

Electronic Supplementary Information (ESI)

CPh₃ as a functional group in P-heterocyclic chemistry: elimination of HCPPh₃ in the reaction of *P*-CPh₃ substituted Li/Cl phosphinidenoid complexes with Ph₂C=O

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Table of contents

	<u>Page</u>
1. X-ray data	2
3. Table S 1. Energetics computed at different levels for the transformation 3→4,8 in model systems	5
3. Table S 2. Energetics computed at different levels for the transformation 8e→11e	5
4. Computed structures: Cartesian coordinates and energies for all computed species	6

X ray data

Crystal structure data of complex 3a

Summary of Data CCDC 1423351; Empirical formula: $C_{31}H_{21}CrO_6P$; Moiety formula: $C_{31}H_{21}CrO_6P$
Formula weight: 572.45; Temperature/K: 123.(2); Crystal system: orthorhombic; Space group: P 21 21 21; $a/\text{\AA}$: 8.5858(5); $b/\text{\AA}$: 19.6165(9); $c/\text{\AA}$: 15.6007(10); $\alpha/^\circ$: 90; $\beta/^\circ$: 90; $\gamma/^\circ$: 90; Volume/ \AA^3 : 2627.5(3); Z : 4; $\rho_{\text{calc}}/\text{mg}/\text{mm}^3$: 1.447; m/mm^{-1} : 0.541; $F(000)$: 1176; Crystal size/ mm^3 : $0.15 \times 0.12 \times 0.04$; Θ range for data collection: 2.90 to 28° ; Index ranges: $-11 \leq h \leq 11$, $-22 \leq k \leq 25$, $-20 \leq l \leq 20$; Reflections collected: 14343; Independent reflections: 6334; [$R_{\text{int}} = 0.0754$]; Data/restraints/parameters: 6334/4/356; Goodness-of-fit on F^2 : 0.623; Final R indexes [$I \geq 2\sigma(I)$]: $R_1 = 0.0409$, $wR_2 = 0.0495$; Final R indexes [all data]: $R_1 = 0.0816$, $wR_2 = 0.0567$; Largest diff. peak/hole / $e \text{\AA}^{-3}$: 0.622/-0.408.

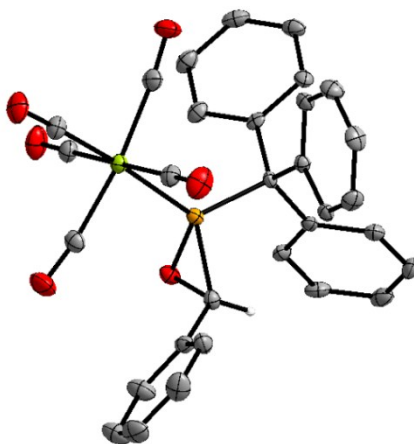


Figure 1. Crystal structure of complex 3a. Diamond 3.0 (ellipsoids 50% probability). Hydrogen atoms, except for that at the endocyclic carbon atom, were removed for clarity.

Crystal structure data of complex 3b

Summary of Data CCDC 1423352; Empirical formula: $C_{31}H_{21}MoO_6P$; Moiety formula: $C_{31}H_{21}CrO_6P$
Formula weight: 616.39; Temperature/K: 123.(2); Crystal system: orthorhombic; Space group: P 21 21 21; $a/\text{\AA}$: 8.6515(3); $b/\text{\AA}$: 15.6935(4); $c/\text{\AA}$: 19.9770(8); $\alpha/^\circ$: 90; $\beta/^\circ$: 90; $\gamma/^\circ$: 90; Volume/ \AA^3 : 2712.32(16); Z : 4; $\rho_{\text{calc}}/\text{mg}/\text{mm}^3$: 1.509; m/mm^{-1} : 0.586; $F(000)$: 1248; Crystal size/ mm^3 : $0.10 \times 0.03 \times 0.02$; Θ range for data collection: 2.88 to 28° ; Index ranges: $-11 \leq h \leq 11$, $-20 \leq k \leq 20$, $-26 \leq l \leq 21$; Reflections collected: 19516; Independent reflections: 6550; [$R_{\text{int}} = 0.0826$]; Data/restraints/parameters: 6550/0/356; Goodness-of-fit on F^2 : 0.840; Final R indexes [$I \geq 2\sigma(I)$]: $R_1 = 0.0432$, $wR_2 = 0.0549$; Final R indexes [all data]: $R_1 = 0.0646$, $wR_2 = 0.0585$; Largest diff. peak/hole / $e \text{\AA}^{-3}$: 0.592/-0.653.

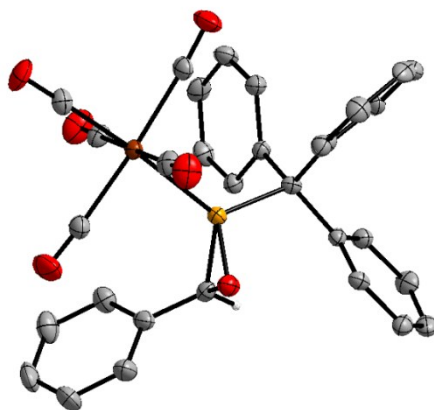


Figure 2. Crystal structure of complex **3b**. Diamond 3.0 (ellipsoids 50% probability). Hydrogen atoms, except for that at the endocyclic carbon atom, were removed for clarity.

Crystal structure data of complex **4f**

Summary of Data CCDC 1423354; Empirical formula: $C_{37}H_{25}O_6PW$; Moiety formula: $C_{37}H_{25}O_6PW$
 Formula weight: 780.39; Temperature/K: 123.15; Crystal system: triclinic; Space group: P -1; $a/\text{\AA}$: 9.4174(14); $b/\text{\AA}$: 10.7473(14); $c/\text{\AA}$: 17.631(2); $\alpha/^\circ$: 98.301(4); $\beta/^\circ$: 94.830(4); $\gamma/^\circ$: 112.865(4);
 Volume/ \AA^3 : 1607.6(4); Z: 2; $\rho_{\text{calc}}/\text{mg/mm}^3$: 1.612; m/mm^{-1} : 3.688; F(000): 768.0; Crystal size/ mm^3 : $0.06 \times 0.04 \times 0.03$; Θ range for data collection: 5.46 to 50.5°; Index ranges: $-11 \leq h \leq 11$, $-12 \leq k \leq 12$, $-21 \leq l \leq 19$; Reflections collected: 14721; Independent reflections: 5711; [$R_{\text{int}} = 0.0995$];
 Data/restraints/parameters: 5711/18/406; Goodness-of-fit on F^2 : 0.962; Final R indexes [$I \geq 2\sigma(I)$]: $R_1 = 0.0498$, $wR_2 = 0.0702$; Final R indexes [all data]: $R_1 = 0.0893$, $wR_2 = 0.0809$; Largest diff. peak/hole / $e \text{\AA}^{-3}$: 1.27/-1.70.

