	-2.847222
H	0.424663	1.253304	0.151099

H	3.569020	-5.740591	1.170546
H	5.728266	-6.587627	2.033236
H	7.484978	-4.991132	2.776624
H	7.054700	-2.544490	2.671720
H	4.898473	-1.699085	1.811841
H	6.214742	2.369253	-2.580630
H	8.326784	3.463581	-3.217704
H	10.344689	3.231249	-1.784596
H	10.230648	1.870422	0.296184
H	8.113946	0.770850	0.940173
H	-3.728052	5.273289	-0.715814
H	-4.196617	7.493885	0.269274
H	-2.352908	8.810785	1.305528
H	-0.045476	7.882129	1.323903
H	0.425107	5.683629	0.338714
H	-2.280122	3.304538	-0.634151
H	-1.427664	4.010444	-1.966773
H	0.033353	3.440517	0.641185

Sum of electronic and zero-point energy: -3954.700878
Sum of electronic and thermal free energies: -3954.809186
Frequency: -514.8898

Supplementary Table 25. **O1R2R^{TS}** representative 4

C	4.248487	-0.198249	0.810126
C	3.019099	1.423318	2.425513
P	1.847186	2.289867	1.275540
P	3.578201	0.263271	-0.860199
C	3.607274	6.505892	0.396652
C	2.597256	5.968294	-0.405177
C	2.098291	4.692066	-0.141244
C	2.593071	3.939513	0.938284
C	3.596479	4.496144	1.746043
C	4.105473	5.767296	1.470609
H	1.320842	4.274820	-0.775009
H	3.989574	3.950305	2.597414
C	-1.695886	3.283937	4.142118
C	-1.128677	4.292049	3.358887
C	-0.073629	4.000999	2.492649
C	0.429489	2.692669	2.395726
C	-0.157273	1.678628	3.173077
C	-1.207288	1.977807	4.045356
H	0.360783	4.800676	1.903632
H	0.187581	0.653050	3.093931
C	7.018671	2.911500	-2.521978
C	5.758923	3.475357	-2.325288
C	4.705703	2.694035	-1.842514
C	4.905225	1.340154	-1.549465
C	6.179677	0.777575	-1.753380
C	7.227189	1.559062	-2.235682
H	3.729029	3.138546	-1.694761
H	6.352341	-0.276559	-1.554536
C	3.907206	-3.534318	-3.513708
C	3.974815	-3.666141	-2.127571
C	3.883127	-2.538118	-1.305102
C	3.729064	-1.264555	-1.872035
C	3.657470	-1.140835	-3.271683
C	3.747262	-2.267782	-4.085165
H	3.935686	-2.673936	-0.230449
H	3.541078	-0.160659	-3.725980
H	-2.509875	3.512873	4.824538
H	4.001176	7.496340	0.187143
H	3.980239	-4.412169	-4.149412
H	7.835668	3.518911	-2.901021
H	4.888508	6.179901	2.100399
H	2.199143	6.540039	-1.238843
H	-1.657400	1.182751	4.632869
H	-1.499550	5.310974	3.426346
H	8.204008	1.111228	-2.394500
H	5.587524	4.524756	-2.546795
H	3.696950	-2.157654	-5.164613
H	4.102195	-4.642643	-1.670677
Rh	1.410108	1.019802	-0.740363
O	-0.643009	1.804814	-0.747676
C	-1.449286	1.132934	-0.043180
N	-1.094710	-0.061907	0.451435
C	0.106079	-0.726023	0.033510
C	0.306760	-0.953972	-1.364648
H	-1.704745	-0.555364	1.112183
H	1.943264	2.219214	-1.612092
H	1.166776	0.242380	-2.153575
H	1.090833	-1.677464	-1.585399
C	-2.884442	-1.209411	-4.264718

C	-1.978248	-0.152936	-4.349724
C	-0.954714	-0.026165	-3.408304
C	-0.824278	-0.952032	-2.366833
C	-1.748266	-2.007864	-2.281042
C	-2.764480	-2.136841	-3.227992
H	-3.678692	-1.310915	-4.998779
H	-2.061817	0.576318	-5.150899
H	-0.258869	0.804128	-3.475090
H	-1.672464	-2.741609	-1.481303
H	-3.465685	-2.962131	-3.153311
C	4.354489	0.972887	1.805630
H	4.876358	1.818411	1.341955
H	4.997553	0.638508	2.629052
H	3.201799	2.071040	3.289792
H	2.470651	0.549680	2.793628
H	3.611590	-0.984338	1.229506
H	5.242308	-0.631532	0.649200
C	-3.286661	-2.563400	2.074556
C	-3.197779	-4.012842	2.588979
N	-4.436902	-2.154894	1.486483
C	-4.623951	-0.826443	1.026796
C	-5.408111	-0.518230	-0.027471
C	-4.110826	0.220644	1.987568
O	-4.349362	0.117109	3.182078
N	-3.402907	1.310462	1.514784
C	-2.822668	1.647748	0.252009
C	-3.365040	2.523087	-0.626217
C	-4.636882	3.243390	-0.627254
N	-1.792635	-4.358798	2.745189
C	-1.037552	-4.369073	1.600267
C	0.469051	-4.046724	1.731309
N	0.702422	-2.990893	0.734715
C	0.622218	-1.664735	1.103335
O	0.877989	-1.296769	2.249780
C	1.320491	-5.299998	1.489044
O	-1.532373	-4.562781	0.493107
O	-2.309637	-1.822406	2.199233
C	-6.154754	-1.411243	-0.922956
C	2.825580	-5.124323	1.604340
C	-5.547553	3.291902	0.451451
C	-6.733413	4.014245	0.343552
C	-7.041928	4.703309	-0.833070
C	-6.150479	4.671640	-1.907795
C	-4.962919	3.953671	-1.802596
C	-5.783430	-2.741991	-1.207942
C	-6.558099	-3.530526	-2.057942
C	-7.715775	-3.012882	-2.643535
C	-8.085946	-1.690306	-2.387680
C	-7.310500	-0.898374	-1.544900
C	3.421755	-4.119117	2.378612
C	4.812645	-4.047415	2.506506
C	5.631449	-4.977249	1.864799
C	5.048803	-5.981969	1.088646
C	3.660851	-6.049548	0.959657
H	-3.670138	-4.708239	1.891416
H	-3.701219	-4.098694	3.557077
H	-5.190021	-2.818162	1.342819
H	-5.585008	0.541717	-0.188727
H	-3.096392	1.891856	2.293482
H	-2.745065	2.712856	-1.499177
H	-1.348105	-3.932594	3.549347
H	0.274092	-3.226041	-0.154017

