Supplementary Material

Multipath kinetics of the reaction of OH radical with 1-pentene

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Table S1. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for conf#1

C	1.6562490	-0.8970980	0.2020180
H	0.9347220	-1.4809710	0.7732210
H	2.6305090	-1.3516660	0.0301130
C	1.3763870	0.3189570	-0.2684940
H	2.1519510	0.8428990	-0.8341240
C	0.0936290	1.0854400	-0.0807660
H	-0.2253000	1.4764510	-1.0601920
H	0.3253910	1.9741140	0.5264680
C	-1.0616090	0.3128980	0.5541330
H	-0.7156230	-0.1717440	1.4778440
H	-1.8341080	1.0316780	0.8582830
C	-1.6849180	-0.7182340	-0.3860870
H	-2.1203350	-0.2199350	-1.2627220
H	-0.9400890	-1.4364090	-0.7481880
H	-2.4855460	-1.2761920	0.1144690

Table S2. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for conf#2

C	-2.109246	-0.666606	0.000003
H	-1.540254	-1.59579	0.000135
H	-3.194609	-0.751786	-0.000044
C	-1.515515	0.527962	-0.000061
H	-2.145394	1.421714	-0.000164
C	-0.033614	0.780838	0.000073
H	0.214237	1.402444	0.875613
H	0.21437	1.402652	-0.875281
C	0.844546	-0.464812	0.000003
H	0.605493	-1.075794	0.881667
H	0.605428	-1.075718	-0.881697
C	2.330513	-0.118858	-0.000035
H	2.594988	0.471892	-0.887085
H	2.594956	0.472201	0.886823
H	2.950677	-1.02296	0.000134

Table S3. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for conf#3

C	2.292412	-0.249487	-0.285189
H	2.644498	0.705149	-0.679724
H	2.962172	-1.103423	-0.375096
C	1.093449	-0.359823	0.287935
H	0.785783	-1.334273	0.676727
C	0.112615	0.767769	0.435094
H	0.597831	1.706999	0.136656
H	-0.169799	0.866966	1.495248
C	-1.165031	0.566803	-0.39319
H	-1.806431	1.448972	-0.260924
H	-0.893423	0.5253	-1.457224
C	-1.945633	-0.688812	-0.011137
H	-1.379636	-1.598922	-0.243911
H	-2.172632	-0.694358	1.063881
H	-2.895237	-0.741106	-0.556711

Table S4. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for conf#4

C	2.410946	-0.196537	-0.081918
H	2.678198	-0.194128	0.983309
H	2.412715	-1.239467	-0.425566
C	3.194272	0.341604	-0.628803
H	1.041916	0.441122	-0.297572
C	0.794941	0.453096	-1.368139
H	1.062450	1.490015	0.031990
H	-0.067814	-0.299731	0.455878
C	-0.113172	-1.343772	0.113782
H	0.188643	-0.319798	1.526976
H	-1.408910	0.347403	0.274091
C	-1.500885	1.375558	0.637945
H	-2.460351	-0.227475	-0.309868
H	-2.405378	-1.249976	-0.686785
H	-3.406500	0.298174	-0.428371

Table S5. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for conf#5

C	2.06874	0.573632	0.120504
H	2.049561	0.835891	1.179476
H	2.85012	1.022014	-0.491315
C	1.171642	-0.26563	-0.397104
H	1.220038	-0.498933	-1.4659
C	0.05639	-0.918315	0.366263
H	0.138061	-0.654361	1.430847
H	0.158441	-2.010976	0.290372
C	-1.327299	-0.512257	-0.160487
H	-1.39718	-0.777607	-1.225691
H	-2.091327	-1.103386	0.361991
C	-1.614424	0.975305	0.021207
H	-1.551092	1.253121	1.082315
H	-0.888088	1.586847	-0.52772
H	-2.618825	1.230982	-0.336676

Table S6. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for OH

O	0	0	0.1083990
H	0	0	-0.8671880

Table S7. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for π-PC1 (conf#1 + OH)

C	0.50171	1.23779	0.52874
H	0.89436	1.94446	1.26504
C	0.75379	1.47420	-0.76257
H	1.33157	2.34518	-1.06708
H	0.38780	0.82139	-1.55565
O	2.17808	-1.44505	-0.27361
H	2.09446	-0.46909	-0.26432
C	-0.25498	0.06888	1.10282
H	0.44864	-0.50982	1.72081
H	-1.00767	0.46109	1.80486
C	-0.93283	-0.85473	0.09148
H	-1.21482	-1.78104	0.60796
H	-0.21338	-1.15414	-0.68549
C	-2.17574	-0.23644	-0.54743

H	-2.61255	-0.91139	-1.29296
H	-2.93883	-0.04024	0.21747
H	-1.94600	0.715762	-1.04014

Table S8. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for π-PC2 (conf#1 + OH)

C	-1.063699	-0.967639	-0.320093
H	-1.900247	-1.057470	-1.019086
C	-1.332402	-0.985343	0.989244
H	-2.353547	-1.098161	1.349180
H	-0.548503	-0.906477	1.742419
O	-1.063961	2.212790	-0.341313
H	-1.139338	1.312059	0.035727
C	0.291028	-0.843466	-0.964865
H	0.461819	-1.763288	-1.544901
H	0.241200	-0.031869	-1.708383
C	1.473891	-0.600155	-0.028009
H	2.395096	-0.756898	-0.604274
H	1.478634	-1.358328	0.768460
C	1.512616	0.804043	0.576723
H	2.443479	0.961681	1.134292
H	1.460470	1.566494	-0.213138
H	0.684014	0.985293	1.272201

Table S9. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for π-PC1 (conf#2 + OH)

C	1.282460	-0.889599	-0.469870
H	1.870798	-1.200649	-1.337507
C	1.913329	-0.718861	0.696619
H	2.984747	-0.891527	0.784185
H	1.383552	-0.417904	1.600780
O	0.771199	2.287341	-0.159768
H	1.388759	1.527737	-0.123883
C	-0.186319	-0.688456	-0.720314
H	-0.301515	0.049041	-1.530359
H	-0.598100	-1.629292	-1.119091
C	-1.006353	-0.244860	0.485906
H	-0.596980	0.693787	0.889179
H	-0.916038	-0.996090	1.283226
C	-2.474845	-0.038094	0.128925

H	-3.056555	0.270727	1.005108
H	-2.581168	0.738948	-0.639010
H	-2.916724	-0.964293	-0.262081

Table S10. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for π-PC2 (conf#2 + OH)

C	1.282460	-0.889599	-0.469870
H	1.870798	-1.200649	-1.337507
C	1.913329	-0.718861	0.696619
H	2.984747	-0.891527	0.784185
H	1.383552	-0.417904	1.600780
O	0.771199	2.287341	-0.159768
H	1.388759	1.527737	-0.123883
C	-0.186319	-0.688456	-0.720314
H	-0.301515	0.049041	-1.530359
H	-0.598100	-1.629292	-1.119091
C	-1.006353	-0.244860	0.485906
H	-0.596980	0.693787	0.889179
H	-0.916038	-0.996090	1.283226
C	-2.474845	-0.038094	0.128925
H	-3.056555	0.270727	1.005108
H	-2.581168	0.738948	-0.639010
H	-2.916724	-0.964293	-0.262081

Table S11. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for π-PC1 (conf#3 + OH)

C	-1.025461	-0.686243	0.497495
H	-0.729959	-0.585395	1.545613
C	-2.249371	-0.287943	0.136451
H	-2.951455	0.124566	0.860156
H	-2.591439	-0.381269	-0.895628
O	-0.181076	2.377046	-0.228589
H	-0.836197	1.678607	-0.020340
C	-0.006891	-1.268642	-0.439663
H	0.329503	-2.236957	-0.037556
H	-0.480442	-1.462423	-1.411264
C	1.225320	-0.372035	-0.638723
H	0.919864	0.560097	-1.138045
H	1.908976	-0.883118	-1.330028
C	1.960074	-0.044581	0.658823

H	2.884038	0.507146	0.451771
H	1.347458	0.582046	1.317530
H	2.226237	-0.963004	1.200200

Table S12. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for π-PC2 (conf#3 + OH)

C	0.393561	0.812656	-0.345530
H	0.014094	0.966290	-1.359077
C	1.276553	1.686387	0.147067
H	1.611994	2.544975	-0.432816
H	1.680516	1.573057	1.155004
O	2.647407	-1.401104	-0.221929
H	2.458124	-0.453551	-0.377164
C	-0.130444	-0.382243	0.398898
H	0.065334	-1.290825	-0.193848
H	0.417522	-0.487439	1.345126
C	-1.637850	-0.297313	0.681146
H	-1.831411	0.580860	1.312690
H	-1.926663	-1.181071	1.265094
C	-2.490384	-0.223591	-0.583703
H	-3.558004	-0.262431	-0.337788
H	-2.313117	0.708014	-1.134978
H	-2.266263	-1.064429	-1.254093

Table S13. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for π-PC1 (conf#4 + OH)

C	-1.258837	-0.924989	0.273946
H	-1.272765	-1.475205	1.220127
C	-2.399564	-0.396716	-0.179085
H	-3.335713	-0.508434	0.365353
H	-2.431565	0.147730	-1.125321
O	-0.427195	2.274340	0.034297
H	-1.098387	1.593338	0.247351
C	0.072229	-0.820555	-0.411134
H	0.363186	-1.815185	-0.784377
H	-0.012334	-0.158390	-1.284244
C	1.176825	-0.313206	0.522564
H	1.306415	-1.030612	1.345771
H	0.867617	0.636762	0.984231
C	2.497633	-0.112099	-0.211973

H	3.284737	0.227911	0.471016
H	2.831884	-1.048690	-0.678441
H	2.384772	0.641445	-1.001752

Table S14. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for π-PC2 (conf#4 + OH)

C	-0.806502	-0.917328	-0.419860
H	-0.779666	-1.228817	-1.468603
C	-1.729586	-1.448469	0.387117
H	-2.449280	-2.180787	0.024584
H	-1.781189	-1.172431	1.442141
O	-2.223560	1.883239	-0.046551
H	-2.351201	0.914268	-0.098864
C	0.234210	0.078163	0.001397
H	0.128123	0.995266	-0.601166
H	0.071913	0.360964	1.051419
C	1.656392	-0.463384	-0.179640
H	1.792559	-0.771847	-1.226230
H	1.771019	-1.368185	0.433250
C	2.716545	0.565649	0.198645
H	3.727085	0.160613	0.069250
H	2.627449	1.464192	-0.426060
H	2.605317	0.873069	1.246738

Table S15. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for π-PC1 (conf#5 + OH)

C	0.880066	-1.061486	-0.349305
H	0.614765	-1.589992	-1.271191
C	2.108142	-0.547660	-0.236759
H	2.843731	-0.653024	-1.032245
H	2.421289	-0.025924	0.670302
O	0.685491	2.311924	0.300991
H	0.927616	1.491849	-0.175780
C	-0.187711	-1.009463	0.707995
H	-0.209896	-1.982604	1.221696
H	0.074935	-0.252381	1.461345
C	-1.580050	-0.727060	0.133243
H	-2.320288	-0.816699	0.938662
H	-1.822255	-1.505869	-0.604991
C	-1.693820	0.649260	-0.515938

H	-2.695934	0.811100	-0.929973
H	-1.502521	1.444585	0.218580
H	-0.975128	0.762023	-1.339742

Table S16. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for π-PC2 (conf#5 + OH)

C	-0.3779470	0.7084500	0.5945600
H	-0.2757620	0.8406930	1.6765180
C	-0.8783440	1.7111750	-0.1333170
H	-1.1870830	2.6499640	0.3243360
H	-0.9815220	1.6227180	-1.2165770
O	-2.9101400	-0.9952780	-0.2555350
H	-2.5654580	-0.1051490	-0.0387990
C	0.0820680	-0.6117120	0.0466750
H	-0.4981990	-1.4185760	0.5204890
H	-0.1223230	-0.6525980	-1.0330550
C	1.5755570	-0.8564490	0.3049010
H	1.8216220	-1.8798620	-0.0068130
H	1.7653980	-0.8024470	1.3868180
C	2.4704600	0.1371540	-0.4297840
H	3.5300070	-0.0717380	-0.2412320
H	2.3007130	0.0810290	-1.5136270
H	2.2629650	1.1664790	-0.1119920

Table S17. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC11+ (conf#1 + OH)

C	-2.245194	0.117248	-0.586464
H	-2.978193	0.381742	0.187621
H	-1.819160	1.051215	-0.971974
H	-2.784110	-0.375028	-1.405006
C	-1.167006	-0.799316	-0.008644
H	-0.486995	-1.147757	-0.797413
H	-1.645261	-1.698265	0.401772
C	-0.349961	-0.142876	1.102119
H	-1.028315	0.315998	1.839574
H	0.213829	-0.911501	1.650663
C	0.639826	0.898942	0.660119
H	1.153178	1.427376	1.468914
C	0.958703	1.219368	-0.601044
H	0.486086	0.743479	-1.458385

H	1.705634	1.984436	-0.808590
O	2.156744	-1.117784	-0.424285
H	2.911136	-0.589623	-0.109408

Table S18. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC12- (conf#1 + OH)