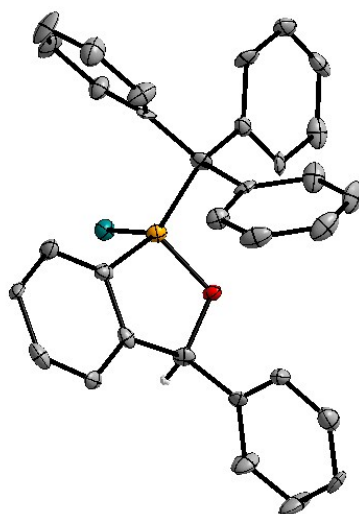


Figure 3. Crystal structure of complex **4f**. Diamond 3.0 (ellipsoids 50% probability). Hydrogen atoms (except those at chiral centres), as well as carbonyl groups at the metal, were removed for clarity.

Crystal structure data of complex 5e

Summary of Data CCDC 1423353; Empirical formula: $C_{59}H_{44}Mo_2O_{13}P_2$; Moiety formula: $C_{55}H_{34}Mo_2O_{12}P_2$, $C_4H_{10}O$ Formula weight: 1214.76; Temperature/K: 123(2); Crystal system: monoclinic; Space group: P 21/c; a/Å: 13.286(8); b/Å: 18.409(9); c/Å: 23.093(10); $\alpha/^\circ$: 90; $\beta/^\circ$: 103.99; $\gamma/^\circ$: 90; Volume/Å³: 5481(5); Z: 4; ρ_{calc} /mg/mm³: 1.472; m/mm⁻¹: 0.580; F(000): 2464; Crystal size/mm³: 0.36 × 0.06 × 0.03; Θ range for data collection: 2.94 to 28°; Index ranges: $-17 \leq h \leq 17$, $-24 \leq k \leq 23$, $-30 \leq l \leq 30$; Reflections collected: 51069; Independent reflections: 13213; [R_{int} = 0.1524]; Data/restraints/parameters: 13213/37/687; Goodness-of-fit on F^2 : 0.789; Final R indexes [$I \geq 2\sigma(I)$]: $R_1 = 0.0492$, $wR_2 = 0.0858$; Final R indexes [all data]: $R_1 = 0.1109$, $wR_2 = 0.0985$; Largest diff. peak/hole / e Å⁻³: 0.893/-0.985.

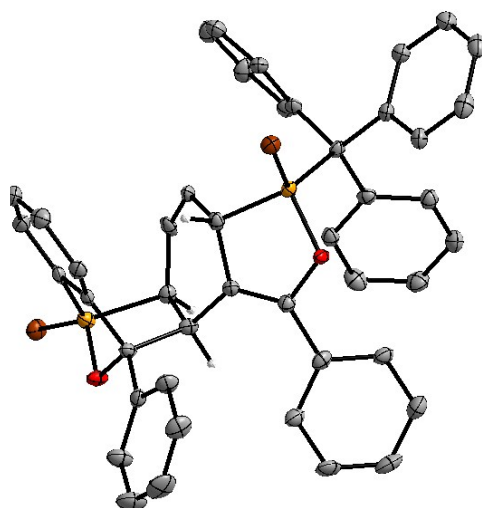


Figure 4. Crystal structure of complex 5e. Diamond 3.0 (ellipsoids 50% probability). Hydrogen atoms (except those at chiral centres), as well as carbonyl groups at the metal, were removed for clarity. The crystal structure contains one molecule of diethylether, which was removed for clarity.

Table S 1. Energetics of reactions involved in mechanistic pathway from **3g,h**.^[a]

	3g	TS ^(3g→6g)	6g	TS ^(3g→7g)	7g	3h	TS ^(3h→6h)	6h	TS ^(3h→7h)
B3LYP-D3	0.00	26.38	-1.44	37.01	28.34	0.00	16.07	17.32	27.94
PWPB95-D3	0.00	25.08	-7.00	34.65	26.39	0.00	22.14	-3.25	33.71
SCS-MP2	0.00	29.42	-9.53	39.93	29.70	0.00	27.43	-5.80	38.95
LPNO-NCEPA1	0.00	30.02	-6.35	38.29	28.24	0.00	27.99	-0.71	38.18
DLPNO-CCSD(T)	0.00	28.91	-6.57	37.72	28.90	0.00	27.15	-2.01	37.11

Table S 1. Continued

7h	TS ^(7h→8h)	8h	7h'	TS ^(7h'→8h')	8h'	TS ^(8h'→4h)	4h	4h'	TS ^(8h'·H2O→4h·H2O)
15.94	27.50	3.03	17.19	26.20	3.01	56.19	-28.37	-24.18	37.97
21.91	33.07	3.12	23.05	30.98	3.57	57.09	-22.41	-22.93	40.51
27.68	40.36	4.17	28.83	36.38	4.25	58.86	-23.09	-23.86	44.10
25.89	40.58	2.10	27.37	36.88	1.49	61.81	-23.66	-24.60	47.20
25.98	39.19	3.02	27.37	35.88	2.72	61.63	-23.48	-24.18	45.01

Table S 1. Continued

TS ^(8h'·2H2O→9h·2H2O)	9h·H₂O	TS ^(9h·2H2O→4h·2H2O)	13	RMSD ^[b]
24.53	23.38	22.23	-26.28	1.80
27.31	27.61	25.92	-25.72	0.79
31.37	30.49	30.12	-27.20	0.36
32.91	33.74	32.37	-25.77	0.32
31.50	29.73	29.99	-26.58	0.00

^[a] ZPE-corrected relative energies (to **3g** or **3h** in the **g** and **h** series, or to **11** in case of **12**), in kcal/mol, using the def2-TZVPP basis set, COSMO(THF) solvation and the geometries and zero-point correction at COSMO_{THF}/B3LYP -D3/def2-TZVPecp. ^[b] Root mean square deviation of the seventeen data set (removing **3g** and **3h**) with respect to the reference DLNPO-CCSD(T) level.

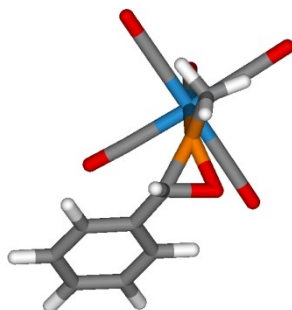
Table S 2. Relative energies for products arising from **8e**.^[a]

	8e	TS ^(8e→10e)	10e	TS ^(10→11e·12)	11e·12	11e+13	TS ^(8e→11e·12)
B3LYP-D3	0.00	25.20	20.67	19.37	5.85	-5.74	31.09
PWPB95-D3	0.00	29.46	22.97	22.75	11.68	1.65	33.97
SCS-MP2	0.00	26.46	18.24	19.14	13.37	4.29	32.46

^[a] ZPE-corrected relative energies (to **8e**), in kcal/mol, using the def2-TZVPP basis set, COSMO(THF) solvation and the geometries and zero-point correction at COSMO_{THF}/B3LYP-D3/def2-TZVPecp.

Calculated structures.