H	-5.322167	2.776427	1.376392
H	-7.418929	4.044194	1.185723
H	-7.968421	5.265329	-0.908689
H	-6.378711	5.208508	-2.823936
H	-4.269899	3.933932	-2.639982
H	-4.861114	-3.147790	-0.805525
H	-6.251729	-4.551431	-2.269193
H	-8.318834	-3.631988	-3.301300
H	-8.978243	-1.275065	-2.847310
H	-7.602830	0.130420	-1.350594
H	2.810407	-3.377824	2.885380
H	5.254183	-3.265966	3.119760
H	6.711192	-4.924035	1.971436
H	5.673535	-6.715804	0.586687
H	3.215758	-6.841033	0.360144
H	1.067450	-5.703721	0.501040
H	0.991434	-6.061257	2.212060
H	0.680886	-3.609890	2.708059

Sum of electronic and zero-point energy: -3954.700668
Sum of electronic and thermal free energies: -3954.816455
Frequency: -724.5988

Supplementary Table 26. **O1R2R^{TS}** representative 5

C	4.023086	3.715705	-0.547896
C	4.907509	1.453594	-1.444043
P	3.607925	0.272264	-0.841067
P	2.379182	3.330210	0.229961
C	6.236463	-3.114432	0.943796
C	5.629582	-2.181942	1.789072
C	4.828703	-1.169408	1.259109
C	4.626592	-1.081501	-0.126933
C	5.242955	-2.019593	-0.971719
C	6.042738	-3.030607	-0.437395
H	4.342673	-0.463832	1.922666
H	5.087372	-1.973991	-2.045216
C	1.436271	-1.582386	-4.490862
C	1.491734	-2.262337	-3.270621
C	2.207902	-1.721045	-2.205838
C	2.861762	-0.483903	-2.335028
C	2.817485	0.179281	-3.569366
C	2.111933	-0.370750	-4.641103
H	2.274130	-2.275006	-1.276902
H	3.333572	1.123546	-3.712010
C	2.411297	6.364777	3.743893
C	2.614452	6.798414	2.430665
C	2.593115	5.881784	1.381530
C	2.364401	4.514127	1.631035
C	2.167464	4.089779	2.952620
C	2.189177	5.012118	4.001340
H	2.738306	6.240243	0.366467
H	2.012672	3.039105	3.167969
C	-0.778441	4.753038	-2.870947
C	-0.697149	5.400623	-1.635998
C	0.241016	4.993303	-0.685121
C	1.116697	3.930861	-0.965066
C	1.001747	3.262005	-2.196187
C	0.068460	3.677102	-3.144554
H	0.287938	5.507983	0.268037
H	1.593360	2.378216	-2.402143
H	0.885780	-2.005549	-5.326913
H	6.858031	-3.902540	1.359648
H	-1.503499	5.080512	-3.610782
H	2.429459	7.079862	4.561159
H	6.512175	-3.751601	-1.100450
H	5.772109	-2.245822	2.863922
H	2.093297	0.149927	-5.594479
H	0.972760	-3.209535	-3.145547
H	2.036136	4.667236	5.019675
H	2.790208	7.849843	2.222921
H	-0.003527	3.141637	-4.086459
H	-1.361432	6.230190	-1.410350
Rh	2.026187	1.134884	0.722998
O	1.863933	-1.007889	1.295271
C	0.891303	-1.629061	0.789736
N	-0.065252	-0.960961	0.120085
C	-0.065272	0.448179	-0.050668
C	-0.241295	1.311408	1.117819
H	-0.754397	-1.508825	-0.380967
H	3.158183	1.402693	1.777944
H	1.081811	1.618573	1.995850
H	-0.503036	2.331437	0.838989
C	-2.765420	-0.350510	4.172362

C	-1.419601	-0.717756	4.140563
C	-0.554390	-0.145837	3.206207
C	-1.034492	0.790285	2.285062
C	-2.383256	1.177710	2.337347
C	-3.243610	0.605959	3.273710
H	-3.435546	-0.802592	4.898245
H	-1.041352	-1.465869	4.829561
H	0.489862	-0.437165	3.183104
H	-2.768532	1.931836	1.656010
H	-4.284912	0.912238	3.290305
C	4.470317	2.892089	-1.764741
H	5.338070	3.405337	-2.197379
H	3.699524	2.915820	-2.540743
H	5.659101	1.472752	-0.645962
H	5.386379	0.995484	-2.316916
H	3.986707	4.775330	-0.821536
H	4.752455	3.618044	0.265262
C	-2.317106	-3.100051	-2.063903
C	-2.667594	-2.344881	-3.360262
N	-2.885850	-2.569694	-0.933610
C	-2.897075	-3.046262	0.416805
C	-3.995388	-2.890143	1.193335
C	-1.612655	-3.368461	1.146185
O	-1.548271	-3.330987	2.367858
N	-0.484159	-3.582400	0.374225
C	0.773550	-3.102625	0.820979
C	1.873544	-3.840426	1.097584
C	2.027339	-5.287852	1.125748
N	-2.386500	-0.917378	-3.304495
C	-3.273778	-0.043220	-2.759447
C	-2.730912	1.392421	-2.552018
N	-1.868909	1.362251	-1.367978
C	-0.637257	0.781934	-1.393962
O	-0.107970	0.417917	-2.448947
C	-3.854547	2.445014	-2.394869
O	-4.397002	-0.392430	-2.387071
O	-1.559677	-4.070146	-2.087223
C	-5.323862	-2.371331	0.875830
C	-4.352001	2.672899	-0.976690
C	0.947229	-6.180885	1.282992
C	1.172381	-7.553467	1.308199
C	2.468935	-8.061175	1.169816
C	3.548774	-7.186511	1.023341
C	3.331314	-5.811513	1.012166
C	-6.047957	-1.775979	1.930902
C	-7.303535	-1.216811	1.714038
C	-7.871627	-1.246926	0.436088
C	-7.181073	-1.857148	-0.613676
C	-5.924365	-2.418847	-0.398355
C	-5.260551	1.801550	-0.356067
C	-5.714713	2.059567	0.939101
C	-5.267409	3.183906	1.637228
C	-4.347026	4.046482	1.037193
C	-3.891939	3.787745	-0.257588
H	-3.731393	-2.476840	-3.583002
H	-2.077581	-2.799306	-4.156850
H	-3.581604	-1.846030	-1.117742
H	-3.811408	-3.096246	2.243997
H	-0.603254	-3.956422	-0.571153
H	2.777607	-3.264052	1.285602
H	-1.420880	-0.604691	-3.405725
H	-2.345100	1.453808	-0.478275