C	-2.415875	0.300372	-0.253596
H	-3.018055	0.057572	0.631952
H	-2.025116	1.316029	-0.120081
H	-3.083232	0.301467	-1.123866
C	-1.289214	-0.719022	-0.421996
H	-0.751719	-0.544990	-1.365302
H	-1.725123	-1.723279	-0.502699
C	-0.294377	-0.715154	0.736572
H	-0.841704	-0.752217	1.692148
H	0.321688	-1.624900	0.708148
C	0.656323	0.448950	0.784501
H	1.315288	0.474739	1.655614
C	0.778123	1.426020	-0.124380
H	0.146243	1.473956	-1.011604
H	1.515912	2.215899	0.004507
O	2.633003	-0.679457	-0.451152
H	2.471912	-0.205621	-1.286205

Table S19. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC12+ (conf#1 + OH)

C	-2.28892	0.21772	-0.48355
H	-2.98872	0.278256	0.360949
H	-1.88964	1.224693	-0.65457
H	-2.85997	-0.07864	-1.37171
C	-1.17652	-0.78641	-0.18146
H	-0.52959	-0.92938	-1.05805
H	-1.6274	-1.76529	0.028824
C	-0.31206	-0.38765	1.012395
H	-0.95537	-0.09952	1.859002
H	0.270042	-1.25333	1.357807
C	0.666733	0.727216	0.767881
H	1.246623	1.037514	1.641213
C	0.897083	1.352741	-0.39444
H	0.356284	1.099894	-1.30522

H	1.634827	2.151649	-0.46032
O	2.217236	-1.00628	-0.49396
H	2.887111	-0.35729	-0.77127

Table S20. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC21+ (conf#1 + OH)

C	1.327993	1.387191	0.181096
H	1.334454	1.767504	-0.850652
H	0.335830	1.571299	0.610690
H	2.050757	1.979649	0.754419
C	1.697743	-0.096352	0.202624
H	1.679873	-0.475953	1.233859
H	2.731928	-0.208397	-0.148356
C	0.802227	-0.965417	-0.679597
H	0.767966	-0.539304	-1.696191
H	1.257810	-1.960033	-0.803336
C	-0.609992	-1.172894	-0.202196
H	-1.266521	-1.698061	-0.900658
C	-1.121762	-0.794780	0.975341
H	-0.533242	-0.264318	1.723120
H	-2.156704	-1.015830	1.227844
O	-2.183051	1.177984	-0.398115
H	-1.315004	1.273081	-0.829423

Table S21. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC22- (conf#1 + OH)

C	1.546865	1.105668	0.411417
H	1.582641	1.727775	-0.49243
H	0.617368	1.355757	0.933175
H	2.394262	1.383587	1.049985
C	1.612371	-0.37497	0.038206
H	1.627401	-0.9978	0.944378
H	2.561055	-0.56918	-0.47967
C	0.473031	-0.8303	-0.87293
H	0.370013	-0.13011	-1.71586
H	0.724437	-1.80375	-1.32208
C	-0.87743	-0.97985	-0.22959
H	-1.68152	-1.27781	-0.90724
C	-1.16836	-0.82668	1.069237
H	-0.41565	-0.53106	1.799019

H	-2.17605	-1.00798	1.441773
O	-1.59256	1.489814	-0.47833
H	-2.38232	1.368854	0.07754

Table S22. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC22+ (conf#1 + OH)

C	1.529548	1.104244	0.460551
H	1.328516	1.801943	-0.363157
H	0.726652	1.210433	1.200232
H	2.462697	1.412077	0.947210
C	1.635648	-0.328012	-0.064842
H	1.761658	-1.030576	0.771320
H	2.545682	-0.410530	-0.673630
C	0.452201	-0.758721	-0.930424
H	0.295980	-0.019115	-1.729771
H	0.694311	-1.704085	-1.440274
C	-0.860478	-0.951106	-0.223188
H	-1.716239	-1.140116	-0.875362
C	-1.066118	-0.942468	1.100178
H	-0.257019	-0.777428	1.811860
H	-2.059345	-1.115160	1.510595
O	-1.824907	1.420511	-0.446002
H	-1.328436	1.664844	0.355350

Table S23. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC11+ (conf#2 + OH)

C	-2.603443	0.327248	0.100906
H	-2.611018	1.130226	-0.648017
H	-3.138745	-0.533351	-0.322723
H	-3.164473	0.676248	0.975954
C	-1.172435	-0.048372	0.474049
H	-1.184324	-0.829855	1.247443
H	-0.657025	0.822264	0.901052
C	-0.383562	-0.542721	-0.731653
H	-0.884034	-1.421203	-1.170941
H	-0.393143	0.229472	-1.516179
C	1.047563	-0.903571	-0.459915
H	1.624022	-1.23772	-1.327203
C	1.660641	-0.854389	0.730836
H	1.142486	-0.53156	1.632348

H	2.703851	-1.150224	0.83489
O	1.591758	1.685168	-0.12801
H	2.535759	1.495188	-0.267883

Table S24. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC12+ (conf#2 + OH)

C	2.612711	0.320466	-0.122026
H	2.608047	1.211124	0.519854
H	3.137342	-0.480124	0.416461
H	3.191598	0.557023	-1.022571
C	1.188586	-0.100052	-0.473064
H	1.214839	-0.974252	-1.139213
H	0.683645	0.708551	-1.017981
C	0.374145	-0.435604	0.770086
H	0.865614	-1.249031	1.328257
H	0.366885	0.430915	1.448274
C	-1.050420	-0.835676	0.518007
H	-1.646034	-1.048857	1.409436
C	-1.633242	-0.964180	-0.681779
H	-1.094320	-0.768029	-1.607499
H	-2.671355	-1.283861	-0.766500
O	-1.635676	1.684480	0.080856
H	-2.521534	1.510975	-0.282709

Table S25. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC21+ (conf#2 + OH)

C	-2.603443	0.327248	0.100906
H	-2.611018	1.130226	-0.648017
H	-3.138745	-0.533351	-0.322723
H	-3.164473	0.676248	0.975954
C	-1.172435	-0.048372	0.474049
H	-1.184324	-0.829855	1.247443
H	-0.657025	0.822264	0.901052
C	-0.383562	-0.542721	-0.731653
H	-0.884034	-1.421203	-1.170941
H	-0.393143	0.229472	-1.516179
C	1.047563	-0.903571	-0.459915
H	1.624022	-1.23772	-1.327203
C	1.660641	-0.854389	0.730836
H	1.142486	-0.53156	1.632348

H	2.703851	-1.150224	0.83489
O	1.591758	1.685168	-0.12801
H	2.535759	1.495188	-0.267883

Table S26. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC22+ (conf#2 + OH)

C	2.612711	0.320466	-0.122026
H	2.608047	1.211124	0.519854
H	3.137342	-0.480124	0.416461
H	3.191598	0.557023	-1.022571
C	1.188586	-0.100052	-0.473064
H	1.214839	-0.974252	-1.139213
H	0.683645	0.708551	-1.017981
C	0.374145	-0.435604	0.770086
H	0.865614	-1.249031	1.328257
H	0.366885	0.430915	1.448274
C	-1.050420	-0.835676	0.518007
H	-1.646034	-1.048857	1.409436
C	-1.633242	-0.964180	-0.681779
H	-1.094320	-0.768029	-1.607499
H	-2.671355	-1.283861	-0.766500
O	-1.635676	1.684480	0.080856
H	-2.521534	1.510975	-0.282709

Table S27. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC11- (conf#3 + OH)

C	1.876492	0.840873	0.456908
H	1.011370	1.358831	0.889401
H	2.400129	0.317677	1.268823
H	2.556805	1.599132	0.050606
C	1.451040	-0.146972	-0.627444
H	2.342790	-0.585071	-1.094739
H	0.914325	0.380569	-1.432736
C	0.560482	-1.285633	-0.103293
H	0.290932	-1.947427	-0.936439
H	1.142188	-1.882760	0.615480
C	-0.691511	-0.785916	0.560202
H	-0.579473	-0.323247	1.542806
C	-1.911510	-0.842697	0.013736
H	-2.069562	-1.294818	-0.966387

H	-2.785345	-0.446294	0.525993
O	-1.518056	1.825310	-0.186924
H	-0.789672	1.543006	-0.768072

Table S28. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC11+ (conf#3 + OH)

C	2.082728	0.530419	0.641729
H	1.361439	0.908744	1.377795
H	2.601486	-0.327293	1.092237
H	2.823095	1.320695	0.471858
C	1.397009	0.133773	-0.663744
H	2.159996	-0.111575	-1.414770
H	0.816080	0.979590	-1.052759
C	0.459816	-1.075463	-0.519720
H	-0.007276	-1.289495	-1.489923
H	1.061280	-1.955003	-0.240550
C	-0.614905	-0.880108	0.508873
H	-0.293595	-0.811390	1.552366
C	-1.922972	-0.791065	0.233133
H	-2.289321	-0.871085	-0.790468
H	-2.664579	-0.654158	1.018073
O	-1.601367	1.691110	-0.288123
H	-1.167720	1.776754	0.579499

Table S29. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC12- (conf#3 + OH)

C	2.029786	0.479902	0.508566
H	1.316086	1.178611	0.959740
H	2.396230	-0.201325	1.289464
H	2.882553	1.067546	0.148471
C	1.388621	-0.299331	-0.636959
H	2.158014	-0.885380	-1.157768
H	0.962434	0.404383	-1.363051
C	0.287394	-1.264559	-0.176027
H	-0.096553	-1.827825	-1.037396
H	0.732016	-1.994088	0.519905
C	-0.856091	-0.586977	0.518239
H	-0.624025	-0.042948	1.436592
C	-2.128474	-0.626768	0.102253
H	-2.408669	-1.173815	-0.799369

H	-2.923606	-0.133164	0.659790
O	-0.875895	1.945032	-0.230092
H	-1.714734	1.834149	-0.712081

Table S30. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC12+ (conf#3 + OH)

C	2.032580	0.484487	0.505877
H	1.316083	1.175778	0.964102
H	2.409126	-0.196770	1.281833
H	2.878295	1.080323	0.142680
C	1.389699	-0.295456	-0.638104
H	2.158702	-0.877972	-1.163458
H	0.958511	0.408054	-1.361552
C	0.293307	-1.264829	-0.173467
H	-0.088579	-1.832790	-1.032693
H	0.742054	-1.989930	0.524431
C	-0.852816	-0.588656	0.518337
H	-0.622713	-0.037577	1.433031
C	-2.125306	-0.636621	0.102956
H	-2.403235	-1.192607	-0.794188
H	-2.922264	-0.141322	0.656244
O	-0.896603	1.951600	-0.220330
H	-1.677932	1.798460	-0.781382

Table S31. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC21- (conf#3 + OH)

C	-2.559684	0.058150	-0.626930
H	-2.211621	0.989327	-1.091095
H	-2.459046	-0.748799	-1.365826
H	-3.626089	0.179381	-0.402683
C	-1.767508	-0.264103	0.638411
H	-2.219626	-1.129379	1.141285
H	-1.828556	0.580236	1.339079
C	-0.289057	-0.580919	0.370982
H	0.214643	-0.838202	1.312123
H	-0.224719	-1.465842	-0.280889
C	0.444603	0.557064	-0.274887
H	0.154806	0.820456	-1.296275
C	1.411165	1.267917	0.319935
H	1.731042	1.040838	1.336933

H	1.904535	2.096402	-0.186222
O	2.796187	-0.894717	-0.238468
H	2.758025	-0.595336	-1.163745

Table S32. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC21+ (conf#3 + OH)

C	-2.544594	-0.126129	-0.760749
H	-2.085537	0.558059	-1.485030
H	-2.442423	-1.149904	-1.147004
H	-3.613850	0.111101	-0.713344
C	-1.897632	0.003123	0.615635
H	-2.462004	-0.595334	1.344131
H	-1.945137	1.048449	0.952189
C	-0.431288	-0.455893	0.644466
H	-0.039285	-0.360952	1.665829
H	-0.398231	-1.523773	0.374329
C	0.443212	0.326907	-0.293141
H	0.282275	0.179573	-1.363494
C	1.392237	1.184995	0.100544
H	1.591374	1.357195	1.159080
H	1.991633	1.741890	-0.617611
O	3.111079	-0.705504	-0.265822
H	2.460947	-1.320283	0.116967

Table S33. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC22- (conf#3 + OH)

C	-2.466459	-0.132554	-0.696743
H	-2.078836	0.618722	-1.395922
H	-2.336144	-1.122338	-1.155363
H	-3.541775	0.047246	-0.580665
C	-1.752449	-0.063287	0.651168
H	-2.239007	-0.749784	1.357189
H	-1.848739	0.947759	1.071076
C	-0.263607	-0.431091	0.574110
H	0.179213	-0.399976	1.578255
H	-0.164035	-1.462140	0.205632
C	0.512440	0.482891	-0.327904
H	0.315152	0.405090	-1.399766
C	1.395050	1.396030	0.097995
H	1.624486	1.503107	1.158925