Cartesian coordinates (in Å) and energies (hartrees) for all computed species.-

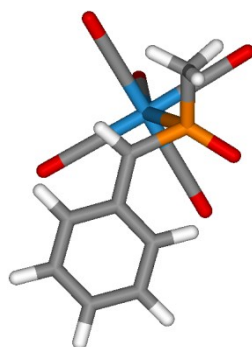


3g: E = -1358.33470326679 au
ZPE = 0.19138974 au

C	0.113797	0.086263	1.279092	C	2.129681	-1.420868	2.762066
O	1.339522	-0.048450	0.492213	H	1.497997	-2.196265	2.331181
C	-0.722091	1.275773	1.010687	H	3.176562	-1.629704	2.535206
C	-0.311227	2.272054	0.126653	H	2.009081	-1.401275	3.846644
C	-1.094205	3.405345	-0.061260	W	2.878302	2.250452	2.900638
C	-2.288211	3.554445	0.634285	C	3.893013	3.887213	3.560313
C	-2.707347	2.555873	1.510251	O	4.472492	4.807590	3.926629
C	-1.931457	1.420449	1.694614	C	2.589696	1.590505	4.833443
H	0.616317	2.152840	-0.414300	O	2.427955	1.211511	5.902122
H	-0.766549	4.174827	-0.748756	C	1.113284	3.336399	3.032635
H	-2.892835	4.441294	0.493674	O	0.172582	3.972618	3.152801
H	-3.639351	2.664096	2.050388	C	3.121568	2.856791	0.937301
H	-2.257130	0.645980	2.379007	O	3.247206	3.182834	-0.151136
H	-0.418032	-0.854631	1.392417	C	4.653609	1.207359	2.829742
P	1.704939	0.213154	2.099101	O	5.645121	0.634356	2.807251

TS(3g-6g): E = -1358.28698322011 au
ZPE = 0.18973676 au
 $\nu = -108.27 \text{ cm}^{-1}$

C	0.111013	0.400265	1.555517	C	2.177283	-1.214983	2.478838
O	2.204287	0.498753	0.338914	H	1.777591	-1.946026	1.773688
C	-0.748223	1.400660	1.096282	H	3.249979	-1.377254	2.590542
C	-2.114272	1.070203	0.879369	H	1.703384	-1.341902	3.453794
C	-3.016901	2.040435	0.501760	W	2.845491	2.231083	3.433286
C	-2.573750	3.348545	0.298841	C	3.710473	3.623288	4.641497
C	-1.227638	3.692723	0.472120	O	4.200652	4.412771	5.318832
C	-0.324090	2.737506	0.868857	C	2.596240	0.958976	5.035036
H	-2.434665	0.048042	1.032873	O	2.459250	0.252687	5.927431
H	-4.058617	1.791476	0.353978	C	0.981685	3.012092	3.825599
H	-3.280800	4.109285	-0.006258	O	-0.060981	3.431841	4.054182
H	-0.904331	4.709010	0.294197	C	3.096826	3.459245	1.795095
H	0.717365	2.985700	0.989589	O	3.234582	4.132200	0.878297
H	-0.322569	-0.597445	1.596920	C	4.672178	1.348588	3.045058
P	1.909821	0.481652	1.851225	O	5.673940	0.835278	2.835406



6g:

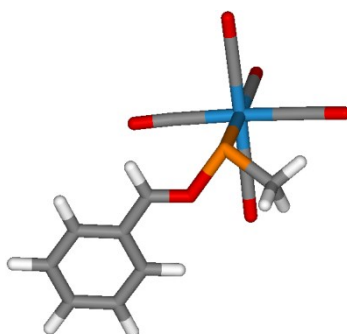
E = -1358.34636887102 au
ZPE = 0.19258566 au

C	0.487072	0.770131	1.955108	C	2.524410	-1.287237	2.013230
O	2.685555	0.812312	0.189644	H	2.223321	-1.971216	1.218657
C	-0.461100	1.649126	1.284318	H	3.602539	-1.352733	2.152372
C	-1.760603	1.760081	1.805133	H	2.015409	-1.549162	2.938546
C	-2.712116	2.551087	1.178969	W	2.325710	2.091306	3.532289
C	-2.383582	3.256869	0.025339	C	3.236878	3.275294	4.903181
C	-1.096831	3.157983	-0.499909	O	3.761127	3.937937	5.676515
C	-0.142784	2.364080	0.117242	C	2.096078	0.560837	4.893496
H	-2.018013	1.217090	2.705977	O	1.960504	-0.306592	5.627215
H	-3.709305	2.621421	1.594423	C	0.473324	2.872118	4.098261
H	-3.123557	3.878889	-0.461714	O	-0.535050	3.302971	4.406437
H	-0.836712	3.702219	-1.398877	C	2.483946	3.543922	2.057245
H	0.850872	2.286713	-0.300529	O	2.568289	4.338361	1.243266
H	0.091972	0.138685	2.741274	C	4.241347	1.438026	3.113731
P	2.098498	0.389285	1.493511	O	5.308004	1.084887	2.906415

TS(3g-7g):

E = -1358.27304448562 au
ZPE = 0.18983653 au
 $\nu = -185.01 \text{ cm}^{-1}$

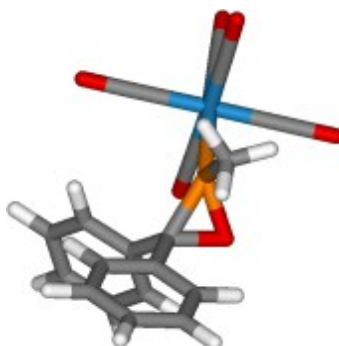
C	-0.307870	0.456655	1.614126	C	2.576166	-1.367827	2.433645
O	0.949668	0.460115	1.272391	H	1.852807	-2.163554	2.249016
C	-1.174433	1.522947	1.255150	H	3.206146	-1.234652	1.551619
C	-0.686294	2.654277	0.572777	H	3.203080	-1.660411	3.278487
C	-1.551049	3.679311	0.245210	W	3.348534	2.209338	3.059820
C	-2.899065	3.593237	0.599301	C	4.708376	3.687127	3.220048
C	-3.392137	2.476489	1.275538	O	5.502862	4.520098	3.300719
C	-2.536765	1.441937	1.602418	C	3.078648	2.138326	5.100852
H	0.362511	2.707946	0.318649	O	2.911769	2.093024	6.234531
H	-1.184160	4.552681	-0.276743	C	1.836527	3.611276	2.959140
H	-3.569888	4.404804	0.348348	O	1.025155	4.421627	2.934619
H	-4.438506	2.423032	1.544078	C	3.479894	2.177244	1.002070
H	-2.900878	0.569298	2.129839	O	3.522580	2.140948	-0.142589
H	-0.710082	-0.410987	2.129727	C	4.880331	0.840879	3.214034
P	1.727577	0.197848	2.879833	O	5.736885	0.084323	3.305053



7g:

E = -1358.28797305667 au
ZPE = 0.19072195 au

C	-0.404971	1.120953	2.331176	C	2.698154	-1.070902	1.772073
O	0.714528	0.678161	1.970335	H	2.001630	-1.835351	1.424771
C	-1.258073	1.827552	1.431203	H	3.049721	-0.478197	0.927321
C	-0.860830	2.106667	0.110268	H	3.557410	-1.575436	2.221265
C	-1.717700	2.792698	-0.726291	W	3.464045	2.018471	3.506898
C	-2.968060	3.206626	-0.258572	C	4.621224	3.640468	3.843097
C	-3.366413	2.936927	1.048653	O	5.272497	4.575746	4.025319
C	-2.514552	2.250192	1.896464	C	3.584284	1.446282	5.483167
H	0.112834	1.786446	-0.233971	O	3.638322	1.110793	6.578802
H	-1.420688	3.013750	-1.742603	C	1.740149	3.055524	3.892974
H	-3.633043	3.746819	-0.920128	O	0.733914	3.583589	4.072395
H	-4.335244	3.264331	1.400534	C	3.249206	2.440578	1.504846
H	-2.807869	2.034890	2.916086	O	3.099654	2.636654	0.383749
H	-0.724469	0.965103	3.363148	C	5.099598	0.839828	3.066997
P	1.943311	-0.055892	3.111950	O	5.989821	0.164089	2.809776