H	-0.054380	-5.790321	1.415586
H	0.335194	-8.232564	1.441230
H	2.636566	-9.134373	1.186012
H	4.557745	-7.576936	0.925668
H	4.169278	-5.127088	0.903785
H	-5.603930	-1.745576	2.922316
H	-7.843681	-0.763298	2.540593
H	-8.851459	-0.811061	0.263941
H	-7.623371	-1.901794	-1.604303
H	-5.425466	-2.919289	-1.219974
H	-5.608541	0.924465	-0.889791
H	-6.421896	1.374761	1.396412
H	-5.628989	3.385092	2.641870
H	-3.987658	4.921039	1.572784
H	-3.176972	4.461757	-0.722209
H	-4.684619	2.143413	-3.040569
H	-3.464671	3.391521	-2.781342
H	-2.095410	1.654740	-3.401714

Sum of electronic and zero-point energy: -3954.701753
Sum of electronic and thermal free energies: -3954.80921
Frequency: -720.8475

Supplementary Table 27. **O1R2S^{TS}** representative 1

C	-5.235182	-1.465943	-1.008636
P	-4.160598	-0.735168	0.314113
P	-1.871262	-1.528450	-2.091163
C	-6.114148	-1.440966	4.440073
C	-6.344271	-2.350275	3.404819
C	-5.790278	-2.131223	2.142891
C	-5.010000	-0.990749	1.907820
C	-4.779877	-0.076063	2.950945
C	-5.331760	-0.306380	4.211403
H	-5.966711	-2.854443	1.352249
H	-4.173494	0.809656	2.777029
C	-4.844171	3.699715	-0.811282
C	-5.793019	3.007807	-0.054943
C	-5.554635	1.688197	0.324699
C	-4.353612	1.051625	-0.037314
C	-3.405350	1.752911	-0.791778
C	-3.656842	3.069252	-1.182752
H	-6.300052	1.159301	0.910418
H	-2.467278	1.284771	-1.063160
C	0.643007	-5.163321	-3.574067
C	-0.297862	-5.309705	-2.550522
C	-1.034916	-4.210472	-2.112440
C	-0.850760	-2.946200	-2.698625
C	0.086512	-2.812064	-3.734003
C	0.831760	-3.913210	-4.162694
H	-1.734849	-4.331981	-1.292888
H	0.247951	-1.851928	-4.209870
C	0.127766	2.012918	-4.314945
C	0.825645	1.265951	-3.361344
C	0.184108	0.234687	-2.680443
C	-1.155908	-0.085350	-2.961419
C	-1.857010	0.683702	-3.901013
C	-1.215579	1.730382	-4.570455
H	0.746617	-0.334497	-1.948659
H	-2.897265	0.473236	-4.126990
H	-5.025708	4.728096	-1.110134
H	-6.543993	-1.616347	5.421962
H	0.622401	2.823785	-4.841676
H	1.223797	-6.017607	-3.910005
H	-5.151323	0.403509	5.013382
H	-6.954940	-3.231557	3.578554
H	-2.926266	3.611899	-1.769439
H	-6.719474	3.492606	0.239124
H	1.560184	-3.788649	-4.958605
H	-0.453259	-6.278747	-2.084384
H	-1.766858	2.315802	-5.300988
H	1.859458	1.492225	-3.120671
Rh	-2.084819	-1.677662	0.309267
O	-0.080085	-2.576816	0.167286
C	0.865215	-1.794189	0.456784
N	0.638537	-0.649625	1.112861
C	-0.680774	-0.229255	1.476165
C	-1.379769	-0.974478	2.451853
H	1.416182	-0.132324	1.525287
H	-2.893335	-2.974803	-0.115222
H	-2.477648	-2.274267	1.745314
H	-2.240142	-0.469034	2.880792
C	0.676119	-3.576868	5.199460
C	1.109401	-2.268842	4.973126