H	1.903678	2.064379	-0.596334
O	2.557451	-1.111274	-0.181997
H	3.176544	-0.473811	-0.578810

Table S34. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC22+ (conf#3 + OH)

C	-2.373098	-0.497950	-0.671500
H	-1.917461	-0.142452	-1.603950
H	-2.192289	-1.578775	-0.595412
H	-3.455232	-0.340930	-0.751897
C	-1.805396	0.232426	0.543487
H	-2.366969	-0.061540	1.440409
H	-1.941648	1.316282	0.422446
C	-0.317581	-0.057197	0.790773
H	0.010779	0.463268	1.700971
H	-0.182624	-1.135335	0.959631
C	0.553486	0.362242	-0.356242
H	0.447052	-0.196240	-1.288739
C	1.420372	1.383028	-0.315987
H	1.550856	1.973269	0.593352
H	2.013530	1.660608	-1.185797
O	2.516652	-1.240862	-0.012138
H	3.034095	-0.566561	0.462910

Table S35. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC11- (conf#4 + OH)

C	2.762053	0.365283	-0.157344
H	3.237682	-0.170821	0.674372
H	2.993970	-0.176742	-1.083454
H	3.216562	1.361060	-0.223582
C	1.254070	0.453650	0.052950
H	0.802137	1.023970	-0.773600
H	1.034496	1.001880	0.980600
C	0.588778	-0.927068	0.110711
H	0.703734	-1.427377	-0.861110
H	1.115428	-1.537876	0.859391
C	-0.865371	-0.837810	0.469947
H	-1.096951	-0.548433	1.498408
C	-1.873696	-1.044583	-0.384136
H	-1.683036	-1.327441	-1.420965

H	-2.911535	-0.941942	-0.074350
O	-2.169466	1.622646	0.020769
H	-1.251765	1.705724	-0.294628

Table S36. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC11+ (conf#4 + OH)

C	-0.925545	-0.963302	0.363469
H	-0.896006	-1.262075	1.416848
H	-2.115877	-0.788961	-0.224650
H	-3.047061	-0.942711	0.318625
C	-2.189606	-0.503719	-1.273968
H	-1.642352	1.759834	-0.114823
H	-1.730984	1.652334	0.848799
C	0.400769	-0.784706	-0.311463
H	0.885518	-1.769520	-0.412589
H	0.243415	-0.391475	-1.325272
C	1.340162	0.141979	0.465103
H	1.471675	-0.252922	1.483391
C	0.863597	1.126561	0.556762
H	2.699620	0.281245	-0.212999
H	3.364706	0.938401	0.359791
O	3.189931	-0.696649	-0.311176
H	2.588848	0.705569	-1.219382

Table S37. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC12- (conf#4 + OH)

C	2.745096	0.193091	-0.187628
H	3.198285	-0.489975	0.543381
H	2.880981	-0.245912	-1.185080
H	3.299096	1.138718	-0.156633
C	1.265820	0.408467	0.114272
H	0.824685	1.111054	-0.603599
H	1.145979	0.870067	1.104566
C	0.474426	-0.902793	0.077408
H	0.538247	-1.351889	-0.924271
H	0.941483	-1.612094	0.779772
C	-0.962777	-0.725456	0.462859
H	-1.148603	-0.293416	1.450186
C	-2.010043	-1.060861	-0.300501
H	-1.867910	-1.506022	-1.286853

H	-3.032400	-0.918002	0.046384
O	-1.718675	1.788363	0.009446
H	-2.105576	1.515885	-0.841874

Table S38. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC12+ (conf#4 + OH)

C	2.718793	0.143617	-0.228493
H	3.162396	-0.845256	-0.050706
H	2.673920	0.301287	-1.314737
H	3.393409	0.897854	0.194088
C	1.326761	0.238148	0.388505
H	0.900873	1.233536	0.218399
H	1.392706	0.101410	1.477160
C	0.373527	-0.812449	-0.185722
H	0.278906	-0.683857	-1.273838
H	0.811764	-1.809970	-0.016453
C	-0.988723	-0.785687	0.439612
H	-1.018837	-0.708803	1.530052
C	-2.144380	-0.882982	-0.229810
H	-2.161179	-0.965592	-1.317961
H	-3.100973	-0.900719	0.292151
O	-1.455585	1.791648	-0.075858
H	-2.404179	1.643044	-0.235834

Table S39. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC21- (conf#4 + OH)

C	2.881078	0.542572	0.180184
H	2.871590	1.382961	-0.526320
H	2.767719	0.954097	1.191754
H	3.863112	0.058770	0.118639
C	1.756721	-0.439717	-0.133172
H	1.789818	-1.287290	0.566549
H	1.898260	-0.858532	-1.140539
C	0.373878	0.216967	-0.050858
H	0.200499	0.610966	0.960829
H	0.347969	1.077941	-0.736482
C	-0.726600	-0.734548	-0.410298
H	-0.705496	-1.140258	-1.427266
C	-1.695608	-1.132544	0.423650
H	-1.742381	-0.763371	1.448715

H	-2.461307	-1.840207	0.110090
O	-2.708040	1.256891	0.036070
H	-2.702280	1.033415	-0.911557

Table S40. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC21+ (conf#4 + OH)

C	-2.894808	-0.410079	0.208066
H	-2.820925	-1.497621	0.075594
H	-2.963753	-0.206756	1.284930
H	-3.827288	-0.073168	-0.260272
C	-1.683665	0.291550	-0.398568
H	-1.780311	1.379820	-0.280690
H	-1.641299	0.094311	-1.479386
C	-0.369910	-0.164001	0.244952
H	-0.390776	0.050847	1.323390
H	-0.270124	-1.253154	0.128762
C	0.820213	0.500383	-0.377483
H	0.992148	0.292506	-1.436887
C	1.644376	1.344836	0.256417
H	1.494294	1.590092	1.309550
H	2.479171	1.818486	-0.257375
O	2.590236	-1.329492	-0.093235
H	2.909735	-0.935558	0.737964

Table S41. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC22- (conf#4 + OH)

C	2.854474	0.451591	0.198591
H	2.813138	1.444963	-0.267600
H	2.825365	0.590522	1.287332
H	3.817088	-0.006079	-0.059296
C	1.685877	-0.411613	-0.267197
H	1.750090	-1.410136	0.187230
H	1.742114	-0.557341	-1.355795
C	0.332136	0.212026	0.087060
H	0.246146	0.332045	1.176156
H	0.269160	1.216826	-0.355030
C	-0.812667	-0.614171	-0.415041
H	-0.899534	-0.710581	-1.501162
C	-1.687453	-1.264285	0.363334
H	-1.630673	-1.195071	1.450322

H	-2.474096	-1.887381	-0.061273
O	-2.431335	1.385625	-0.022941
H	-3.242315	0.855947	-0.117841

Table S42. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC22+ (conf#4 + OH)

C	-2.893797	-0.411706	0.207428
H	-2.822557	-1.497258	0.058448
H	-2.957576	-0.224330	1.287501
H	-3.827706	-0.066047	-0.251601
C	-1.683929	0.296635	-0.393924
H	-1.779225	1.383379	-0.261875
H	-1.644982	0.113223	-1.477306
C	-0.368715	-0.168102	0.240036
H	-0.385516	0.035319	1.320768
H	-0.271098	-1.256113	0.112178
C	0.820374	0.500983	-0.379224
H	0.992352	0.299125	-1.439768
C	1.643252	1.343420	0.259017
H	1.492889	1.582762	1.313461
H	2.477052	1.821278	-0.252443
O	2.589244	-1.328032	-0.093383
H	2.909312	-0.934461	0.737710

Table S43. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC11- (conf#5 + OH)

C	1.326845	1.405505	-0.006345
H	0.938089	1.585045	-1.020440
H	0.515017	1.559724	0.717129
H	2.094808	2.161506	0.193174
C	1.893897	-0.007255	0.107925
H	2.192615	-0.198768	1.148566
H	2.802911	-0.092683	-0.501645
C	0.900797	-1.087267	-0.336526
H	0.676777	-0.973697	-1.407363
H	1.374496	-2.072515	-0.209677
C	-0.382710	-1.063841	0.442981
H	-0.286674	-1.006108	1.532164
C	-1.607349	-1.123348	-0.093026
H	-1.748198	-1.184780	-1.172835

H	-2.501047	-1.131327	0.527319
O	-2.195631	1.387734	-0.019939
H	-1.282618	1.508968	-0.336931

Table S44. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC11+ (conf#5 + OH)

C	-1.557691	1.102920	-0.463225
H	-1.134553	1.790086	0.282070
H	-0.866007	1.037251	-1.316443
H	-2.491102	1.541491	-0.834470
C	-1.796875	-0.274610	0.149473
H	-2.243570	-0.940271	-0.603326
H	-2.524917	-0.190624	0.966571
C	-0.517082	-0.923492	0.689160
H	-0.071440	-0.293190	1.471857
H	-0.782231	-1.884790	1.154891
C	0.502935	-1.176953	-0.385606
H	0.120344	-1.601853	-1.320058
C	1.814442	-0.947238	-0.273218
H	2.240970	-0.541874	0.646301
H	2.502397	-1.169971	-1.087179
O	1.695351	1.757111	0.332546
H	1.012922	1.513100	-0.320087

Table S45. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC12- (conf#5 + OH)

C	-1.633142	0.705958	0.846736
H	-2.101737	0.022123	1.567457
H	-0.651906	0.992751	1.244204
H	-2.248213	1.611228	0.785524
C	-1.496685	0.036736	-0.517068
H	-1.097838	0.755921	-1.245116
H	-2.488554	-0.271088	-0.873578
C	-0.580532	-1.197895	-0.474699
H	-0.866790	-1.836616	0.373514
H	-0.723292	-1.783169	-1.393832
C	0.869048	-0.827684	-0.361739
H	1.323573	-0.385345	-1.253616
C	1.622398	-0.986229	0.731943
H	1.213338	-1.434844	1.638639

H	2.672154	-0.693875	0.744613
O	1.351590	1.870071	-0.431859
H	1.470021	1.677033	0.516030

Table S46. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC12+ (conf#5 + OH)

C	-1.602999	0.805443	0.742980
H	-2.080206	0.248121	1.560491
H	-0.610783	1.131098	1.075242
H	-2.202284	1.702579	0.547718
C	-1.500109	-0.065414	-0.505250
H	-1.122020	0.532896	-1.345604
H	-2.498457	-0.425766	-0.787243
C	-0.577643	-1.278638	-0.293442
H	-0.808108	-1.745024	0.675398
H	-0.774101	-2.026361	-1.074079
C	0.877664	-0.914036	-0.340994
H	1.293859	-0.736974	-1.336818
C	1.675314	-0.793095	0.725822
H	1.295508	-0.962001	1.734029
H	2.731396	-0.540802	0.630204
O	1.179007	1.837409	-0.389328
H	2.109782	1.597395	-0.539412

Table S47. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC21- (conf#5 + OH)

C	2.447628	0.515821	-0.387570
H	2.276561	0.548887	-1.472160
H	2.029803	1.433699	0.043841
H	3.530269	0.518426	-0.214426
C	1.794629	-0.722631	0.219534
H	1.980121	-0.748780	1.303465
H	2.254231	-1.627359	-0.199998
C	0.281798	-0.779364	-0.034546
H	0.078477	-0.747175	-1.114001
H	-0.111116	-1.736480	0.338058
C	-0.450163	0.342376	0.639496
H	-0.379697	0.376472	1.732249
C	-1.146689	1.294909	0.007960
H	-1.225768	1.305661	-1.079128

H	-1.650495	2.090725	0.554426
O	-2.918809	-0.585929	-0.392379
H	-2.995130	-0.633310	0.577472

Table S48. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC21+ (conf#5 + OH)

C	-2.516431	0.588491	0.052083
H	-2.530418	0.839710	1.122389
H	-1.997474	1.397916	-0.473226
H	-3.553661	0.559172	-0.303400
C	-1.818225	-0.749283	-0.177585
H	-1.817680	-0.989626	-1.250207
H	-2.374976	-1.550461	0.326626
C	-0.371270	-0.761284	0.336625
H	-0.358727	-0.510644	1.408347
H	0.035025	-1.779034	0.228638
C	0.505230	0.196162	-0.414020
H	0.623354	0.000659	-1.483608
C	1.132370	1.250833	0.121504
H	1.038836	1.484661	1.183365
H	1.755098	1.906441	-0.484640
O	3.108679	-0.450443	-0.061565
H	2.721138	-0.904759	0.706595

Table S49. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC22- (conf#5 + OH)

C	2.475544	0.469897	-0.184941
H	2.430316	0.629327	-1.270978
H	2.055925	1.359493	0.300877
H	3.530859	0.389873	0.101877
C	1.701331	-0.786433	0.204039
H	1.760881	-0.939374	1.291646
H	2.164760	-1.665738	-0.262652
C	0.225840	-0.732146	-0.216439
H	0.151617	-0.565521	-1.300553
H	-0.252261	-1.696918	-0.000881
C	-0.525919	0.347401	0.502846
H	-0.610547	0.233598	1.587701
C	-1.051473	1.434809	-0.075947
H	-0.979524	1.585383	-1.153794