3h:

E = -1588.95595747058 au
ZPE = 0.27180954 au

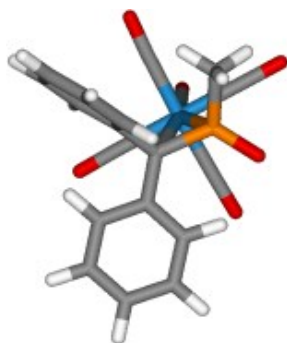
C	0.149013	0.009682	1.198413	H	-0.454274	-4.389903	-0.190052
O	1.512804	-0.095634	0.659893	H	-2.695691	-4.536922	0.859258
C	-0.553752	1.268027	0.792712	H	-3.617678	-2.573070	2.060253
C	-0.484226	1.697728	-0.530943	H	-2.322049	-0.489449	2.203531
C	-1.140105	2.857638	-0.922728	P	1.570484	0.174200	2.302746
C	-1.871158	3.595283	0.003952	C	1.911435	-1.427673	3.077165
C	-1.942771	3.168906	1.325661	H	1.352670	-2.236307	2.612194
C	-1.283709	2.009814	1.718421	H	2.981909	-1.625398	3.001357
H	0.097183	1.131452	-1.246965	H	1.648955	-1.353142	4.133815
H	-1.074936	3.190171	-1.950909	W	2.638172	2.226820	3.219264
H	-2.375899	4.502870	-0.301561	C	3.612146	3.860087	3.942300
H	-2.500710	3.743157	2.054214	O	4.173035	4.777473	4.344077
H	-1.326633	1.688565	2.750521	C	3.293566	1.130554	4.832769
C	-0.638438	-1.257155	1.103162	O	3.653272	0.529004	5.739130
C	-0.123986	-2.364852	0.429877	C	0.941209	2.732401	4.284220
C	-0.864128	-3.539440	0.340078	O	0.008020	3.012452	4.884712
C	-2.121203	-3.621954	0.927005	C	1.963260	3.366678	1.624516
C	-2.639013	-2.518382	1.600596	O	1.617773	4.039073	0.768928
C	-1.905904	-1.342404	1.684785	C	4.326081	1.704945	2.143331
H	0.854640	-2.302059	-0.024203	O	5.260300	1.416369	1.549647

TS(3h-6h):

E = -1588.91207118021 au
ZPE = 0.2711822 au
 $\nu = -67.57 \text{ cm}^{-1}$

C	-0.069926	0.024261	1.446897	C	-1.787065	2.573831	-0.680991
O	2.121738	-0.235571	0.792217	C	-2.036664	3.572274	0.259805
C	-0.731002	1.236414	1.035597	C	-1.650599	3.404164	1.587664
C	-1.165228	1.400659	-0.293863	C	-0.974940	2.259059	1.968083

H	-0.965610	0.620757	-1.015622	P	1.620803	0.137613	2.206928
H	-2.084208	2.712988	-1.711821	C	1.685965	-1.271568	3.366533
H	-2.535107	4.483841	-0.043666	H	1.244389	-2.183882	2.972735
H	-1.864993	4.172431	2.318423	H	2.735292	-1.453834	3.604029
H	-0.684153	2.111989	2.994222	H	1.171974	-0.984990	4.286329
C	-0.647597	-1.236504	1.038477	W	2.723615	2.238688	3.157081
C	0.094551	-2.401664	0.750404	C	3.823965	3.836470	3.740547
C	-0.549148	-3.586489	0.452794	O	4.458446	4.741758	4.062536
C	-1.943280	-3.655181	0.453305	C	3.374041	1.155568	4.779301
C	-2.693348	-2.518257	0.730438	O	3.736529	0.552583	5.685186
C	-2.058297	-1.316572	0.999181	C	1.189621	2.936425	4.331860
H	1.169043	-2.331753	0.693982	O	0.370703	3.349670	5.023417
H	0.034886	-4.463336	0.205944	C	2.042638	3.255062	1.490249
H	-2.439050	-4.590178	0.226368	O	1.689357	3.815913	0.556691
H	-3.774350	-2.563689	0.731263	C	4.359300	1.574396	2.073325
H	-2.648226	-0.441947	1.230368	O	5.285600	1.228205	1.498931



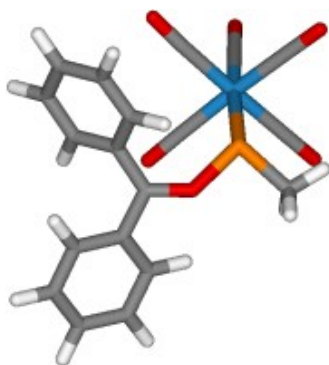
6h: $E = -1588.96052318868$ au
 $ZPE = 0.27317685$ au

C	0.090704	0.173992	2.014569	H	0.897980	-4.116776	0.370220
O	1.498298	-1.282263	4.019549	H	-0.401823	-3.682775	-1.697436
C	-0.982722	1.226142	2.001914	H	-1.477846	-1.468517	-2.019053
C	-0.952231	2.402843	1.256609	H	-1.239719	0.277041	-0.321546
C	-2.024614	3.288508	1.276363	P	1.019041	0.027062	3.481381
C	-3.152744	3.005490	2.036086	C	0.409990	1.147989	4.764025
C	-3.205238	1.824838	2.771134	H	-0.427093	0.672727	5.275916
C	-2.131581	0.945805	2.752776	H	1.220681	1.299073	5.475892
H	-0.090218	2.639862	0.653554	H	0.096198	2.102835	4.352479
H	-1.973885	4.200144	0.695084	W	2.669365	1.263038	1.861061
H	-3.985269	3.696912	2.054941	C	4.421673	2.078884	1.240528
H	-4.080560	1.588510	3.362513	O	5.414801	2.535391	0.900576
H	-2.180297	0.026609	3.322883	C	3.591242	1.205988	3.710639
C	-0.017177	-0.901512	1.005214	O	4.120093	1.185569	4.722150
C	0.571890	-2.166484	1.178982	C	1.940571	3.131369	2.348666
C	0.433740	-3.151358	0.213503	O	1.567963	4.167451	2.655776
C	-0.297684	-2.910122	-0.946522	C	1.952978	1.354461	-0.093117
C	-0.899134	-1.669416	-1.126381	O	1.586017	1.377214	-1.171566
C	-0.761762	-0.678755	-0.164978	C	3.412623	-0.629205	1.455435
H	1.132358	-2.375018	2.077349	O	3.863055	-1.653943	1.237976

TS(3h-7h): $E = -1588.89608214184$ au
 $ZPE = 0.27106839$ au
 $\nu = -195.40$ cm⁻¹