C	0.444331	-1.456066	4.055419
C	-0.671127	-1.942529	3.351412
C	-1.099816	-3.253978	3.587155
C	-0.431451	-4.065792	4.504186
H	1.197836	-4.210866	5.910840
H	1.968545	-1.876066	5.509957
H	0.790784	-0.440881	3.889826
H	-1.946550	-3.647961	3.032760
H	-0.775070	-5.082972	4.669686
C	2.893931	2.018545	2.396627
C	2.317676	3.326825	2.947901
N	3.927810	2.109144	1.517189
C	4.388200	0.964835	0.811205
C	5.686878	0.654777	0.621390
C	3.294392	0.186402	0.128936
O	2.459722	0.750356	-0.578187
N	3.277015	-1.157718	0.386376
C	2.245842	-2.057529	-0.026634
C	2.464823	-3.137252	-0.811349
C	3.683631	-3.563362	-1.490778
N	1.037095	3.558883	2.286722
C	1.068164	3.755790	0.927442
C	-0.204094	3.305676	0.179771
N	-0.232733	1.845433	0.310541
C	-0.967195	1.221733	1.281253
O	-1.798789	1.818788	1.975901
C	-0.173362	3.727134	-1.292300
O	2.080920	4.142374	0.355631
O	2.380004	0.934880	2.697266
C	6.903640	1.313788	1.100026
C	-0.666939	5.130200	-1.580907
C	4.741309	-2.694395	-1.830624
C	5.861881	-3.174304	-2.501977
C	5.957981	-4.528530	-2.838977
C	4.912583	-5.399219	-2.521475
C	3.781508	-4.918058	-1.867315
C	6.936535	2.236315	2.165846
C	8.139874	2.810248	2.566656
C	9.332766	2.484331	1.914426
C	9.318262	1.565324	0.862847
C	8.117743	0.982091	0.466530
C	-1.281062	5.391310	-2.815829
C	-1.749501	6.666427	-3.133601
C	-1.612447	7.709918	-2.215486
C	-0.999487	7.464849	-0.985840
C	-0.528081	6.187769	-0.673012
H	2.974911	4.182003	2.777009
H	2.150346	3.206049	4.019616
H	4.163722	3.029511	1.159232
H	5.867028	-0.198767	-0.031478
H	3.967824	-1.508775	1.039172
H	1.601836	-3.785550	-0.943381
H	0.225673	3.083381	2.668938
H	0.511810	1.332015	-0.153911
H	4.661799	-1.638150	-1.604647
H	6.661750	-2.490272	-2.771475
H	6.837645	-4.899273	-3.357117
H	4.975949	-6.449252	-2.791581
H	2.960191	-5.590440	-1.636595
H	6.024486	2.482166	2.695993
H	8.148830	3.512775	3.395074
H	10.267622	2.938947	2.228897

H	10.241330	1.300248	0.355790
H	8.112995	0.263462	-0.349728
H	-1.392365	4.580316	-3.532968
H	-2.223554	6.844010	-4.095348
H	-1.978338	8.703894	-2.456694
H	-0.883850	8.270221	-0.265571
H	-0.044625	6.027271	0.285659
H	-0.775697	3.010525	-1.853718
H	0.855299	3.614858	-1.653349
H	-1.100609	3.679555	0.680889
C	-3.500404	-1.904796	-2.909516
C	-4.753047	-1.142610	-2.438491
H	-5.281416	-2.549341	-0.858048
H	-6.240408	-1.054971	-0.860937
H	-4.616040	-0.060597	-2.544998
H	-5.567867	-1.411416	-3.121612
H	-3.367217	-1.781406	-3.990200
H	-3.638586	-2.978132	-2.735360

Sum of electronic and zero-point energy: -3954.709895
Sum of electronic and thermal free energies: -3954.819637
Frequency: -407.5109

Supplementary Table 28. **O1R2S^{TS}** representative 2

C	-3.949602	1.939958	-0.142670
P	-4.103232	0.307347	0.713089
P	-2.026312	-0.399939	-1.848446
C	-8.142563	-1.141640	-1.046570
C	-6.996904	-1.908699	-1.253942
C	-5.776929	-1.511215	-0.701735
C	-5.690773	-0.337419	0.053493
C	-6.852975	0.428256	0.266459
C	-8.069603	0.025960	-0.279374
H	-4.894148	-2.113672	-0.866386
H	-6.812244	1.327901	0.874664
C	-5.006715	1.186198	5.166173
C	-5.471933	0.014298	4.561512
C	-5.214098	-0.226095	3.213636
C	-4.488915	0.708404	2.455522
C	-4.016106	1.880006	3.066470
C	-4.280956	2.114046	4.418560
H	-5.585057	-1.134538	2.747366
H	-3.412581	2.589711	2.513331
C	-4.775432	-3.090127	-4.449057
C	-4.007747	-3.632787	-3.414492
C	-3.193239	-2.806852	-2.641418
C	-3.123432	-1.427714	-2.902274
C	-3.883627	-0.894830	-3.952149
C	-4.711725	-1.721758	-4.714763
H	-2.631710	-3.228461	-1.812433
H	-3.845794	0.164281	-4.184926
C	2.124580	-1.020465	-3.851182
C	1.403265	-2.103448	-3.344066
C	0.163105	-1.900179	-2.741869
C	-0.377802	-0.607901	-2.640792
C	0.351216	0.472674	-3.160402
C	1.595199	0.265781	-3.757539
H	-0.375569	-2.748529	-2.337067
H	-0.035095	1.481661	-3.109332
H	-5.208732	1.372288	6.217073
H	-9.091898	-1.450992	-1.474510
H	3.092600	-1.179416	-4.318191
H	-5.418672	-3.731398	-5.044770
H	-8.961464	0.620646	-0.104017
H	-7.040351	-2.816106	-1.848863
H	-3.912564	3.023147	4.885051
H	-6.037852	-0.710710	5.139316
H	-5.304978	-1.293526	-5.517552
H	-4.051353	-4.697361	-3.202387
H	2.149237	1.115984	-4.144441
H	1.809448	-3.108939	-3.406249
Rh	-2.202709	-0.945159	0.482959
O	-0.456424	-2.257087	0.215924
C	0.652954	-1.715520	0.472241
N	0.725064	-0.504276	1.037220
C	-0.443569	0.232979	1.409626
C	-1.192179	-0.253685	2.514304
H	1.620388	-0.154201	1.382205
H	-3.207647	-2.106991	0.163629
H	-2.431543	-1.348236	2.045757
H	-1.891959	0.459652	2.942471
C	0.668339	-2.852835	5.404014
C	-0.525290	-3.254593	4.802434