H	-1.556846	2.203941	0.507490
O	-2.790338	-0.748740	-0.145207
H	-3.324416	0.054688	-0.016421

Table S50. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for σ-PC22+ (conf#5 + OH)

C	-2.515162	0.456382	-0.052085
H	-2.603009	0.792889	0.990106
H	-2.044946	1.265246	-0.625104
H	-3.526995	0.303188	-0.445465
C	-1.691649	-0.825922	-0.134005
H	-1.618540	-1.156169	-1.180434
H	-2.201363	-1.629560	0.413638
C	-0.277099	-0.662873	0.438635
H	-0.336853	-0.325103	1.483884
H	0.232373	-1.636268	0.432143
C	0.546806	0.307276	-0.353608
H	0.722347	0.046434	-1.401237
C	1.044914	1.458330	0.115734
H	0.873139	1.763625	1.149671
H	1.627751	2.125631	-0.517113
O	2.894270	-0.721932	-0.130257
H	3.075077	-0.173624	0.653954

Table S51. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS11- (Conf#1 + OH)

C	2.217011	-0.676495	0.219723
H	2.952197	0.042246	0.605827
H	1.676586	-1.090285	1.079882
H	2.766397	-1.494645	-0.261221
C	1.270930	0.004666	-0.768475
H	0.584451	-0.724223	-1.219714
H	1.859489	0.425605	-1.594065
C	0.454385	1.131229	-0.139605
H	1.120188	1.818413	0.407534
H	-0.010806	1.737991	-0.932117
C	-0.647459	0.701710	0.782892
H	-1.171194	1.506816	1.305617
C	-1.087188	-0.564550	0.963641
H	-0.576855	-1.420021	0.529746

H	-1.901418	-0.776128	1.653100
O	-2.216232	-0.481059	-0.907709
H	-2.815254	0.243337	-0.661975

Table S52. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS12+ (Conf#1 + OH)

C	-2.31560	0.40683	-0.21913
H	-2.93891	0.17295	0.65421
H	-1.88340	1.40197	-0.05737
H	-2.97239	0.45898	-1.09597
C	-1.23600	-0.66068	-0.40092
H	-0.67979	-0.50408	-1.33512
H	-1.72091	-1.64066	-0.49568
C	-0.24402	-0.72229	0.75894
H	-0.78277	-0.63710	1.71689
H	0.26431	-1.69429	0.77610
C	0.83363	0.32604	0.74995
H	1.53157	0.28095	1.58743
C	0.90792	1.39600	-0.08201
H	0.22331	1.52104	-0.91824
H	1.68398	2.14833	0.04749
O	2.09787	-0.73414	-0.61414
H	2.81649	-0.11037	-0.80769

Table S53. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS21- (Conf#1 + OH)

C	1.393878	1.360770	0.009133
H	1.608208	1.565375	-1.049139
H	0.352749	1.643193	0.204051
H	2.041326	2.010073	0.610424
C	1.656979	-0.111182	0.326998
H	1.480001	-0.307691	1.393898
H	2.717063	-0.332474	0.146430
C	0.823538	-1.079018	-0.512008
H	0.922949	-0.822087	-1.580118
H	1.239203	-2.095961	-0.427120
C	-0.636713	-1.175756	-0.174889
H	-1.225658	-1.839175	-0.813294
C	-1.280388	-0.531081	0.825884
H	-0.751040	0.109847	1.527407

H	-2.319816	-0.754464	1.048044
O	-2.038305	1.128248	-0.345346
H	-1.502307	1.014983	-1.148525

Table S54. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS22- (Conf#1 + OH)

C	1.681232	0.972332	0.363001
H	1.789608	1.538404	-0.571217
H	0.800672	1.373248	0.875173
H	2.568191	1.158734	0.981060
C	1.537435	-0.519447	0.063489
H	1.474905	-1.093586	0.999610
H	2.446150	-0.869846	-0.444287
C	0.344910	-0.863995	-0.827880
H	0.351890	-0.232618	-1.727390
H	0.440612	-1.902282	-1.182244
C	-1.017125	-0.751438	-0.203149
H	-1.848790	-1.011739	-0.859027
C	-1.277754	-0.565751	1.114550
H	-0.488319	-0.344358	1.830241
H	-2.297429	-0.613213	1.493071
O	-1.330647	1.358377	-0.539469
H	-2.204500	1.500046	-0.139298

Table S55. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS11 (Conf#2 + OH)

C	-2.655717	0.426714	0.011256
H	-2.705668	0.878013	-0.988569
H	-3.224188	-0.512623	-0.014653
H	-3.156752	1.105139	0.711765
C	-1.207559	0.181144	0.423181
H	-1.178962	-0.246445	1.435659
H	-0.658445	1.131218	0.456267
C	-0.493943	-0.758391	-0.540935
H	-1.025564	-1.722921	-0.592930
H	-0.546004	-0.342313	-1.560374
C	0.946090	-1.025203	-0.227727
H	1.475556	-1.689020	-0.916936
C	1.640347	-0.475286	0.795182
H	1.157247	0.139257	1.549724

H	2.682931	-0.734801	0.964706
O	1.924062	1.365001	-0.340371
H	2.412037	0.980612	-1.087425

Table S56. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS12 (Conf#2 + OH)

C	2.641555	0.217278	-0.146174
H	2.673289	1.234779	0.264957
H	3.102064	-0.457350	0.588148
H	3.256862	0.200237	-1.053358
C	1.203857	-0.199177	-0.442722
H	1.197801	-1.208168	-0.879048
H	0.758774	0.480747	-1.181066
C	0.341952	-0.177760	0.813976
H	0.736112	-0.895924	1.551269
H	0.402955	0.812362	1.285812
C	-1.110378	-0.490473	0.601119
H	-1.749010	-0.390495	1.480118
C	-1.640380	-1.052138	-0.514093
H	-1.047290	-1.211019	-1.412371
H	-2.690936	-1.336533	-0.548305
O	-1.595156	1.454682	-0.181092
H	-2.499011	1.347526	-0.520052

Table S57. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS21 (Conf#2 + OH)

C	-2.655717	0.426714	0.011256
H	-2.705668	0.878013	-0.988569
H	-3.224188	-0.512623	-0.014653
H	-3.156752	1.105139	0.711765
C	-1.207559	0.181144	0.423181
H	-1.178962	-0.246445	1.435659
H	-0.658445	1.131218	0.456267
C	-0.493943	-0.758391	-0.540935
H	-1.025564	-1.722921	-0.592930
H	-0.546004	-0.342313	-1.560374
C	0.946090	-1.025203	-0.227727
H	1.475556	-1.689020	-0.916936
C	1.640347	-0.475286	0.795182
H	1.157247	0.139257	1.549724

H	2.682931	-0.734801	0.964706
O	1.924062	1.365001	-0.340371
H	2.412037	0.980612	-1.087425

Table S58. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS22 (Conf#2 + OH)

C	2.641555	0.217278	-0.146174
H	2.673289	1.234779	0.264957
H	3.102064	-0.457350	0.588148
H	3.256862	0.200237	-1.053358
C	1.203857	-0.199177	-0.442722
H	1.197801	-1.208168	-0.879048
H	0.758774	0.480747	-1.181066
C	0.341952	-0.177760	0.813976
H	0.736112	-0.895924	1.551269
H	0.402955	0.812362	1.285812
C	-1.110378	-0.490473	0.601119
H	-1.749010	-0.390495	1.480118
C	-1.640380	-1.052138	-0.514093
H	-1.047290	-1.211019	-1.412371
H	-2.690936	-1.336533	-0.548305
O	-1.595156	1.454682	-0.181092
H	-2.499011	1.347526	-0.520052

Table S59. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS11+ (Conf#3 + OH)

C	2.132368	0.542285	0.609386
H	1.429315	0.970552	1.335269
H	2.634480	-0.310014	1.088105
H	2.891042	1.305074	0.399125
C	1.421817	0.113232	-0.671922
H	2.167799	-0.189456	-1.419020
H	0.858110	0.956606	-1.089057
C	0.449310	-1.060787	-0.469171
H	-0.023800	-1.309428	-1.427872
H	1.025454	-1.941506	-0.142638
C	-0.615639	-0.778811	0.543648
H	-0.296398	-0.647527	1.581042
C	-1.928131	-0.641836	0.249450
H	-2.297999	-0.823819	-0.757922

H	-2.668826	-0.466758	1.026350
O	-1.649705	1.455286	-0.333793
H	-1.279879	1.769496	0.508615

Table S60. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS12+ (Conf#3 + OH)

C	2.087633	0.340524	0.647973
H	1.440148	1.093194	1.113099
H	2.270475	-0.462911	1.376125
H	3.049024	0.819966	0.429632
C	1.450381	-0.203255	-0.627801
H	2.175846	-0.828094	-1.166129
H	1.180566	0.629448	-1.285804
C	0.204184	-1.057183	-0.368183
H	-0.251194	-1.358698	-1.320639
H	0.517918	-1.980611	0.147120
C	-0.846327	-0.424310	0.496817
H	-0.518338	-0.028662	1.458919
C	-2.176223	-0.513526	0.254263
H	-2.548215	-0.938477	-0.677565
H	-2.908962	-0.148353	0.972440
O	-0.876431	1.554417	-0.422485
H	-1.713710	1.914367	-0.085729

Table S61. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS21- (Conf#3 + OH)

C	-2.585813	0.364449	-0.531179
H	-2.151866	1.355096	-0.715594
H	-2.581001	-0.192155	-1.478366
H	-3.630228	0.512169	-0.232188
C	-1.811862	-0.392885	0.545371
H	-2.334424	-1.329663	0.780638
H	-1.785157	0.199640	1.470331
C	-0.371392	-0.737440	0.135032
H	0.115383	-1.318407	0.928341
H	-0.401663	-1.374130	-0.762642
C	0.458338	0.474581	-0.153642
H	0.206243	1.059781	-1.041879
C	1.509953	0.865586	0.601314
H	1.758334	0.345487	1.524486

H	2.059690	1.777535	0.380213
O	2.857780	-0.528200	-0.390845
H	2.687115	-0.255506	-1.307957

Table S62. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS22- (Conf#3 + OH)

C	-2.377233	-0.065577	-0.721801
H	-1.917790	0.621608	-1.443355
H	-2.305685	-1.083269	-1.129223
H	-3.439493	0.195460	-0.647240
C	-1.695212	0.020104	0.641866
H	-2.255062	-0.582611	1.369459
H	-1.716791	1.057956	1.002922
C	-0.242333	-0.475953	0.627858
H	0.186695	-0.409245	1.635813
H	-0.215644	-1.531790	0.328272
C	0.617734	0.313699	-0.314752
H	0.469724	0.143025	-1.381698
C	1.403890	1.345418	0.075121
H	1.551137	1.564443	1.132569
H	1.930392	1.966235	-0.648293
O	2.306270	-1.031065	-0.183947
H	3.021282	-0.519440	-0.597396

Table S63. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS11+ (Conf#4 + OH)

C	2.744681	0.299030	-0.214164
H	3.251609	-0.663831	-0.065575
H	2.694362	0.490489	-1.293991
H	3.363514	1.082191	0.239539
C	1.346654	0.277152	0.395332
H	0.851765	1.245895	0.251328
H	1.416456	0.105479	1.479676
C	0.463947	-0.810334	-0.227864
H	0.350931	-0.624309	-1.304518
H	0.968746	-1.783250	-0.110722
C	-0.886692	-0.881314	0.408507
H	-0.910910	-1.055132	1.488905
C	-2.053965	-0.694740	-0.247264
H	-2.074434	-0.577493	-1.328857

H	-3.010922	-0.779520	0.262701
O	-1.852151	1.482961	-0.141304
H	-1.771658	1.557028	0.824663

Table S64. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS12+ (Conf#4 + OH)

C	2.736874	0.001830	-0.221743
H	3.075417	-1.022414	-0.013837
H	2.709408	0.132314	-1.311678
H	3.485183	0.694308	0.181382
C	1.362211	0.259838	0.387192
H	1.041666	1.288150	0.187200
H	1.413108	0.146283	1.480120
C	0.307218	-0.699298	-0.161241
H	0.222297	-0.591097	-1.251331
H	0.632406	-1.734367	0.035772
C	-1.051215	-0.527428	0.452623
H	-1.078621	-0.299951	1.520654
C	-2.212891	-0.818275	-0.180466
H	-2.223359	-1.077526	-1.238630
H	-3.167044	-0.785104	0.343228
O	-1.335647	1.533610	-0.197023
H	-2.278465	1.680515	-0.014890

Table S65. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS21- (Conf#4 + OH)

C	-2.945487	-0.447027	0.177367
H	-2.986043	-1.297376	-0.516216
H	-2.859908	-0.848579	1.195520
H	-3.895219	0.096030	0.105308
C	-1.762114	0.459266	-0.147096
H	-1.747626	1.319595	0.536305
H	-1.871143	0.866638	-1.162564
C	-0.423938	-0.281400	-0.041825
H	-0.284635	-0.670600	0.975825
H	-0.444934	-1.151505	-0.716581
C	0.736425	0.589002	-0.402699
H	0.761540	0.979140	-1.424831
C	1.748903	0.898621	0.438257
H	1.726027	0.583983	1.479794