C	-0.314025	-0.058312	1.123981	C	-2.306887	1.265451	1.892731
O	0.993440	0.018646	1.120360	H	0.377809	2.254101	0.059308
C	-1.082505	1.180836	1.212329	H	-0.834138	4.404332	0.172111
C	-0.553496	2.327067	0.599308	H	-2.976073	4.549462	1.404318
C	-1.242313	3.527496	0.656485	H	-3.904210	2.541546	2.517071
C	-2.447922	3.606678	1.345241	H	-2.695903	0.400892	2.411722
C	-2.975675	2.474270	1.965697	C	-0.912638	-1.349327	0.864607

C	-0.114355	-2.506201	0.959954	H	2.912899	-1.401875	2.674268
C	-0.653185	-3.750818	0.695030	H	2.527433	-0.925132	4.338007
C	-1.989245	-3.864348	0.313048	W	3.163653	2.382871	2.735879
C	-2.782980	-2.726660	0.182896	C	4.610046	3.790490	2.740242
C	-2.253622	-1.477591	0.452684	O	5.452132	4.579936	2.740045
H	0.922165	-2.410123	1.241405	C	3.216773	2.232693	4.789040
H	-0.036185	-4.635215	0.780740	O	3.238985	2.129289	5.931960
H	-2.408292	-4.839960	0.102603	C	1.704930	3.836175	2.885219
H	-3.811085	-2.816265	-0.141206	O	0.915023	4.662253	2.983379
H	-2.863271	-0.598788	0.310316	C	3.025684	2.409323	0.683655
P	1.366358	0.529986	2.860737	O	2.927683	2.393375	-0.459405
C	2.109487	-1.085230	3.339948	C	4.588014	0.904600	2.593285
H	1.358459	-1.872051	3.416169	O	5.376696	0.075727	2.509974



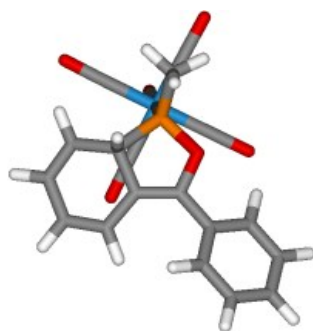
7h: $E = -1588.91488494789$ au
 $ZPE = 0.27213601$ au

C	0.038131	0.183175	0.189394	H	0.407011	-4.311996	-0.761098
O	1.299956	0.242992	0.350188	H	-1.953983	-4.744799	-0.153701
C	-0.798628	1.377552	0.107759	H	-3.394080	-2.889614	0.628998
C	-0.571594	2.460255	0.968267	H	-2.487191	-0.607390	0.789175
C	-1.406170	3.563612	0.927633	P	2.504334	1.554303	0.375952
C	-2.441754	3.622289	-0.000820	C	3.892106	0.362939	0.606503
C	-2.656403	2.563690	-0.878003	H	3.943000	-0.400773	-0.169409
C	-1.853067	1.436487	-0.813800	H	3.830125	-0.112565	1.586165
H	0.244106	2.424810	1.676511	H	4.811182	0.953507	0.570949
H	-1.238806	4.388165	1.607569	W	2.614973	2.488884	-2.076046
H	-3.075262	4.498513	-0.047376	C	2.830835	3.225199	-3.935413
H	-3.450209	2.616456	-1.611100	O	2.962506	3.631682	-5.008657
H	-2.017066	0.614212	-1.495270	C	4.144270	1.172658	-2.473092
C	-0.521346	-1.158294	0.093547	O	4.993986	0.442614	-2.721778
C	0.295992	-2.221224	-0.325257	C	1.256399	1.076213	-2.678606
C	-0.221504	-3.500341	-0.419168	O	0.492543	0.266540	-2.964391
C	-1.552738	-3.742155	-0.080849	C	1.089820	3.845829	-1.770350
C	-2.365832	-2.698873	0.351763	O	0.264953	4.638048	-1.679557
C	-1.858746	-1.411237	0.434077	C	3.970892	3.838771	-1.302245
H	1.323343	-2.025434	-0.597364	O	4.726756	4.579218	-0.858892

TS(7h-8h): $E = -1588.89251812705$ au
 $ZPE = 0.27083095$ au
 $\nu = -189.58$ cm⁻¹

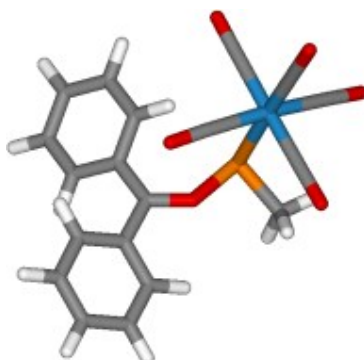
C	-0.067330	0.146468	-0.269480	H	-0.447562	4.432159	-1.813917
O	1.218441	0.385197	-0.088087	H	-2.738455	4.619675	-0.953692
C	-0.878892	1.222014	-0.664228	H	-3.866595	2.671401	0.095068
C	-0.212854	2.363399	-1.234876	H	-2.693769	0.527297	0.296559
C	-0.922749	3.583551	-1.340001	C	-0.510432	-1.193111	0.078263
C	-2.205261	3.680909	-0.867784	C	0.213896	-1.952273	1.010829
C	-2.861441	2.564126	-0.289678	C	-0.204363	-3.228380	1.346900
C	-2.217200	1.361048	-0.198600	C	-1.336916	-3.774260	0.745369
H	0.587371	2.183794	-1.937947	C	-2.049876	-3.037663	-0.196877

C	-1.640470	-1.756968	-0.533237	W	2.686805	2.018819	2.591771
H	1.091503	-1.526277	1.473567	C	3.393802	1.898365	4.493460
H	0.351530	-3.801930	2.076980	O	3.818456	1.801430	5.559396
H	-1.657406	-4.775112	1.004514	C	3.425945	0.147753	2.148145
H	-2.918216	-3.467929	-0.678254	O	3.825304	-0.888161	1.861657
H	-2.174986	-1.200054	-1.290013	C	0.871057	1.214799	3.146564
P	1.827051	2.021045	0.213279	O	-0.148418	0.778927	3.442264
C	3.121671	2.019044	-1.079572	C	1.908805	3.907842	2.908602
H	3.854826	1.228484	-0.916585	O	1.469751	4.953848	3.073359
H	2.693237	1.908835	-2.077626	C	4.436987	2.871274	1.920085
H	3.631440	2.982477	-1.018147	O	5.398152	3.352057	1.519762



8h: $E = -1588.95153936872$ au
 $ZPE = 0.27220645$ au

C	-0.185863	0.778738	0.274403	H	-0.431457	-3.307939	-1.859093
O	1.199999	0.651149	0.339383	H	-2.729768	-3.732556	-1.032272
C	-0.645151	2.030856	0.525098	H	-3.833753	-2.066509	0.434410
C	0.458820	2.975491	0.998724	H	-2.656658	-0.007877	1.071220
C	0.208605	4.415868	0.691196	P	1.936382	2.159088	0.238123
C	-1.016635	4.836632	0.351822	C	3.186523	2.036127	1.539049
C	-2.127427	3.913765	0.195761	H	3.972277	1.349130	1.226370
C	-1.951278	2.575737	0.271928	H	2.744153	1.695272	2.474521
H	0.579681	2.860210	2.087462	H	3.628097	3.025188	1.676127
H	1.021800	5.117935	0.818477	W	2.619878	2.874748	-2.059771
H	-1.195565	5.890152	0.175386	C	3.183293	3.477325	-3.919682
H	-3.101977	4.314494	-0.050316	O	3.511569	3.825016	-4.964171
H	-2.774474	1.910751	0.053699	C	4.580440	2.493107	-1.568595
C	-0.888264	-0.448965	-0.077510	O	5.669993	2.268906	-1.291567
C	-0.263062	-1.408832	-0.885654	C	2.424507	0.927116	-2.720006
C	-0.925149	-2.578899	-1.229249	O	2.319342	-0.152022	-3.086794
C	-2.216341	-2.817406	-0.766605	C	0.627796	3.205364	-2.524627
C	-2.838309	-1.879189	0.052357	O	-0.464379	3.376083	-2.818800
C	-2.180332	-0.708233	0.400005	C	2.830805	4.817465	-1.400934
H	0.739818	-1.229123	-1.244387	O	2.969924	5.900514	-1.052705