C	-1.138012	-2.442968	3.846031
C	-0.566855	-1.219651	3.481500
C	0.637461	-0.822274	4.087350
C	1.247318	-1.633993	5.042767
H	1.146146	-3.486355	6.145994
H	-0.980550	-4.203569	5.071358
H	-2.054211	-2.770008	3.362711
H	1.103501	0.116472	3.803762
H	2.178720	-1.313123	5.500919
C	3.696627	1.691634	1.817964
C	3.504376	3.163114	2.193918
N	4.668759	1.401180	0.911554
C	4.754618	0.119739	0.310364
C	5.908198	-0.511326	0.010780
C	3.422366	-0.416467	-0.144601
O	2.648967	0.280468	-0.792701
N	3.143189	-1.691697	0.274692
C	1.923021	-2.398522	0.113880
C	1.894849	-3.702744	-0.238610
C	3.011758	-4.527140	-0.699283
N	2.234726	3.599166	1.623045
C	2.128159	3.594644	0.253362
C	0.691221	3.429575	-0.273312
N	0.341545	2.021707	-0.036206
C	-0.470543	1.667252	1.013201
O	-1.177146	2.495366	1.606372
C	0.585763	3.846802	-1.746816
O	3.114835	3.603289	-0.472216
O	2.939171	0.831880	2.280426
C	7.295931	-0.122933	0.271470
C	0.706393	5.346930	-1.918164
C	4.090510	-3.999728	-1.440837
C	5.115880	-4.830190	-1.885019
C	5.093169	-6.197558	-1.591842
C	4.023492	-6.735811	-0.872013
C	2.985994	-5.911152	-0.442382
C	7.679200	0.829053	1.238240
C	9.023056	1.136327	1.434211
C	10.012102	0.508535	0.671357
C	9.649235	-0.444718	-0.282845
C	8.306868	-0.761185	-0.473870
C	1.932077	5.948451	-2.229697
C	2.027320	7.335362	-2.358659
C	0.900409	8.138903	-2.172619
C	-0.325530	7.548544	-1.856453
C	-0.418654	6.162040	-1.731428
H	4.306028	3.804611	1.821765
H	3.452761	3.243885	3.281411
H	5.125736	2.178272	0.446142
H	5.796989	-1.434190	-0.557899
H	3.868506	-2.163221	0.801818
H	0.928910	-4.192406	-0.147856
H	1.397859	3.382916	2.152990
H	0.974020	1.320559	-0.422872
H	4.093624	-2.947376	-1.703313
H	5.931045	-4.413680	-2.470335
H	5.897716	-6.841496	-1.934770
H	3.993743	-7.799202	-0.653588
H	2.149529	-6.334101	0.108224
H	6.926735	1.304452	1.856281
H	9.301497	1.865396	2.189803
H	11.058402	0.755433	0.825684

H	10.411558	-0.943988	-0.873709
H	8.030362	-1.507745	-1.214774
H	2.811018	5.323711	-2.352341
H	2.983749	7.788607	-2.604934
H	0.975751	9.217902	-2.274790
H	-1.207976	8.166242	-1.713043
H	-1.377197	5.704498	-1.491443
H	-0.389423	3.516703	-2.119000
H	1.361209	3.324347	-2.315256
H	-0.001896	4.022607	0.328175
C	-2.472888	1.360151	-2.189478
C	-3.845996	1.826147	-1.673809
H	-4.833723	2.527078	0.128670
H	-3.070568	2.444345	0.271090
H	-4.023625	2.825070	-2.089748
H	-4.647691	1.187877	-2.062887
H	-1.689350	1.942252	-1.695240
H	-2.385095	1.548276	-3.264952

Sum of electronic and zero-point energy: -3954.712898
Sum of electronic and thermal free energies: -3954.823304
Frequency: -670.9373

Supplementary Table 29. **O1R2S^{TS}** representative 3

C	4.825922	2.613331	-0.911010
P	4.117820	1.012067	-0.300012
P	1.347808	2.819259	-1.230647
C	6.647426	-0.548942	3.243242
C	6.015121	-1.441263	2.373998
C	5.299580	-0.961245	1.278449
C	5.205793	0.420575	1.044290
C	5.837230	1.311944	1.921800
C	6.560610	0.825897	3.012125
H	4.830348	-1.668037	0.601035
H	5.761273	2.384568	1.770853
C	5.153655	-1.444908	-4.081048
C	6.133065	-1.223773	-3.105157
C	5.812792	-0.541584	-1.932119
C	4.501408	-0.075079	-1.725387
C	3.528084	-0.294033	-2.705653
C	3.852977	-0.982057	-3.877595
H	6.578925	-0.377810	-1.180414
H	2.511202	0.039978	-2.552132
C	-1.094761	6.405986	0.425482
C	-0.114741	5.789024	1.209140
C	0.576314	4.680048	0.721769
C	0.301990	4.180650	-0.562431
C	-0.686979	4.801164	-1.340367
C	-1.384657	5.904559	-0.844220
H	1.320020	4.192728	1.343042
H	-0.920146	4.426075	-2.331192
C	-1.029374	0.849734	-4.664673
C	-1.628122	1.082842	-3.423242
C	-0.910982	1.718598	-2.413452
C	0.410376	2.142026	-2.638849
C	0.999712	1.918518	-3.890188
C	0.280682	1.271001	-4.897011
H	-1.404498	1.900892	-1.463949
H	2.019249	2.234558	-4.089047
H	5.408046	-1.978821	-4.992339
H	7.205782	-0.921973	4.096888
H	-1.585091	0.348080	-5.452057
H	-1.630848	7.271789	0.804699
H	7.052641	1.523242	3.683923
H	6.077049	-2.512625	2.543517
H	3.080498	-1.152031	-4.621980
H	7.146495	-1.583559	-3.258634
H	-2.150524	6.373205	-1.455273
H	0.110090	6.168599	2.202095
H	0.745544	1.102254	-5.864537
H	-2.651141	0.780064	-3.223059
Rh	1.977803	1.263484	0.469942
O	0.065466	1.807944	1.381240
C	-0.896693	1.028051	1.142855
N	-0.661613	-0.207093	0.655105
C	0.639262	-0.624397	0.207282
C	1.638038	-0.949802	1.180975
H	-1.473843	-0.755405	0.394954
H	2.722446	2.489818	1.150647
H	2.466181	0.412814	1.769117
H	2.473246	-1.502697	0.756420
C	0.578561	-2.455075	5.070793
C	1.424069	-3.169453	4.219009