H	2.550041	1.570422	0.138517
O	2.761014	-0.984472	0.023127
H	2.841052	-0.882752	-0.940117

Table S66. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS22- (Conf#4 + OH)

C	-2.844875	-0.315993	0.186898
H	-2.889685	-1.327105	-0.238550
H	-2.842931	-0.411834	1.280646
H	-3.757189	0.217270	-0.105821
C	-1.596145	0.417075	-0.293416
H	-1.579754	1.439096	0.110150
H	-1.619365	0.512424	-1.388775
C	-0.310760	-0.305172	0.124265
H	-0.245194	-0.354896	1.219750
H	-0.328139	-1.337138	-0.249641
C	0.904705	0.386288	-0.413690
H	1.058105	0.328232	-1.492909
C	1.675205	1.233924	0.308938
H	1.524239	1.346194	1.382459
H	2.479108	1.805394	-0.152740
O	2.261988	-1.236481	0.027785
H	3.136114	-0.822525	-0.064825

Table S67. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS11- (Conf#5 + OH)

C	1.593875	1.232115	0.032308
H	1.302074	1.531082	-0.985613
H	0.792078	1.522152	0.724193
H	2.489689	1.803300	0.301205
C	1.856477	-0.269858	0.095809
H	2.106368	-0.556453	1.127459
H	2.729166	-0.521299	-0.520685
C	0.664400	-1.108747	-0.378978
H	0.435911	-0.882953	-1.431145
H	0.947395	-2.172544	-0.336997
C	-0.569068	-0.915648	0.451225
H	-0.429549	-0.884051	1.535671
C	-1.818936	-0.774828	-0.044542
H	-2.007565	-0.847530	-1.114677

H	-2.683658	-0.730581	0.611251
O	-1.879878	1.401711	-0.050209
H	-1.003377	1.546981	-0.443920

Table S68. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS12- (Conf#5 + OH)

C	-2.075578	0.523336	0.535466
H	-2.400212	-0.028830	1.428063
H	-1.335468	1.272541	0.834411
H	-2.948261	1.046751	0.126308
C	-1.476959	-0.430885	-0.494136
H	-1.224261	0.123685	-1.406842
H	-2.230344	-1.180742	-0.768531
C	-0.219098	-1.151036	0.022946
H	-0.268591	-1.268730	1.115216
H	-0.185940	-2.166603	-0.401301
C	1.086516	-0.512877	-0.354900
H	1.254201	-0.361265	-1.421975
C	2.136795	-0.365979	0.492574
H	2.030884	-0.583463	1.556153
H	3.100622	-0.008501	0.137403
O	0.801414	1.613902	-0.367173
H	1.085999	1.868587	0.526777

Table S69. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS21- (Conf#5 + OH)

C	2.409556	0.694791	-0.251037
H	2.265957	0.862616	-1.327100
H	1.897425	1.503910	0.284455
H	3.482045	0.769138	-0.036226
C	1.858553	-0.668781	0.156252
H	2.008986	-0.825848	1.234363
H	2.414869	-1.463090	-0.358345
C	0.366791	-0.827074	-0.173199
H	0.198040	-0.669754	-1.247330
H	0.055631	-1.856755	0.056230
C	-0.491542	0.120238	0.603506
H	-0.481744	0.010885	1.692711
C	-1.280369	1.069253	0.051182
H	-1.263105	1.253730	-1.021032

H	-1.858502	1.755198	0.666257
O	-2.865463	-0.370256	-0.352076
H	-2.973828	-0.708538	0.552393

Table S70. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS22- (Conf#5 + OH)

	Cartesian coordinates (angstroms)		
C	2.368245	0.556781	-0.118408
H	2.341027	0.757250	-1.198206
H	1.889723	1.402184	0.391083
H	3.419002	0.523040	0.193009
C	1.658102	-0.755778	0.201476
H	1.690049	-0.942832	1.284807
H	2.191616	-1.588013	-0.276109
C	0.198623	-0.787987	-0.274764
H	0.151270	-0.584449	-1.353711
H	-0.224608	-1.785750	-0.108837
C	-0.648956	0.213142	0.450952
H	-0.801877	0.032811	1.517072
C	-1.043745	1.398751	-0.072218
H	-0.869917	1.627412	-1.123279
H	-1.565991	2.141571	0.529081
O	-2.529382	-0.667807	-0.136449
H	-3.178852	0.009785	0.114456

Table S71. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS11+ (Conf#1 + OH)

C	2.217011	-0.676495	0.219723
H	2.952197	0.042246	0.605827
H	1.676586	-1.090285	1.079882
H	2.766397	-1.494645	-0.261221
C	1.270930	0.004666	-0.768475
H	0.584451	-0.724223	-1.219714
H	1.859489	0.425605	-1.594065
C	0.454385	1.131229	-0.139605
H	1.120188	1.818413	0.407534
H	-0.010806	1.737991	-0.932117
C	-0.647459	0.701710	0.782892
H	-1.171194	1.506816	1.305617
C	-1.087188	-0.564550	0.963641

H	-0.576855	-1.420021	0.529746
H	-1.901418	-0.776128	1.653100
O	-2.216232	-0.481059	-0.907709
H	-2.815254	0.243337	-0.661975

Table S72. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS12- (Conf#1 + OH)

C	-2.351786	0.397305	-0.158524
H	-2.941335	0.105035	0.720473
H	-1.920504	1.384118	0.049261
H	-3.040802	0.497767	-1.005897
C	-1.273452	-0.648542	-0.442792
H	-0.756594	-0.423326	-1.387147
H	-1.755988	-1.623327	-0.588255
C	-0.243850	-0.781122	0.678378
H	-0.758235	-0.772557	1.653371
H	0.273141	-1.745927	0.611134
C	0.824951	0.275848	0.718621
H	1.535671	0.188732	1.540619
C	0.868626	1.404709	-0.036000
H	0.150944	1.589898	-0.834153
H	1.653296	2.141894	0.115548
O	2.315122	-0.618399	-0.505332
H	2.092502	-0.284302	-1.390408

Table S73. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS21+ (Conf#1 + OH)

C	1.393878	1.360770	0.009133
H	1.608208	1.565375	-1.049139
H	0.352749	1.643193	0.204051
H	2.041326	2.010073	0.610424
C	1.656979	-0.111182	0.326998
H	1.480001	-0.307691	1.393898
H	2.717063	-0.332474	0.146430
C	0.823538	-1.079018	-0.512008
H	0.922949	-0.822087	-1.580118
H	1.239203	-2.095961	-0.427120
C	-0.636713	-1.175756	-0.174889
H	-1.225658	-1.839175	-0.813294
C	-1.280388	-0.531081	0.825884

H	-0.751040	0.109847	1.527407
H	-2.319816	-0.754464	1.048044
O	-2.038305	1.128248	-0.345346
H	-1.502307	1.014983	-1.148525

Table S74. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS22+ (Conf#1 + OH)

C	1.667032	0.985111	0.358229
H	1.572185	1.596733	-0.548171
H	0.889290	1.305096	1.062123
H	2.636656	1.204210	0.821139
C	1.556451	-0.501316	0.016839
H	1.559278	-1.103158	0.936967
H	2.452559	-0.799571	-0.543099
C	0.340709	-0.862137	-0.835652
H	0.327180	-0.244645	-1.743902
H	0.432290	-1.905877	-1.174951
C	-1.005943	-0.735090	-0.181141
H	-1.858093	-0.959965	-0.822275
C	-1.234710	-0.593279	1.148663
H	-0.423501	-0.444487	1.860361
H	-2.249588	-0.604440	1.539090
O	-1.520479	1.305150	-0.576528
H	-1.115660	1.755166	0.183308

Table S75. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS11- (Conf#3 + OH)

C	1.944522	0.809743	0.526506
H	1.100456	1.337749	0.987428
H	2.420548	0.187815	1.297102
H	2.674442	1.559304	0.199775
C	1.482871	-0.047669	-0.648748
H	2.353600	-0.475347	-1.163549
H	0.968107	0.579452	-1.391963
C	0.551961	-1.203263	-0.238556
H	0.193991	-1.719197	-1.139325
H	1.140070	-1.927334	0.345856
C	-0.619610	-0.761410	0.586432
H	-0.421437	-0.475094	1.621144
C	-1.884308	-0.644904	0.120484

H	-2.136249	-0.949918	-0.894865
H	-2.706524	-0.377215	0.777509
O	-1.697306	1.484040	-0.246809
H	-0.861172	1.472484	-0.741345

Table S76. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS12- (Conf#3 + OH)

C	2.080412	0.394770	0.593216
H	1.424120	1.179273	0.987509
H	2.271840	-0.337635	1.390562
H	3.036547	0.861719	0.329326
C	1.448922	-0.272673	-0.625181
H	2.179378	-0.939361	-1.103370
H	1.171739	0.495319	-1.355820
C	0.209162	-1.107192	-0.283296
H	-0.232240	-1.521791	-1.200081
H	0.528035	-1.964100	0.333241
C	-0.853350	-0.389153	0.496796
H	-0.543906	0.092818	1.424303
C	-2.180811	-0.497296	0.242144
H	-2.539895	-1.034596	-0.637035
H	-2.919494	-0.038586	0.895279
O	-0.892183	1.617631	-0.314449
H	-1.464675	1.495162	-1.090401

Table S77. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS21+ (Conf#3 + OH)

C	2.573267	-0.455374	-0.543380
H	2.092920	-1.434528	-0.659603
H	2.569433	0.044146	-1.521939
H	3.617257	-0.631132	-0.258699
C	1.860027	0.397599	0.502506
H	2.427065	1.323142	0.670004
H	1.827411	-0.137204	1.461692
C	0.424995	0.779475	0.102144
H	-0.006955	1.433361	0.872168
H	0.469922	1.355159	-0.836313
C	-0.461426	-0.414133	-0.086428
H	-0.256333	-1.062707	-0.940358
C	-1.507719	-0.716378	0.714929

H	-1.729339	-0.117447	1.597525
H	-2.077487	-1.631320	0.577930
O	-2.975261	0.278529	-0.545022
H	-2.466671	1.083163	-0.740855

Table S78. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS22+ (Conf#3 + OH)

C	-2.364528	-0.192551	-0.721580
H	-1.873870	0.342305	-1.544238
H	-2.310301	-1.268409	-0.936129
H	-3.421289	0.099362	-0.720062
C	-1.708455	0.125501	0.620333
H	-2.285790	-0.341364	1.429614
H	-1.729827	1.210127	0.796044
C	-0.257743	-0.368504	0.720555
H	0.141436	-0.135569	1.717302
H	-0.229815	-1.459083	0.600062
C	0.627173	0.253851	-0.319818
H	0.513816	-0.099220	-1.344696
C	1.392355	1.349159	-0.094983
H	1.484222	1.770266	0.907701
H	1.953966	1.823606	-0.896521
O	2.350030	-1.037131	-0.221240
H	2.824390	-0.649713	0.533802

Table S79. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS11- (Conf#4 + OH)

C	2.786134	0.311288	-0.225244
H	3.284649	-0.654475	-0.068405
H	2.730623	0.488572	-1.307388
H	3.415942	1.093521	0.214328
C	1.393551	0.307274	0.396416
H	0.913171	1.285387	0.255786
H	1.468471	0.156276	1.482515
C	0.499390	-0.787388	-0.196608
H	0.406543	-0.653980	-1.284626
H	0.992842	-1.760029	-0.035931
C	-0.860857	-0.825367	0.425682
H	-0.898817	-0.876538	1.516626
C	-2.024517	-0.751083	-0.257691

H	-2.035861	-0.737695	-1.347147
H	-2.982994	-0.826636	0.247888
O	-2.092136	1.418550	0.003202
H	-1.319689	1.608857	-0.554591

Table S80. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS12- (Conf#4 + OH)

C	2.749515	-0.006267	-0.220609
H	3.088339	-1.007038	0.080141
H	2.738870	0.029038	-1.318243
H	3.489946	0.721290	0.132257
C	1.365732	0.297539	0.344608
H	1.039646	1.300914	0.049570
H	1.402467	0.283865	1.443662
C	0.322271	-0.714181	-0.125194
H	0.258565	-0.716497	-1.222866
H	0.649104	-1.723788	0.175044
C	-1.046070	-0.492704	0.451222
H	-1.091321	-0.162903	1.490830
C	-2.197903	-0.866348	-0.157588
H	-2.191575	-1.257676	-1.176002
H	-3.158373	-0.768034	0.343234
O	-1.432039	1.567032	-0.102778
H	-1.930626	1.456341	-0.930038

Table S81. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS21+ (Conf#4 + OH)

C	2.997876	0.407980	0.178207
H	3.038159	1.315453	-0.438670
H	2.952590	0.717638	1.230619
H	3.932216	-0.145591	0.028216
C	1.785955	-0.442069	-0.190087
H	1.766309	-1.356874	0.417604
H	1.857710	-0.761553	-1.239485
C	0.466176	0.313382	0.011928
H	0.363598	0.607221	1.066589
H	0.504483	1.239139	-0.585050
C	-0.718457	-0.502197	-0.403415
H	-0.769855	-0.793144	-1.455653
C	-1.720558	-0.877646	0.422909