7h': $E = -1588.91269593453$ au
 $ZPE = 0.27217059$ au

C	-0.084541	0.229016	-0.114998	H	-4.536506	-0.916563	-0.492181
O	-0.237689	0.381362	1.142667	H	-4.640682	-0.168265	-2.850329
C	1.224227	0.135461	-0.738750	H	-2.631779	0.784214	-3.939009
C	2.332948	0.813596	-0.211865	H	-0.520305	0.966829	-2.687381
C	3.586678	0.661959	-0.781816	P	0.885221	0.434059	2.533692
C	3.757071	-0.188840	-1.868389	C	-0.360857	-0.299696	3.676394
C	2.666885	-0.881258	-2.393965	H	-1.311610	0.232728	3.674762
C	1.407892	-0.715539	-1.844819	H	-0.528952	-1.350851	3.437521
H	2.202566	1.500479	0.606634	H	0.065891	-0.240951	4.680936
H	4.428647	1.206446	-0.375929	W	1.027342	3.003368	3.073894
H	4.738700	-0.315720	-2.306372	C	1.147643	4.953835	3.563128
H	2.802794	-1.553517	-3.230586	O	1.205073	6.071924	3.844618
H	0.571665	-1.271999	-2.241845	C	1.719344	2.377908	4.911019
C	-1.322865	0.108780	-0.879603	O	2.095521	1.990778	5.923704
C	-2.474648	-0.397324	-0.258120	C	-0.904318	2.950619	3.786740
C	-3.656407	-0.506363	-0.969582	O	-1.978805	2.936329	4.187286
C	-3.713038	-0.087724	-2.298400	C	0.297298	3.367470	1.188517
C	-2.582704	0.440401	-2.914359	O	-0.119548	3.481730	0.123963
C	-1.389972	0.534614	-2.213759	C	2.960395	3.090445	2.378656
H	-2.424068	-0.718377	0.772744	O	4.039660	3.165307	1.990954

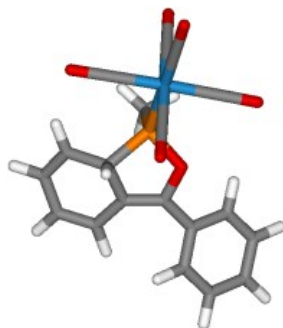
TS(7h'-8h'):

$E = -1588.89763715872$ au

$ZPE = 0.27067203$ au

$\nu = -227.45$ cm⁻¹

C	-0.474445	1.015040	0.174848	H	-1.811834	-3.400929	0.012957
O	0.749169	0.645074	-0.184528	H	-3.698492	-2.996546	1.565370
C	-0.806383	2.365767	0.037092	H	-4.071402	-0.729604	2.493157
C	0.289393	3.297696	-0.077741	H	-2.570801	1.121100	1.869980
C	0.028931	4.598892	-0.593482	P	1.884960	1.697548	-0.946165
C	-1.234249	4.949735	-0.974512	C	2.031448	0.747859	-2.506652
C	-2.321076	4.040281	-0.843494	H	2.336192	-0.280909	-2.300487
C	-2.116303	2.787544	-0.342070	H	1.084956	0.744574	-3.048910
H	1.080264	3.227220	0.657188	H	2.795425	1.224977	-3.122990
H	0.838391	5.314984	-0.644828	W	3.976688	1.724145	0.507516
H	-1.423497	5.945269	-1.356493	C	5.619069	1.658234	1.688831
H	-3.309753	4.339304	-1.164842	O	6.547758	1.603655	2.368129
H	-2.930954	2.078764	-0.303431	C	5.121159	1.817072	-1.204067
C	-1.360850	-0.076719	0.550904	O	5.740314	1.863159	-2.168147
C	-1.139562	-1.369840	0.053071	C	3.943094	-0.333091	0.362515
C	-1.982585	-2.409104	0.411106	O	3.902177	-1.473678	0.264137
C	-3.046085	-2.180585	1.282299	C	2.712445	1.617841	2.129923
C	-3.259802	-0.905852	1.799334	O	1.967321	1.550550	2.999098
C	-2.423094	0.140119	1.440188	C	3.935975	3.784670	0.585352
H	-0.311455	-1.545441	-0.618947	O	3.907995	4.930763	0.621409



8h':

$E = -1588.95183336101$ au

$ZPE = 0.27201207$ au

C	-0.290672	0.910755	0.299594	C	0.218787	3.251657	0.224023
O	1.102803	0.900418	0.421295	C	-0.091477	4.471429	-0.583828
C	-0.823841	2.143110	0.119304	C	-1.331514	4.677677	-1.046363

C	-2.396541	3.707562	-0.845570	H	-2.732436	0.214565	1.275026
C	-2.156531	2.496259	-0.296730	P	1.776598	2.325212	-0.136572
H	0.321179	3.547765	1.280471	C	1.749038	2.086728	-1.938886
H	0.687258	5.209972	-0.726384	H	2.471418	1.312404	-2.196883
H	-1.561127	5.586048	-1.589722	H	0.756809	1.797282	-2.284213
H	-3.389243	3.949666	-1.201967	H	2.046294	3.016517	-2.425214
H	-2.947225	1.761806	-0.244374	W	3.943653	2.951132	0.919643
C	-0.906175	-0.410498	0.318134	C	5.728911	3.459461	1.763196
C	-0.203273	-1.512092	-0.189912	O	6.736157	3.745806	2.233658
C	-0.792755	-2.767630	-0.226805	C	4.832633	2.902057	-0.940022
C	-2.086370	-2.949980	0.254072	O	5.319330	2.873832	-1.976250
C	-2.781496	-1.868179	0.787423	C	4.350311	0.938101	1.177710
C	-2.197030	-0.609921	0.825397	O	4.565449	-0.175893	1.319154
H	0.801742	-1.372649	-0.563004	C	3.009749	2.983390	2.762001
H	-0.241578	-3.606266	-0.633062	O	2.490184	3.000453	3.781925
H	-2.544735	-3.930137	0.224568	C	3.481638	4.941734	0.649630
H	-3.778473	-2.006812	1.185922	O	3.218554	6.046349	0.495761

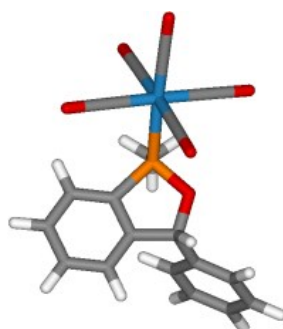
TS(8h'-4h):