C	1.801963	-2.625963	2.990393
C	1.323482	-1.368637	2.583880
C	0.518895	-0.634288	3.468733
C	0.143689	-1.180047	4.696998
H	0.282981	-2.874685	6.028027
H	1.798493	-4.146737	4.511176
H	2.458570	-3.186481	2.332781
H	0.229953	0.378295	3.220129
H	-0.480375	-0.599163	5.370283
C	-4.272650	-2.352966	1.736880
C	-3.574205	-3.672488	2.100310
N	-4.407603	-2.150898	0.398317
C	-4.773176	-0.941705	-0.272573
C	-5.713460	-0.916251	-1.242776
C	-3.912697	0.283630	-0.100639
O	-3.779917	1.119373	-0.988226
N	-3.240362	0.366896	1.104063
C	-2.301741	1.404221	1.365474
C	-2.607052	2.673818	1.725932
C	-3.901634	3.294974	1.962371
N	-2.157786	-3.581738	1.741395
C	-1.747767	-3.795566	0.462270
C	-0.275142	-3.506037	0.166659
N	-0.232005	-2.580109	-0.959586
C	0.470470	-1.400100	-1.090381
O	0.760204	-0.985563	-2.200772
C	0.484745	-4.821985	-0.148764
O	-2.508020	-4.170505	-0.431820
O	-4.562588	-1.523447	2.602174
C	-6.636755	-1.950320	-1.701155
C	1.985535	-4.634171	-0.213163
C	-5.119737	2.594089	2.105306
C	-6.305844	3.284996	2.329156
C	-6.310960	4.681418	2.411892
C	-5.113718	5.389060	2.282622
C	-3.922876	4.701939	2.069522
C	-6.969545	-3.107422	-0.965458
C	-7.865060	-4.040322	-1.480148
C	-8.443766	-3.847736	-2.738317
C	-8.134559	-2.702045	-3.475329
C	-7.249581	-1.760770	-2.957281
C	2.593883	-3.901053	-1.244713
C	3.974339	-3.691238	-1.253124
C	4.774043	-4.222077	-0.237563
C	4.184461	-4.968942	0.785015
C	2.802275	-5.170810	0.793024
H	-4.007045	-4.525096	1.569834
H	-3.667328	-3.821185	3.175960
H	-4.119599	-2.923595	-0.203339
H	-5.753352	0.022108	-1.791370
H	-3.627693	-0.157618	1.892006
H	-1.748213	3.333640	1.829075
H	-1.521144	-3.161382	2.408125
H	-0.517454	-2.977142	-1.849693
H	-5.143191	1.513307	2.062151
H	-7.233117	2.731173	2.443462
H	-7.242818	5.212666	2.583550
H	-5.108790	6.472943	2.353189
H	-2.991391	5.250361	1.968064
H	-6.550806	-3.258645	0.021803
H	-8.117863	-4.920362	-0.895614
H	-9.138538	-4.581621	-3.136465

H	-8.588441	-2.539233	-4.448504
H	-7.018398	-0.865845	-3.529646
H	1.997651	-3.488639	-2.052077
H	4.422446	-3.120671	-2.058602
H	5.848772	-4.062720	-0.251509
H	4.797434	-5.402139	1.570765
H	2.350102	-5.753274	1.592734
H	0.084123	-5.221936	-1.088365
H	0.235733	-5.551873	0.630518
H	0.191478	-3.026059	1.025447
C	2.758974	3.828415	-1.916705
C	4.116367	3.151902	-2.169886
H	4.776416	3.348444	-0.101295
H	5.881221	2.420216	-1.134724
H	4.028701	2.355993	-2.917101
H	4.772710	3.909007	-2.615866
H	2.398232	4.307184	-2.834491
H	2.891149	4.629397	-1.179968

Sum of electronic and zero-point energy: -3954.689797
Sum of electronic and thermal free energies: -3954.79828
Frequency: -639.7879