H	-1.685130	-0.646121	1.486651
H	-2.520795	-1.527690	0.080557
O	-2.998287	0.806671	-0.079099
H	-2.318940	1.501455	-0.075838

Table S82. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS22+ (Conf#4 + OH)

C	-2.860437	-0.302820	0.194871
H	-2.880066	-1.368516	-0.068335
H	-2.897157	-0.226315	1.289592
H	-3.767090	0.163581	-0.208345
C	-1.602502	0.364446	-0.352496
H	-1.601716	1.433658	-0.099176
H	-1.594424	0.301070	-1.450134
C	-0.325100	-0.281673	0.195630
H	-0.303034	-0.189929	1.291383
H	-0.321940	-1.352200	-0.046487
C	0.902724	0.350354	-0.386467
H	1.068347	0.198602	-1.454025
C	1.669026	1.257849	0.266443
H	1.486364	1.487421	1.317439
H	2.497392	1.760604	-0.227308
O	2.369581	-1.191740	-0.084736
H	2.654411	-1.002993	0.825397

Table S83. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS11+ (Conf#5 + OH)

C	1.649956	1.159881	0.169081
H	1.190709	1.612373	-0.719569
H	1.000446	1.366959	1.031208
H	2.608234	1.657697	0.357095
C	1.840398	-0.342861	-0.022819
H	2.198680	-0.792745	0.914707
H	2.620283	-0.521738	-0.774268
C	0.562256	-1.060461	-0.469438
H	0.249478	-0.695963	-1.457889
H	0.780269	-2.135233	-0.573413
C	-0.578426	-0.891586	0.488110
H	-0.335193	-0.899325	1.555631
C	-1.867072	-0.718949	0.114613

H	-2.159362	-0.787567	-0.931259
H	-2.663257	-0.652197	0.851773
O	-1.756143	1.414649	-0.287826
H	-1.083810	1.654405	0.371313

Table S84. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS12+ (Conf#5 + OH)

C	-2.155952	0.506876	0.432458
H	-2.507575	-0.001336	1.340830
H	-1.472091	1.310276	0.725682
H	-3.027922	0.952623	-0.061789
C	-1.450184	-0.483342	-0.491405
H	-1.171016	0.024373	-1.423667
H	-2.149624	-1.285360	-0.760336
C	-0.189707	-1.099494	0.146645
H	-0.220278	-0.991980	1.239764
H	-0.164534	-2.179787	-0.063547
C	1.110050	-0.550105	-0.362591
H	1.214947	-0.495942	-1.448549
C	2.197151	-0.316148	0.409733
H	2.138121	-0.387637	1.495118
H	3.154294	-0.036224	-0.028089
O	0.697430	1.597271	-0.173952
H	1.558084	1.966103	-0.432843

Table S85. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS21+ (Conf#5 + OH)

C	2.412734	0.742794	-0.196073
H	2.291652	0.937408	-1.270442
H	1.860454	1.518246	0.348768
H	3.476355	0.844864	0.048931
C	1.898963	-0.649339	0.158007
H	2.019486	-0.830323	1.235752
H	2.497837	-1.410373	-0.359299
C	0.422815	-0.850338	-0.221318
H	0.291280	-0.670703	-1.298355
H	0.151340	-1.898483	-0.023196
C	-0.488757	0.052079	0.552136
H	-0.524809	-0.098887	1.634321

C	-1.269995	1.010362	0.005201
H	-1.226616	1.224932	-1.061684
H	-1.863558	1.676406	0.625252
O	-3.029746	-0.256973	-0.152225
H	-2.590015	-1.070650	-0.449968

Table S86. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for TS22+ (Conf#5 + OH)

C	-2.380191	0.554971	0.053911
H	-2.385027	0.811058	1.122371
H	-1.887831	1.374193	-0.484233
H	-3.421162	0.502305	-0.286095
C	-1.659913	-0.770457	-0.176954
H	-1.655737	-1.011836	-1.249716
H	-2.207206	-1.579548	0.324258
C	-0.214932	-0.774686	0.344551
H	-0.207627	-0.518586	1.414381
H	0.212925	-1.778532	0.238918
C	0.653990	0.190705	-0.404546
H	0.832848	-0.035610	-1.457040
C	1.035523	1.401473	0.070696
H	0.810225	1.692824	1.097758
H	1.597741	2.100005	-0.544927
O	2.611448	-0.617036	-0.041265
H	2.812411	-0.232020	0.828503

Table S87. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P11+ (Conf#1 + OH)

C	2.165506	-0.734215	0.222463
H	2.812244	-0.077898	0.820529
H	1.535506	-1.303485	0.918877
H	2.805953	-1.445217	-0.312933
C	1.316165	0.082494	-0.747506
H	0.662827	-0.578862	-1.332506
H	1.966693	0.597737	-1.466708
C	0.448049	1.134014	-0.034974
H	1.094308	1.844184	0.498408
H	-0.087947	1.708111	-0.808705
C	-0.532043	0.530989	0.920851
H	-0.540022	0.826847	1.968001

C	-1.425934	-0.577557	0.476443
H	-0.855339	-1.502205	0.288523
H	-2.170827	-0.805355	1.253927
O	-2.063902	-0.301017	-0.771534
H	-2.542639	0.529926	-0.678800

Table S88. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P12+ (Conf#1 + OH)

C	-2.207134	0.464458	-0.202839
H	-2.741582	0.439819	0.756571
H	-1.690657	1.429960	-0.273030
H	-2.954129	0.422036	-1.005235
C	-1.230060	-0.706518	-0.301400
H	-0.739035	-0.715386	-1.283969
H	-1.798577	-1.643142	-0.233840
C	-0.152455	-0.704407	0.788798
H	-0.553929	-0.280779	1.720862
H	0.168539	-1.731283	1.008868
C	1.125739	0.064365	0.416813
H	1.782121	0.042988	1.305084
C	0.906904	1.484346	0.021662
H	0.701726	1.727088	-1.018908
H	0.795710	2.258544	0.776907
O	1.734583	-0.673559	-0.641743
H	2.495183	-0.174844	-0.957567

Table S89. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P21+ (Conf#1 + OH)

C	1.830635	1.186863	-0.282368
H	2.231823	0.984512	-1.284757
H	0.850099	1.664607	-0.408577
H	2.496952	1.902944	0.212997
C	1.711630	-0.106468	0.518898
H	1.302842	0.107147	1.516028
H	2.709794	-0.533992	0.681688
C	0.845880	-1.161051	-0.186296
H	1.343269	-1.466940	-1.117478
H	0.812200	-2.065614	0.449501
C	-0.544296	-0.711866	-0.507110
H	-1.050197	-1.130007	-1.378412

C	-1.418033	-0.061847	0.510039
H	-0.838162	0.648695	1.123586
H	-1.839287	-0.807067	1.206815
O	-2.544028	0.582493	-0.069024
H	-2.222003	1.161988	-0.768183

Table S89. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P22- (Conf#1 + OH)

C	1.833839	0.719680	0.443437
H	1.963369	1.373814	-0.428536
H	1.084012	1.188229	1.089696
H	2.784977	0.676479	0.988313
C	1.401198	-0.679879	0.009571
H	1.209035	-1.300161	0.897071
H	2.229241	-1.161881	-0.528396
C	0.175412	-0.717901	-0.904821
H	0.377851	-0.165308	-1.833785
H	-0.027087	-1.761469	-1.183465
C	-1.124742	-0.139996	-0.320293
H	-1.943702	-0.458370	-0.989448
C	-1.424705	-0.620795	1.058683
H	-1.003146	-0.099112	1.915325
H	-1.915669	-1.578284	1.215226
O	-1.015118	1.283063	-0.363331
H	-1.803946	1.654899	0.045189

Table S90. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P11+ (Conf#2 + OH)

C	2.666871	-0.446684	-0.026511
H	2.593763	-1.072384	-0.925905
H	3.237204	0.454297	-0.288839
H	3.238929	-1.002292	0.726177
C	1.279490	-0.082320	0.490727
H	1.364148	0.524749	1.403565
H	0.730878	-0.994615	0.759336
C	0.458585	0.694119	-0.553140
H	1.016051	1.586878	-0.865939
H	0.361860	0.049395	-1.442407
C	-0.892303	1.088435	-0.050366
H	-1.125240	2.137397	0.125334

C	-1.822391	0.057517	0.495619
H	-1.478621	-0.310856	1.476785
H	-2.824150	0.488939	0.645850
O	-1.889225	-1.111399	-0.318194
H	-2.142536	-0.836717	-1.206380

Table S91. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P12+ (Conf#2 + OH)

C	-2.65542	-0.01319	-0.08643
H	-2.85418	-1.00121	0.349725
H	-2.95293	0.744993	0.650908
H	-3.29766	0.102329	-0.96793
C	-1.18038	0.128417	-0.45055
H	-1.00711	1.110441	-0.91257
H	-0.90135	-0.6302	-1.19294
C	-0.27785	-0.02352	0.770327
H	-0.46802	0.790341	1.4851
H	-0.5037	-0.96985	1.283631
C	1.220442	-0.03476	0.437894
H	1.768293	-0.11673	1.39319
C	1.679617	1.191115	-0.27564
H	1.591353	1.24803	-1.35835
H	1.950012	2.08523	0.28067
O	1.448755	-1.2064	-0.34387
H	2.366741	-1.20053	-0.63409

Table S92. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P21+ (Conf#2 + OH)

C	2.666871	-0.446684	-0.026511
H	2.593763	-1.072384	-0.925905
H	3.237204	0.454297	-0.288839
H	3.238929	-1.002292	0.726177
C	1.279490	-0.082320	0.490727
H	1.364148	0.524749	1.403565
H	0.730878	-0.994615	0.759336
C	0.458585	0.694119	-0.553140
H	1.016051	1.586878	-0.865939
H	0.361860	0.049395	-1.442407
C	-0.892303	1.088435	-0.050366
H	-1.125240	2.137397	0.125334

C	-1.822391	0.057517	0.495619
H	-1.478621	-0.310856	1.476785
H	-2.824150	0.488939	0.645850
O	-1.889225	-1.111399	-0.318194
H	-2.142536	-0.836717	-1.206380

Table S93. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P22+ (Conf#2 + OH)

C	-2.65542	-0.01319	-0.08643
H	-2.85418	-1.00121	0.349725
H	-2.95293	0.744993	0.650908
H	-3.29766	0.102329	-0.96793
C	-1.18038	0.128417	-0.45055
H	-1.00711	1.110441	-0.91257
H	-0.90135	-0.6302	-1.19294
C	-0.27785	-0.02352	0.770327
H	-0.46802	0.790341	1.4851
H	-0.5037	-0.96985	1.283631
C	1.220442	-0.03476	0.437894
H	1.768293	-0.11673	1.39319
C	1.679617	1.191115	-0.27564
H	1.591353	1.24803	-1.35835
H	1.950012	2.08523	0.28067
O	1.448755	-1.2064	-0.34387
H	2.366741	-1.20053	-0.63409

Table S94. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P11+ (Conf#3 + OH)

C	-2.352497	0.159040	-0.683164
H	-1.764805	0.055841	-1.604449
H	-2.874420	-0.791700	-0.507218
H	-3.109918	0.933688	-0.851674
C	-1.458654	0.510971	0.502387
H	-2.077457	0.684307	1.393660
H	-0.918869	1.447194	0.303328
C	-0.431647	-0.591019	0.828238
H	0.145839	-0.280243	1.709898
H	-0.987019	-1.504222	1.096155
C	0.512616	-0.884704	-0.290939
H	0.203302	-1.530724	-1.111107

C	1.915561	-0.385462	-0.246832
H	2.469424	-0.846312	0.587266
H	2.447900	-0.632698	-1.177598
O	1.987162	1.018030	0.018968
H	1.456455	1.467673	-0.648146

Table S95. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P12+ (Conf#3 + OH)

C	2.158275	0.179958	0.697569
H	1.615374	1.005205	1.174657
H	2.181936	-0.667248	1.397491
H	3.190520	0.513854	0.538354
C	1.504658	-0.216495	-0.623862
H	2.146234	-0.936178	-1.150566
H	1.413825	0.666230	-1.268055
C	0.121727	-0.849019	-0.453593
H	-0.309809	-1.073726	-1.439128
H	0.204077	-1.798720	0.095068
C	-0.868507	0.043501	0.301482
H	-0.493629	0.191061	1.328497
C	-2.229330	-0.558844	0.363746
H	-2.856304	-0.539221	-0.525903
H	-2.535037	-1.164409	1.212966
O	-0.886246	1.296744	-0.384033
H	-1.588152	1.834594	-0.003170

Table S96. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P21- (Conf#3 + OH)

C	-2.165581	-0.734161	0.221996
H	-1.535702	-1.303544	0.918432
H	-2.812518	-0.078037	0.820066
H	-2.805854	-1.445065	-0.313732
C	-1.316052	0.082883	-0.747523
H	-1.966422	0.598500	-1.466595
H	-0.662678	-0.578273	-1.332715
C	-0.447932	1.133945	-0.034330
H	0.088277	1.708415	-0.807639
H	-1.094198	1.843893	0.499340
C	0.531944	0.530260	0.921294
H	0.539484	0.825121	1.968727