Supplementary Table 30. **O1R2S^{TS}** representative 4

C	-4.321455	0.630593	-1.921967
P	-4.040656	0.551597	-0.089738
P	-2.469062	-2.188005	-1.264861
C	-8.219395	-0.943171	1.236888
C	-7.128026	-1.810654	1.292642
C	-5.853366	-1.359570	0.943742
C	-5.664185	-0.035850	0.525790
C	-6.768400	0.832847	0.467168
C	-8.036957	0.381021	0.826764
H	-5.011552	-2.038401	0.999045
H	-6.635143	1.864993	0.154617
C	-3.436888	4.882973	1.398312
C	-3.254017	4.592602	0.046340
C	-3.499208	3.304552	-0.432861
C	-3.929253	2.296605	0.441156
C	-4.114408	2.596276	1.801802
C	-3.872980	3.884175	2.275633
H	-3.330996	3.096552	-1.483660
H	-4.438754	1.818559	2.487576
C	-5.121694	-5.552748	0.509870
C	-3.998514	-5.078041	1.195461
C	-3.205255	-4.080456	0.631940
C	-3.518474	-3.552262	-0.634583
C	-4.632669	-4.049185	-1.323731
C	-5.434480	-5.039388	-0.749031
H	-2.345826	-3.697633	1.175672
H	-4.894932	-3.669126	-2.305372
C	1.489549	-4.174746	-2.662546
C	1.272569	-2.808056	-2.847791
C	0.061928	-2.230077	-2.466402
C	-0.943403	-3.013122	-1.872754
C	-0.729309	-4.391675	-1.711739
C	0.477791	-4.966172	-2.116511
H	-0.098162	-1.168128	-2.608942
H	-1.497419	-5.019080	-1.272726
H	-3.237578	5.885608	1.764663
H	-9.209422	-1.293560	1.514683
H	2.444324	-4.614907	-2.932205
H	-5.746415	-6.321917	0.954988
H	-8.882292	1.062112	0.788630
H	-7.258985	-2.841468	1.608585
H	-4.020272	4.106783	3.328539
H	-2.914994	5.362256	-0.635759
H	-6.302367	-5.407334	-1.288720
H	-3.746337	-5.478433	2.173284
H	0.630905	-6.034401	-1.991063
H	2.057161	-2.185834	-3.267497
Rh	-2.150617	-0.575799	0.484028
O	-0.431827	-1.787923	1.013532
C	0.657825	-1.401233	0.509121
N	0.742636	-0.229952	-0.156447
C	-0.338800	0.700942	-0.214246
C	-0.772986	1.345041	0.982000
H	1.570852	-0.025347	-0.711880
H	-3.103108	-1.412859	1.409768
H	-1.954778	0.423802	1.783910
H	-1.432946	2.184762	0.785830
C	1.967618	2.251022	4.159984
C	1.219200	3.247672	3.531832

C	0.275213	2.907651	2.562238
C	0.085886	1.566629	2.180009
C	0.786278	0.567336	2.873918
C	1.724110	0.911712	3.848587
H	2.716220	2.513725	4.900181
H	1.363297	4.290095	3.802102
H	-0.323278	3.687385	2.094821
H	0.555614	-0.474918	2.697333
H	2.257333	0.125837	4.376912
C	4.681500	1.645767	1.168467
C	4.460856	2.215653	-0.231840
N	5.097461	0.337742	1.251626
C	5.281052	-0.580801	0.168804
C	6.356434	-0.589640	-0.649932
C	4.170169	-1.555916	-0.104596
O	4.227211	-2.417077	-0.970251
N	3.077801	-1.399176	0.731707
C	1.900242	-2.177556	0.694643
C	1.808324	-3.525080	0.797685
C	2.816714	-4.546663	1.037678
N	3.193734	2.926848	-0.269056
C	2.162078	2.492818	-1.033987
C	0.875234	3.346713	-0.946184
N	-0.234340	2.706353	-1.642418
C	-0.568827	1.371440	-1.553155
O	-1.081630	0.804009	-2.516780
C	1.138659	4.745593	-1.557361
O	2.239981	1.508102	-1.772191
O	4.492419	2.335907	2.159978
C	7.552136	0.246490	-0.679363
C	0.054511	5.767699	-1.296158
C	4.109419	-4.291643	1.538612
C	4.997510	-5.335708	1.773558
C	4.625336	-6.656381	1.503430
C	3.345271	-6.929373	1.015362
C	2.450117	-5.886692	0.795906
C	7.951074	1.125447	0.351744
C	9.107091	1.889045	0.221509
C	9.889705	1.800888	-0.934552
C	9.515252	0.930711	-1.960574
C	8.364195	0.158594	-1.829836
C	-0.771954	6.230218	-2.326380
C	-1.715072	7.234587	-2.089071
C	-1.843556	7.786756	-0.812675
C	-1.032390	7.321215	0.226953
C	-0.094406	6.318087	-0.014924
H	4.440066	1.456911	-1.011074
H	5.289166	2.902854	-0.440767
H	5.268509	0.020994	2.202154
H	6.285274	-1.331955	-1.442670
H	3.060172	-0.580947	1.329066
H	0.801257	-3.903156	0.649948
H	3.026768	3.585902	0.482668
H	-0.391154	3.047174	-2.586033
H	4.407928	-3.277564	1.771107
H	5.987186	-5.120689	2.166439
H	5.326969	-7.466851	1.678790
H	3.044509	-7.953268	0.812904
H	1.452012	-6.099807	0.423661
H	7.371140	1.198317	1.262717
H	9.402785	2.554085	1.027838
H	10.789215	2.402155	-1.030149

H	10.121714	0.849390	-2.857723
H	8.078885	-0.521998	-2.627932
H	-0.659831	5.823526	-3.329112
H	-2.339696	7.591424	-2.902995
H	-2.567265	8.575478	-0.629152
H	-1.121408	7.749946	1.221328
H	0.547314	5.974715	0.794634
H	1.306855	4.625141	-2.635374
H	2.083735	5.115530	-1.146441
H	0.627023	3.472652	0.110627
C	-3.281153	-1.568795	-2.804532
C	-4.559462	-0.738729	-2.586796
H	-5.194269	1.276527	-2.071950
H	-3.449911	1.109023	-2.377154
H	-4.999921	-0.551437	-3.573345
H	-5.308812	-1.308538	-2.024213
H	-2.520773	-0.956121	-3.296194
H	-3.481768	-2.426243	-3.456193

Sum of electronic and zero-point energy: -3954.698835
Sum of electronic and thermal free energies: -3954.8088
Frequency: -639.0016