C	1.425951	-0.577873	0.476085
H	0.855475	-1.502474	0.287540
H	2.170870	-0.806166	1.253390
O	2.063795	-0.300369	-0.771713
H	2.542920	0.530262	-0.678244

Table S97. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P22-(Conf#3 + OH)

C	-2.190336	0.185753	-0.686164
H	-1.659767	0.998302	-1.199081
H	-2.211467	-0.681849	-1.359929
H	-3.223637	0.516645	-0.527789
C	-1.520560	-0.172305	0.639731
H	-2.158742	-0.876765	1.189377
H	-1.440023	0.728134	1.265209
C	-0.139286	-0.806205	0.477885
H	0.303452	-1.006064	1.463626
H	-0.221414	-1.770444	-0.044209
C	0.859903	0.053582	-0.301470
H	0.496334	0.178783	-1.334095
C	1.074629	1.393989	0.315126
H	1.596303	1.454647	1.269060
H	0.647921	2.298126	-0.110839
O	2.075956	-0.700801	-0.318475
H	2.757292	-0.161993	-0.734180

Table S98. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P11+ (Conf#4 + OH)

C	2.755694	0.367032	-0.183455
H	3.259568	-0.596007	-0.340326
H	2.638982	0.849573	-1.162744
H	3.41055	0.997187	0.429957
C	1.398301	0.163823	0.482572
H	0.914198	1.13533	0.652195
H	1.528423	-0.306731	1.467477
C	0.458939	-0.708493	-0.368868
H	0.292014	-0.204297	-1.332074
H	0.97339	-1.660243	-0.578687
C	-0.854628	-0.972849	0.286318
H	-0.913856	-1.697158	1.098411

C	-2.080257	-0.242715	-0.140679
H	-2.311476	-0.451086	-1.19698
H	-2.948544	-0.548158	0.461404
O	-1.909985	1.178972	-0.094174
H	-1.631659	1.409028	0.79943

Table S99. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P12+ (Conf#4 + OH)

C	2.745771	-0.206606	-0.164220
H	2.921055	-1.210288	0.246164
H	2.776956	-0.281740	-1.259323
H	3.573876	0.438419	0.153228
C	1.401309	0.345870	0.300494
H	1.247483	1.354486	-0.100989
H	1.393432	0.434473	1.397078
C	0.237383	-0.540637	-0.134324
H	0.209866	-0.619787	-1.231365
H	0.368467	-1.556953	0.264940
C	-1.121045	-0.012616	0.332663
H	-1.094424	0.076081	1.433416
C	-2.243503	-0.907896	-0.065015
H	-2.576925	-0.903877	-1.101220
H	-2.615142	-1.676107	0.607976
O	-1.270413	1.284973	-0.246651
H	-2.160822	1.596825	-0.054285

Table S100. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P21- (Conf#4 + OH)

C	2.814962	-0.487198	-0.101118
H	3.224062	-0.239900	0.887577
H	2.586542	-1.560994	-0.111299
H	3.595038	-0.298766	-0.848458
C	1.560868	0.332895	-0.387441
H	1.174527	0.089115	-1.387085
H	1.804473	1.404599	-0.395416
C	0.453085	0.078870	0.652900
H	0.211063	-0.993752	0.658242
H	0.847460	0.332230	1.648199
C	-0.783508	0.863401	0.367168

H	-0.813291	1.923842	0.617356
C	-1.851817	0.296379	-0.506288
H	-1.453939	0.029059	-1.498923
H	-2.657054	1.030658	-0.657295
O	-2.378180	-0.931028	0.002898
H	-2.654980	-0.773944	0.912598

Table S101. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P22-(Conf#4 + OH)

C	-2.762437	-0.175161	0.144591
H	-2.922203	-1.171102	-0.289040
H	-2.815406	-0.273000	1.236941
H	-3.586712	0.471965	-0.178267
C	-1.410406	0.389237	-0.282121
H	-1.281401	1.396959	0.137419
H	-1.384749	0.498979	-1.376692
C	-0.252050	-0.498178	0.161512
H	-0.216027	-0.561208	1.259164
H	-0.390655	-1.520492	-0.218637
C	1.110003	-0.006856	-0.330099
H	1.079302	0.053349	-1.431720
C	1.483391	1.325313	0.226570
H	1.719377	1.401951	1.286901
H	1.438043	2.230833	-0.372010
O	2.051617	-1.006821	0.068540
H	2.936490	-0.679800	-0.125091

Table S102. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P11-(Conf#5 + OH)

C	1.616643	1.246258	-0.009075
H	1.321821	1.505160	-1.036907
H	0.812369	1.554095	0.672837
H	2.506876	1.834977	0.240500
C	1.887572	-0.250986	0.110124
H	2.130197	-0.500917	1.152615
H	2.764359	-0.519972	-0.493830
C	0.693125	-1.107057	-0.344673
H	0.482835	-0.898258	-1.405047
H	0.989330	-2.168197	-0.286460
C	-0.541449	-0.876848	0.463075

H	-0.469298	-0.954272	1.549611
C	-1.818402	-0.377516	-0.120328
H	-1.884277	-0.658899	-1.183995
H	-2.684676	-0.802158	0.401277
O	-1.975653	1.042773	0.017820
H	-1.189242	1.463156	-0.347896

Table S103. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P12-(Conf#5 + OH)

C	-2.186583	0.571941	0.051354
H	-2.178596	0.807465	1.124571
H	-1.672198	1.384903	-0.469620
H	-3.231786	0.547082	-0.280786
C	-1.512094	-0.774359	-0.207732
H	-1.488369	-0.973239	-1.289805
H	-2.121581	-1.572444	0.238560
C	-0.091469	-0.903388	0.343584
H	-0.084127	-0.706593	1.428283
H	0.246061	-1.941066	0.209135
C	0.946623	0.010747	-0.314556
H	0.788421	-0.018707	-1.408168
C	2.342934	-0.403505	0.006073
H	2.581375	-1.431704	0.267336
H	3.154363	0.300249	-0.165109
O	0.752464	1.387263	0.016099
H	0.990254	1.497328	0.944471

Table S104. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P21-(Conf#5 + OH)

C	2.119837	0.969689	-0.210326
H	1.826430	1.259762	-1.228417
H	1.522113	1.562124	0.495069
H	3.172772	1.241769	-0.070883
C	1.900026	-0.524795	0.008688
H	2.205271	-0.799633	1.028784
H	2.535619	-1.099191	-0.678844
C	0.434804	-0.942929	-0.203464
H	0.121643	-0.688315	-1.226395
H	0.371148	-2.039467	-0.116505

C	-0.494066	-0.293438	0.768658
H	-0.330003	-0.443127	1.836636
C	-1.564323	0.639033	0.315162
H	-1.136450	1.481263	-0.251659
H	-2.110325	1.053665	1.175905
O	-2.470600	0.022009	-0.604842
H	-2.791089	-0.790277	-0.197268

Table S105. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P22-(Conf#5 + OH)

C	-2.188624	0.594334	0.015272
H	-2.128112	0.907080	1.066760
H	-1.706254	1.371091	-0.590508
H	-3.247495	0.558593	-0.268679
C	-1.528893	-0.769958	-0.183490
H	-1.524765	-1.024576	-1.253764
H	-2.140523	-1.535763	0.312091
C	-0.105842	-0.884048	0.362705
H	-0.092310	-0.674199	1.443035
H	0.254743	-1.912493	0.229123
C	0.916109	0.026938	-0.317960
H	0.771683	-0.031749	-1.410282
C	0.844099	1.450371	0.122335
H	0.909492	1.677142	1.185037
H	0.801501	2.271658	-0.588075
O	2.200481	-0.527721	0.015116
H	2.877105	0.109156	-0.238838

Table S106. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P12-(Conf#1 + OH)

C	-2.327127	0.409131	-0.111176
H	-2.902034	0.128596	0.781078
H	-1.913934	1.409949	0.067890
H	-3.023640	0.470833	-0.956170
C	-1.222182	-0.615493	-0.369433
H	-0.736301	-0.396737	-1.333383
H	-1.680864	-1.604249	-0.491813
C	-0.171613	-0.668587	0.752279

H	-0.593665	-0.237510	1.672407
H	0.099288	-1.707614	0.977286
C	1.139649	0.056134	0.435800
H	1.774129	0.029274	1.330735
C	0.970344	1.472789	-0.005799
H	0.143704	1.761244	-0.651695
H	1.786756	2.179452	0.118715
O	1.901993	-0.677297	-0.540180
H	1.496183	-0.538706	-1.403636

Table S107. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P22+ (Conf#1 + OH)

C	1.759713	0.795304	0.449511
H	1.735465	1.500512	-0.392334
H	1.043863	1.130462	1.214085
H	2.755090	0.847534	0.906434
C	1.447272	-0.628355	-0.012086
H	1.359097	-1.278390	0.869496
H	2.298800	-1.010653	-0.591271
C	0.194472	-0.765181	-0.882166
H	0.351577	-0.264949	-1.847660
H	0.031400	-1.831649	-1.095515
C	-1.108507	-0.195319	-0.299275
H	-1.934514	-0.579421	-0.923755
C	-1.344291	-0.591908	1.118389
H	-0.990870	-1.549667	1.493820
H	-2.071975	-0.037816	1.706789
O	-1.209415	1.218468	-0.466246
H	-0.594567	1.639040	0.143642

Table S107. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P11- (Conf#3 + OH)

C	1.863162	0.988091	0.381832
H	1.011096	1.376778	0.956209
H	2.559170	0.533278	1.099212
H	2.372544	1.835259	-0.092394
C	1.415448	-0.040995	-0.653338
H	2.287654	-0.408396	-1.210715
H	0.753059	0.428378	-1.397355
C	0.683549	-1.242745	-0.022222

H	0.493262	-1.981743	-0.818322
H	1.346599	-1.721287	0.710959
C	-0.611398	-0.862832	0.619934
H	-0.709840	-0.854847	1.704279
C	-1.722073	-0.282982	-0.188525
H	-1.597204	-0.550525	-1.251357
H	-2.695863	-0.663552	0.144255
O	-1.828101	1.141535	-0.051696
H	-0.967794	1.523152	-0.257287

Table S108. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P12-(Conf#3 + OH)

C	-2.159478	0.216209	-0.694017
H	-1.614962	1.060522	-1.134044
H	-2.179324	-0.601618	-1.428062
H	-3.192774	0.541700	-0.524632
C	-1.510753	-0.235591	0.612342
H	-2.157877	-0.970066	1.110551
H	-1.422238	0.623621	1.288941
C	-0.130653	-0.863441	0.420132
H	0.290023	-1.144452	1.398633
H	-0.216900	-1.790749	-0.167011
C	0.869814	0.050426	-0.291765
H	0.498022	0.257806	-1.309288
C	2.225322	-0.563181	-0.372610
H	2.354716	-1.641649	-0.315727
H	3.075893	0.056582	-0.646839
O	0.927912	1.342047	0.314925
H	1.376607	1.245391	1.163593

Table S109. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P21+ (Conf#3 + OH)

C	2.220844	-0.934470	-0.286557
H	1.401111	-1.604481	-0.576490
H	2.680656	-0.549750	-1.207019
H	2.972783	-1.529007	0.245561
C	1.711270	0.213116	0.580282

H	2.554428	0.836390	0.907564
H	1.243772	-0.187847	1.491264
C	0.694464	1.108792	-0.157148
H	0.411575	1.933749	0.517321
H	1.184181	1.558210	-1.031633
C	-0.533780	0.373786	-0.581766
H	-0.657858	0.044708	-1.613658
C	-1.440274	-0.225085	0.437278
H	-1.435010	0.399051	1.349591
H	-1.102475	-1.230968	0.740820
O	-2.764863	-0.412745	-0.041486
H	-3.049405	0.415071	-0.443972

Table S110. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P22+ (Conf#3 + OH)

C	-2.168779	0.214428	-0.703144
H	-1.622212	1.040978	-1.175389
H	-2.175137	-0.633522	-1.401753
H	-3.204852	0.543248	-0.560432
C	-1.533209	-0.181319	0.628687
H	-2.184297	-0.898566	1.145997
H	-1.469474	0.703651	1.277163
C	-0.147259	-0.812754	0.474813
H	0.276037	-1.019080	1.471115
H	-0.227384	-1.776612	-0.046639
C	0.850235	0.049162	-0.296128
H	0.506012	0.173184	-1.332018
C	1.057434	1.388549	0.328411
H	0.821016	1.558007	1.377714
H	1.599335	2.161555	-0.210674
O	2.102260	-0.638510	-0.445809
H	2.512337	-0.693156	0.425552

Table S111. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P11- (Conf#4 + OH)

C	3.130564	0.127125	0.162247
H	3.328428	0.845946	-0.644127
H	3.148268	0.676579	1.112887
H	3.951470	-0.599545	0.176847
C	1.784375	-0.559737	-0.042893

H	1.610708	-1.293288	0.756752
H	1.792940	-1.121824	-0.987613
C	0.619429	0.429933	-0.067009
H	0.600384	1.003098	0.874917
H	0.810668	1.179963	-0.859605
C	-0.704541	-0.219862	-0.280363
H	-0.760359	-1.131474	-0.879328
C	-1.976125	0.520061	-0.051300
H	-1.849169	1.230071	0.785363
H	-2.257370	1.118253	-0.934436
O	-3.083612	-0.340687	0.176465
H	-2.829292	-0.967396	0.862529

Table S112. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P12-(Conf#4 + OH)

C	2.752365	-0.188519	-0.168843
H	2.935309	-1.202211	0.212574
H	2.781018	-0.233345	-1.265812
H	3.577775	0.452013	0.163985
C	1.406413	0.341740	0.316633
H	1.245234	1.362604	-0.051548
H	1.404400	0.400083	1.415087
C	0.243055	-0.534802	-0.132986
H	0.234706	-0.616783	-1.232501
H	0.369839	-1.555324	0.259674
C	-1.117512	-0.008659	0.323855
H	-1.086860	0.125093	1.419827
C	-2.232565	-0.926297	-0.045005
H	-2.049255	-1.978124	-0.251712
H	-3.258514	-0.571219	0.020577
O	-1.364097	1.310039	-0.167619
H	-1.551408	1.236121	-1.111122

Table S113. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P21+ (Conf#4 + OH)

C	-3.018470	-0.409578	0.091691
H	-2.986539	-1.317708	-0.525008
H	-3.038664	-0.719403	1.145038
H	-3.957954	0.112550	-0.124582
C	-1.811963	0.479887	-0.189467

H	-1.868231	1.394972	0.416082
H	-1.819298	0.797735	-1.241739
C	-0.484398	-0.222142	0.104363
H	-0.461396	-0.545998	1.157879
H	-0.450934	-1.154001	-0.494613
C	0.707807	0.628750	-0.179176
H	0.678732	1.288290	-1.048014
C	2.032300	0.353846	0.445311
H	1.899094	-0.012781	1.476439
H	2.647988	1.259781	0.478740
O	2.814094	-0.587322	-0.307449
H	2.292800	-1.389447	-0.416957

Table S114. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P22+ (Conf#4 + OH)

C	2.768539	-0.164620	-0.139330
H	2.928267	-1.181753	0.241757
H	2.827005	-0.203945	-1.235150
H	3.590084	0.465839	0.221086
C	1.413522	0.373813	0.311717
H	1.290070	1.406524	-0.043524
H	1.379485	0.417803	1.410455
C	0.254436	-0.486646	-0.185060
H	0.239048	-0.494057	-1.287718
H	0.392842	-1.526164	0.142507
C	-1.104705	-0.016246	0.323336
H	-1.083890	0.001183	1.424284
C	-1.483628	1.330994	-0.194038
H	-0.928603	1.803246	-1.002393
H	-2.385579	1.815075	0.172373
O	-2.129060	-0.974994	0.022636
H	-2.305238	-0.927570	-0.924521

Table S115. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P11+ (Conf#5 + OH)

C	1.737240	1.119625	0.233667
H	1.357732	1.654989	-0.647748
H	1.055710	1.312262	1.073970
H	2.714076	1.543150	0.495445
C	1.838031	-0.376722	-0.050922

H	2.175393	-0.905674	0.852056
H	2.596061	-0.553570	-0.825574
C	0.502801	-0.978532	-0.519214
H	0.177021	-0.460843	-1.432319
H	0.671990	-2.036144	-0.783495
C	-0.577374	-0.881373	0.506878
H	-0.448959	-1.391803	1.462010
C	-1.887280	-0.240017	0.197695
H	-2.445962	-0.818328	-0.556653
H	-2.511394	-0.186800	1.102771
O	-1.736899	1.053669	-0.389071
H	-1.126981	1.555527	0.163486

Table S116. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P12+ (Conf#5 + OH)

C	-2.211763	0.544117	0.107411
H	-2.214535	0.708956	1.193023
H	-1.715436	1.401664	-0.355606
H	-3.253794	0.512335	-0.234384
C	-1.499608	-0.764331	-0.232612
H	-1.460512	-0.894264	-1.324910
H	-2.093273	-1.603996	0.155369
C	-0.081636	-0.898758	0.329866
H	-0.071729	-0.685558	1.409290
H	0.254234	-1.936860	0.199553
C	0.968440	0.003252	-0.329388
H	0.864572	-0.101507	-1.424989
C	2.354288	-0.373661	0.070468
H	2.737176	-0.030125	1.029819
H	2.903207	-1.137006	-0.475340
O	0.683417	1.349669	0.052049
H	1.404420	1.905289	-0.262691

Table S117. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P21+ (Conf#5 + OH)

C	-1.995671	1.118033	0.011499
H	-1.861999	1.385937	1.068608
H	-1.188064	1.590199	-0.562556
H	-2.943980	1.549641	-0.329719
C	-1.982719	-0.396931	-0.167505

H	-2.101615	-0.647483	-1.231022
H	-2.835012	-0.842320	0.363946
C	-0.685490	-1.046280	0.356053
H	-0.588674	-0.817965	1.428907
H	-0.785268	-2.137837	0.261830
C	0.538538	-0.589778	-0.364723
H	0.732325	-0.969081	-1.370130
C	1.416286	0.512103	0.121547
H	1.190125	0.731924	1.178835
H	1.256940	1.442678	-0.446627
O	2.802068	0.223800	-0.050515
H	2.963010	-0.658978	0.300831

Table S118. Optimized geometry (cartesian coordinates, Angstroms) obtained at the M06-2X/aug-cc-pVDZ level for P22+ (Conf#5 + OH)

C	-2.202710	0.590211	0.010245
H	-2.190504	0.880581	1.070008
H	-1.700390	1.381833	-0.558999
H	-3.248859	0.553180	-0.316824
C	-1.528399	-0.766750	-0.188778
H	-1.505022	-1.011533	-1.261082
H	-2.141971	-1.541625	0.290007
C	-0.107675	-0.877335	0.371451
H	-0.111604	-0.654950	1.451863
H	0.243780	-1.910487	0.254971
C	0.922432	0.018449	-0.316203
H	0.800216	-0.070019	-1.406132
C	0.840064	1.452368	0.088488
H	0.432146	1.731113	1.058571
H	1.347760	2.213399	-0.498949
O	2.255457	-0.474362	-0.087782
H	2.488519	-0.278265	0.827598

Table S119. Electronic energies (E, hartrees) and zero-point vibrational energy corrections (zp, hartrees) obtained at the M06-2x/aug-cc-pVDZ level for the stationary points along the OH addition paths belonging to conf#1 and conf#2.

	conf#1		conf#2	
	E (hartrees)	zp (hartrees)	E (hartrees)	zp (hartrees)
Conf + OH	-272.1591408	0.145971	-272.1603278	0.146219
π-PC1	-272.1678471	0.148409	-272.1692117	0.148461
π-PC2	-272.1682813	0.148169	-272.1692117	0.148461
σ-PC$_{11-}$	-	-	-	-
σ-PC$_{11+}$	-272.1677154	0.148227	-272.1689946	0.147869
σ-PC$_{12-}$	-272.1673224	0.148231	-	-
σ-PC$_{12+}$	-272.1677680	0.148446	-272.1690680	0.148585
σ-PC$_{21-}$	-	-	-	-
σ-PC$_{21+}$	-272.1673449	0.148068	-272.1689946	0.147869
σ-PC$_{22-}$	-272.1674298	0.148058	-	-
σ-PC$_{22+}$	-272.1679140	0.148139	-272.1690680	0.148585
TS$_{11-}$	-	-	-	-
TS$_{11+}$	-272.1662680	0.148806	-272.1673192	0.148301
TS$_{12-}$	-272.1649572	0.148876	-	-
TS$_{12+}$	-272.1653960	0.148961	-272.1671298	0.148508
TS$_{21-}$	-	-	-	-
TS$_{21+}$	-272.1659137	0.149070	-272.1673192	0.148301
TS$_{22-}$	-272.1657387	0.148566	-	-
TS$_{22+}$	-272.1658172	0.148748	-272.1671298	0.148508
P$_{11-}$	-	-	-	-
P$_{11+}$	-272.2152274	0.152076	-272.2147898	0.152159
P$_{12-}$	-272.2131627	0.151162	-	-
P$_{12+}$	-272.2102016	0.151565	-272.2151329	0.151188
P$_{21-}$	-	-	-	-
P$_{21+}$	-272.2139733	0.152084	-272.2147898	0.152159
P$_{22-}$	-272.2133661	0.151090	-	
P$_{22+}$	-272.2137240	0.151523	-272.2151329	0.151188

Table S120. Electronic energies (E, hartrees) and zero-point vibrational energy corrections (zp, hartrees) obtained at the M06-2x/aug-cc-pVDZ level for the stationary points along the OH addition paths belonging to conf#3 and conf#4.

	conf#3		conf#4	
	E (hartrees)	zp (hartrees)	E (hartrees)	zp (hartrees)
Conf + OH	-272.1593926	0.145710	-272.160132	0.145696
π-PC1	-272.1682456	0.148369	-272.1685819	0.1479050
π-PC2	-272.1671642	0.148319	-272.1678517	0.1474640
σ-PC$_{11-}$	-272.1675151	0.148173	-272.1673969	0.1474770
σ-PC$_{11+}$	-272.1675193	0.148202	-272.1682635	0.1478740
σ-PC$_{12-}$	-272.1683748	0.148634	-272.1680476	0.1481740
σ-PC$_{12+}$	-272.1683962	0.148785	-272.1679171	0.1480420
σ-PC$_{21-}$	-272.1669759	0.148058	-272.1675744	0.1473670
σ-PC$_{21+}$	-272.1662987	0.147765	-272.1669756	0.1470840
σ-PC$_{22-}$	-272.1672650	0.148065	-272.1679543	0.1478980
σ-PC$_{22+}$	-272.1672725	0.147721	-272.1680049	0.1477520
TS$_{11-}$	-272.1655031	0.148659	-272.1657232	0.1483390
TS$_{11+}$	-272.1665094	0.148828	-272.1671191	0.1481830
TS$_{12-}$	-272.1661212	0.148602	-272.1657878	0.1478090
TS$_{12+}$	-272.1661820	0.149008	-272.1661699	0.1483140
TS$_{21-}$	-272.1655326	0.148718	-272.1661299	0.1479880
TS$_{21+}$	-272.1649640	0.148310	-272.1656382	0.1483570
TS$_{22-}$	-272.1656165	0.148643	-272.1662323	0.1481490
TS$_{22+}$	-272.1655179	0.148861	-272.1661560	0.1485800
P$_{11-}$	-272.2142834	0.152239	-272.2143416	0.1513510
P$_{11+}$	-272.2143966	0.152021	-272.2147479	0.1523120
P$_{12-}$	-272.2152012	0.151019	-272.2153348	0.1507850
P$_{12+}$	-272.2155280	0.151329	-272.2156303	0.1512160
P$_{21-}$	-272.2152273	0.152078	-272.2145956	0.1518790
P$_{21+}$	-272.2145706	0.151714	-272.2132775	0.1520110
P$_{22-}$	-272.2152375	0.151410	-272.2156106	0.1512600
P$_{22+}$	-272.2148064	0.151324	-272.2149888	0.1505890

Table S121. Electronic energies (E, hartrees) and zero-point vibrational energy corrections (zp, hartrees) obtained at the M06-2x/aug-cc-pVDZ level for the stationary points along the OH addition paths belonging to conf#5.

	conf#5	
	E (hartrees)	zp (hartrees)
Conf + OH	-272.1603721	0.145530
π-PC1	-272.1688021	0.148319
π-PC2	-272.1681721	0.147539
σ-PC$_{11-}$	-272.1679481	0.148240
σ-PC$_{11+}$	-272.1682812	0.148218
σ-PC$_{12-}$	-272.1679304	0.147499
σ-PC$_{12+}$	-272.1663701	0.147472
σ-PC$_{21-}$	-272.1679079	0.147920
σ-PC$_{21+}$	-272.1674711	0.147923
σ-PC$_{22-}$	-272.1682062	0.147643
σ-PC$_{22+}$	-272.1682640	0.147892
TS$_{11-}$	-272.1665569	0.148866
TS$_{11+}$	-272.1663972	0.148706
TS$_{12-}$	-272.1630793	0.148423
TS$_{12+}$	-272.1630852	0.148419
TS$_{21-}$	-272.1664426	0.148216
TS$_{21+}$	-272.1659292	0.148354
TS$_{22-}$	-272.1664698	0.148624
TS$_{22+}$	-272.1663493	0.148855
P$_{11-}$	-272.2145107	0.152391
P$_{11+}$	-272.2157653	0.151707
P$_{12-}$	-272.2132495	0.151121
P$_{12+}$	-272.2131803	0.151155
P$_{21-}$	-272.2148741	0.151839
P$_{21+}$	-272.2146129	0.152091
P$_{22-}$	-272.2140619	0.151259
P$_{22+}$	-272.2133938	0.151314