Supplementary Table 31. **O1R2S^{TS}** representative 5

C	4.739652	1.052686	-1.369163
P	4.077175	0.758201	0.336664
P	1.720832	2.698553	-1.119627
C	6.943115	3.569941	2.649904
C	5.631720	3.973353	2.394127
C	4.744329	3.110896	1.748048
C	5.167820	1.837421	1.341196
C	6.493444	1.441712	1.589980
C	7.371646	2.301639	2.248901
H	3.724974	3.431746	1.564941
H	6.837457	0.458272	1.281996
C	4.818037	-3.664603	1.428567
C	4.701899	-3.297094	0.087343
C	4.569759	-1.951259	-0.260619
C	4.544555	-0.963003	0.735659
C	4.660861	-1.341009	2.083933
C	4.804288	-2.684560	2.426107
H	4.449859	-1.688900	-1.306105
H	4.628265	-0.585011	2.863281
C	2.068577	6.745385	1.118580
C	1.207883	5.740160	1.570372
C	1.107767	4.537974	0.871998
C	1.856414	4.333834	-0.302521
C	2.705072	5.352733	-0.756944
C	2.814896	6.549508	-0.043942
H	0.454983	3.749609	1.236463
H	3.294313	5.226083	-1.658870
C	-2.138141	2.888627	-3.721234
C	-1.204999	1.860686	-3.899009
C	-0.061850	1.800829	-3.099134
C	0.178249	2.787691	-2.125833
C	-0.766139	3.810486	-1.948063
C	-1.916872	3.856697	-2.738604
H	0.635543	0.981084	-3.230074
H	-0.606831	4.577695	-1.198203
H	4.910412	-4.713655	1.691752
H	7.629654	4.238824	3.161000
H	-3.034299	2.921442	-4.333833
H	2.155667	7.676737	1.670790
H	8.389899	1.980739	2.449068
H	5.290180	4.958172	2.699604
H	4.893814	-2.966510	3.471185
H	4.696318	-4.056666	-0.686325
H	3.484029	7.327225	-0.400778
H	0.622337	5.888311	2.473271
H	-2.637009	4.655777	-2.587584
H	-1.372527	1.094744	-4.651183
Rh	1.828713	0.992523	0.546833
O	-0.332776	1.385833	0.805807
C	-1.049554	0.719278	0.008917
N	-0.548813	-0.335317	-0.656783
C	0.796642	-0.788569	-0.476927
C	1.247493	-1.309007	0.778030
H	-1.109272	-0.748651	-1.400919
H	2.225607	2.063346	1.626941
H	1.878517	-0.142078	1.742170
H	2.182612	-1.849333	0.663658
C	-1.043942	-3.212239	3.878724
C	-0.025086	-3.885212	3.202937
C	0.713328	-3.225493	2.220781

C	0.420411	-1.892639	1.877679
C	-0.586355	-1.217945	2.579187
C	-1.309566	-1.877476	3.571574
H	-1.618819	-3.720889	4.646733
H	0.211235	-4.915736	3.454073
H	1.539336	-3.737967	1.731461
H	-0.768885	-0.169802	2.382128
H	-2.089734	-1.344264	4.107054
C	-3.548118	-2.383806	0.376826
C	-3.283794	-2.968073	-1.016064
N	-4.300267	-1.244369	0.480221
C	-5.037944	-0.590099	-0.540445
C	-6.376248	-0.410417	-0.473348
C	-4.310708	0.077635	-1.662563
O	-4.811718	0.216807	-2.769001
N	-3.005050	0.517372	-1.434350
C	-2.466771	1.069146	-0.243068
C	-3.115958	1.860090	0.640428
C	-4.474320	2.398470	0.531250
N	-1.951995	-3.558268	-1.006987
C	-0.960995	-3.056421	-1.782408
C	0.458937	-3.557646	-1.441262
N	1.464977	-2.635732	-1.953433
C	1.491270	-1.282499	-1.739584
O	2.102551	-0.541259	-2.510196
C	0.684269	-4.969609	-2.027090
O	-1.150614	-2.233489	-2.681462
O	-3.103677	-2.952774	1.366336
C	-7.321414	-0.860084	0.546609
C	1.994522	-5.593134	-1.598527
C	-4.998662	2.864883	-0.689506
C	-6.300317	3.354360	-0.755596
C	-7.101894	3.383608	0.390293
C	-6.586425	2.940033	1.610930
C	-5.277693	2.466915	1.683696
C	-7.125613	-1.988356	1.371084
C	-8.078961	-2.343487	2.322801
C	-9.240152	-1.582008	2.479663
C	-9.453749	-0.467427	1.663944
C	-8.509845	-0.117413	0.703106
C	3.061594	-5.727884	-2.494056
C	4.258944	-6.327755	-2.093100
C	4.403096	-6.797279	-0.785731
C	3.345829	-6.659232	0.118890
C	2.153155	-6.060268	-0.285936
H	-3.328888	-2.244012	-1.827515
H	-4.044807	-3.734925	-1.207346
H	-4.539912	-1.013772	1.440805
H	-6.785404	0.231333	-1.248464
H	-2.600225	0.884792	-2.293971
H	-2.569644	2.088985	1.552574
H	-1.708062	-4.020065	-0.135709
H	1.888766	-2.890485	-2.839614
H	-4.380521	2.846312	-1.580268
H	-6.690933	3.714070	-1.703150
H	-8.118874	3.761450	0.334044
H	-7.202282	2.965536	2.504987
H	-4.876023	2.128158	2.635810
H	-6.247484	-2.611486	1.247211
H	-7.917485	-3.222473	2.940263
H	-9.978633	-1.861828	3.225428
H	-10.359131	0.122751	1.772636
H	-8.674680	0.751141	0.071665

H	2.949331	-5.384469	-3.520303
H	5.072734	-6.436661	-2.804445
H	5.328877	-7.273180	-0.475590
H	3.445688	-7.031423	1.134837
H	1.328953	-5.969860	0.418969
H	0.618945	-4.909419	-3.120736
H	-0.153302	-5.596681	-1.701570
H	0.548151	-3.619959	-0.353418
C	3.029703	2.660347	-2.426122
C	4.465542	2.466807	-1.910182
H	5.818927	0.873505	-1.304553
H	4.302417	0.311340	-2.042294
H	5.145100	2.636194	-2.753722
H	4.721787	3.223706	-1.158702
H	2.762369	1.827079	-3.081084
H	2.946513	3.577479	-3.018929

Sum of electronic and zero-point energy: -3954.700608
Sum of electronic and thermal free energies: -3954.808933

Frequency: -713.3412