E = -1588.85225908241 au

ZPE = 0.26632047 au

$\nu = -1282.36 \text{ cm}^{-1}$

C	-0.265695	0.812373	-0.035671	H	0.101184	-3.762309	0.034940
O	1.137989	0.865664	0.017857	H	-2.329750	-4.085168	0.428219
C	-0.810649	2.112777	-0.042072	H	-3.802282	-2.094638	0.627449
C	0.269514	3.177890	-0.139085	H	-2.891500	0.146753	0.440337
C	-0.069441	4.537701	-0.150038	P	1.809706	2.312333	-0.433136
C	-1.382893	4.936070	-0.136873	C	1.873166	2.188196	-2.251005
C	-2.419487	3.953097	-0.178992	H	2.612205	1.436317	-2.531889
C	-2.183107	2.615845	-0.164313	H	0.897788	1.914678	-2.655699
H	-0.376062	2.506924	1.012990	H	2.183186	3.154178	-2.653583
H	0.725714	5.271758	-0.195219	W	3.887929	2.976946	0.771325
H	-1.638303	5.985814	-0.133081	C	5.559743	3.530530	1.800184
H	-3.445876	4.291048	-0.253522	O	6.499966	3.837701	2.383264
H	-3.002558	1.922989	-0.263038	C	5.032310	2.321782	-0.814439
C	-0.845105	-0.485554	0.091826	O	5.658518	1.962403	-1.703432
C	-0.021926	-1.631498	-0.005937	C	3.959894	1.083030	1.609612
C	-0.554383	-2.903865	0.115358	O	3.986938	0.034060	2.062135
C	-1.917770	-3.088761	0.336784	C	2.655133	3.629017	2.290556
C	-2.742312	-1.970462	0.442825	O	1.938167	3.995135	3.104768
C	-2.223853	-0.691588	0.323751	C	3.765826	4.836219	-0.102770
H	1.036219	-1.504664	-0.181939	O	3.687860	5.868368	-0.596301



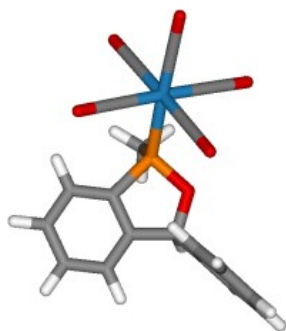
4h:

E = -1588.99496853877 au

ZPE = 0.27341079 au

C	-0.687975	-0.027864	0.209032	C	-1.722417	3.614710	-0.332584
O	0.588335	-0.371329	0.838928	C	-1.827366	2.228444	-0.301821
C	-0.742555	1.477737	0.135210	H	-1.455376	-0.408093	0.885676
C	0.429752	2.113202	0.536835	H	1.451157	3.991318	0.819344
C	0.539926	3.499796	0.504532	H	-0.475843	5.328471	0.032432
C	-0.543784	4.248815	0.063458	H	-2.563575	4.207790	-0.667681

H	-2.740527	1.741242	-0.620366	H	3.482937	-0.093017	-0.121788
C	-0.800934	-0.738588	-1.118142	H	2.318664	0.650835	-1.250052
C	-1.360455	-2.014227	-1.163307	H	3.429439	1.669028	-0.299886
C	-1.410956	-2.720996	-2.360180	W	2.580810	0.940201	3.395169
C	-0.902484	-2.153944	-3.524176	C	3.334769	0.908236	5.284589
C	-0.353413	-0.875140	-3.488716	O	3.762345	0.879317	6.351012
C	-0.306765	-0.170889	-2.292143	C	4.385986	1.592196	2.647101
H	-1.755484	-2.456439	-0.256305	O	5.382719	1.962716	2.219282
H	-1.847213	-3.711506	-2.383870	C	3.143856	-1.026155	3.109426
H	-0.938913	-2.702847	-4.456607	O	3.449335	-2.117549	2.945682
H	0.035697	-0.425509	-4.393502	C	0.728575	0.307503	4.054735
H	0.108698	0.828235	-2.275271	O	-0.306188	-0.041187	4.397891
P	1.629410	0.873631	1.076011	C	1.984332	2.899475	3.643145
C	2.825404	0.759792	-0.292454	O	1.648325	3.985757	3.782571

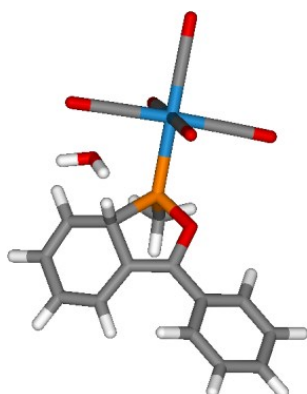


4h':

E = -1588.99656487286 au

ZPE = 0.27388816 au

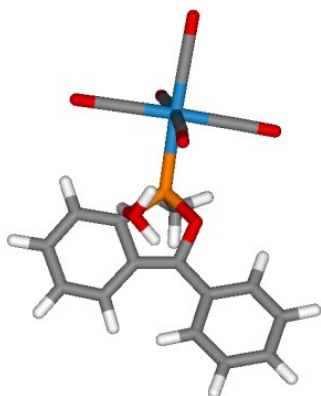
C	0.165598	-0.081049	0.097769	H	-1.735797	-3.919445	1.929300
O	1.615604	0.009805	0.254340	H	-1.781087	-2.949956	4.208222
C	-0.345385	1.338509	0.002556	H	-0.933115	-0.653263	4.588570
C	0.657909	2.300677	-0.084560	H	-0.060936	0.669543	2.699263
C	0.348150	3.653195	-0.177318	P	2.268353	1.479369	-0.069876
C	-0.987871	4.035817	-0.188320	C	2.714440	1.409239	-1.835853
C	-1.994879	3.073728	-0.103681	H	3.592375	0.775893	-1.964623
C	-1.680271	1.722079	-0.007034	H	1.885321	1.022929	-2.429192
H	-0.028540	-0.613265	-0.837530	H	2.958770	2.418264	-2.173182
H	1.130071	4.398905	-0.237096	W	4.085498	2.151399	1.519093
H	-1.248005	5.084147	-0.255541	C	5.574988	2.636194	2.817819
H	-3.032276	3.382535	-0.104387	O	6.414713	2.907438	3.553890
H	-2.465277	0.980496	0.072081	C	5.046364	3.155329	-0.002739
C	-0.393550	-0.877423	1.245961	O	5.574917	3.710780	-0.854769
C	-0.866644	-2.169488	1.037652	C	5.048355	0.403210	0.987784
C	-1.368384	-2.915616	2.100588	O	5.571949	-0.569437	0.686069
C	-1.392967	-2.371393	3.379412	C	3.085663	1.138857	3.017762
C	-0.917376	-1.079075	3.593464	O	2.535213	0.583268	3.852582
C	-0.424367	-0.335584	2.530943	C	3.067364	3.871396	2.028276
H	-0.841221	-2.594045	0.041103	O	2.498160	4.822486	2.317799



8h'·H₂O:

E = -1665.2996533887 au
ZPE = 0.29482449 au

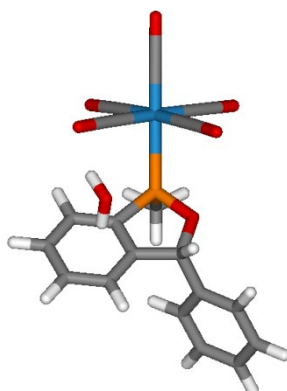
C	-0.357981	0.787315	-0.116023	H	-3.891638	-2.067021	0.799431
O	1.032779	0.774606	0.039511	H	-2.839853	0.152648	0.803267
C	-0.875828	2.014506	-0.365119	P	1.731459	2.171413	-0.558561
C	0.172771	3.118277	-0.280209	C	1.762557	1.849614	-2.348704
C	-0.107408	4.309246	-1.137183	H	2.505815	1.078475	-2.551376
C	-1.334030	4.509734	-1.637392	H	0.785447	1.526413	-2.707520
C	-2.410089	3.553072	-1.429487	H	2.056655	2.761451	-2.869826
C	-2.193989	2.361267	-0.829410	W	3.872257	2.805081	0.540373
H	0.260814	3.455043	0.765723	C	5.634250	3.309627	1.430387
H	0.681544	5.036236	-1.285190	O	6.631231	3.592122	1.926487
H	-1.544244	5.400463	-2.216699	C	4.652493	3.287134	-1.300883
H	-3.391461	3.787135	-1.821265	O	5.077619	3.551851	-2.332377
H	-2.992010	1.635047	-0.772110	C	4.495609	0.852703	0.299545
C	-0.981444	-0.528261	-0.048284	O	4.827698	-0.234383	0.158231
C	-0.265375	-1.659428	-0.465823	C	3.033807	2.291121	2.363808
C	-0.858290	-2.913867	-0.452951	O	2.576130	1.983056	3.365105
C	-2.169860	-3.066030	-0.012040	C	3.171988	4.738547	0.747456
C	-2.879749	-1.953606	0.431574	O	2.780760	5.810319	0.836592
C	-2.291437	-0.696640	0.420629	O	0.715980	4.431468	2.768868
H	0.753423	-1.543803	-0.808224	H	0.187048	3.934860	3.404968
H	-0.295440	-3.775508	-0.789084	H	0.239739	5.261455	2.645023
H	-2.630947	-4.045306	-0.002761				



TS(8h'·H₂O→4h·H₂O): E = -1665.233300426757 au
ZPE = 0.29343369 au
 $\nu = -377.86 \text{ cm}^{-1}$

C	-0.371262	0.877302	-0.204752	H	-2.586186	-3.935388	0.558568
O	1.062471	0.885632	-0.040035	H	-4.014576	-1.902507	0.468894
C	-0.827946	2.130446	-0.604062	H	-3.028460	0.296980	0.151458
C	0.239436	3.135100	-0.613953	P	1.772460	2.215051	-0.705979
C	-0.025485	4.479766	-0.940827	C	1.958547	1.755792	-2.464926
C	-1.312722	4.890228	-1.194139	H	2.739568	1.000711	-2.565088
C	-2.352357	3.923871	-1.205068	H	1.015932	1.369181	-2.853369
C	-2.139078	2.597191	-0.930610	H	2.248897	2.642365	-3.031275
H	0.081666	3.126360	1.148556	W	3.888470	2.888988	0.475589
H	0.792858	5.188155	-0.984771	C	5.622192	3.357815	1.445268
H	-1.531211	5.926383	-1.411933	O	6.592340	3.615400	2.001768
H	-3.357143	4.244127	-1.454459	C	4.712131	3.373446	-1.373104
H	-2.965748	1.905592	-0.992879	O	5.142435	3.644202	-2.395934
C	-0.986252	-0.408153	-0.010018	C	4.485276	0.917832	0.265411
C	-0.191880	-1.573320	0.062371	O	4.797906	-0.175946	0.149440
C	-0.764545	-2.820139	0.264840	C	2.928013	2.432712	2.199195
C	-2.143162	-2.960354	0.403037	O	2.288501	2.196066	3.135708
C	-2.941286	-1.818941	0.346665	C	3.236898	4.834720	0.676587
C	-2.380840	-0.566680	0.150656	O	2.867021	5.911060	0.805446
H	0.879178	-1.483870	-0.046799	O	-0.249305	2.657969	2.040074
H	-0.125350	-3.693892	0.311630	H	-0.567139	1.794190	1.641779

H 0.507116 2.479290 2.644234

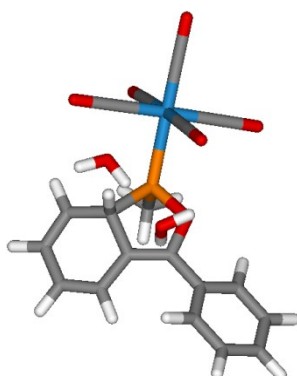


4h·H₂O:

E = -1665.34348979905 au

ZPE = 0.29676346 au

C	-0.107989	-0.393500	-0.308487	H	0.517016	0.204821	-4.900740
O	1.253520	-0.426135	0.227722	H	0.451961	1.031860	-2.583234
C	-0.620896	1.010208	-0.102301	P	1.860088	1.006590	0.745571
C	0.313236	1.888961	0.438368	C	2.981496	1.551888	-0.580362
C	-0.019834	3.212727	0.707163	H	3.868904	0.918315	-0.580142
C	-1.306040	3.653432	0.422709	H	2.495341	1.505514	-1.553347
C	-2.244427	2.776065	-0.123956	H	3.288093	2.578845	-0.373824
C	-1.907430	1.452264	-0.391939	W	2.809770	1.031991	3.065414
H	-0.678076	-1.097382	0.300456	C	3.605080	1.045214	4.941684
H	0.705247	3.889052	1.141668	O	4.058259	1.050951	5.996806
H	-1.584053	4.677937	0.631607	C	4.439972	-0.029507	2.354885
H	-3.246500	3.125631	-0.335167	O	5.339454	-0.613859	1.956555
H	-2.638183	0.776247	-0.817848	C	1.788772	-0.730144	3.435659
C	-0.113259	-0.865494	-1.741175	O	1.195456	-1.689009	3.622128
C	-0.435254	-2.190276	-2.026285	C	1.161696	2.058249	3.719455
C	-0.412442	-2.656333	-3.337118	O	0.221752	2.619045	4.069143
C	-0.063905	-1.797190	-4.373384	C	3.732076	2.813268	2.604539
C	0.253415	-0.469718	-4.096027	O	4.221035	3.812704	2.327689
C	0.223837	-0.006320	-2.787590	O	-2.205866	0.994966	2.981904
H	-0.706076	-2.859325	-1.218268	H	-2.228100	1.250243	2.050813
H	-0.667989	-3.687044	-3.547493	H	-1.614304	1.632278	3.400488
H	-0.044930	-2.156639	-5.394377				



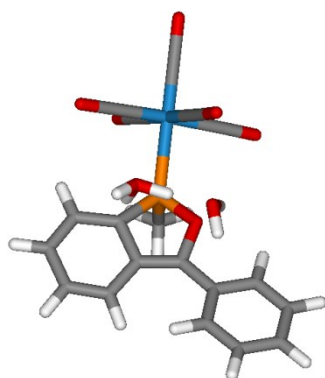
8h'·2H₂O:

E = -1741.65278397889 au

ZPE = 0.31988942 au

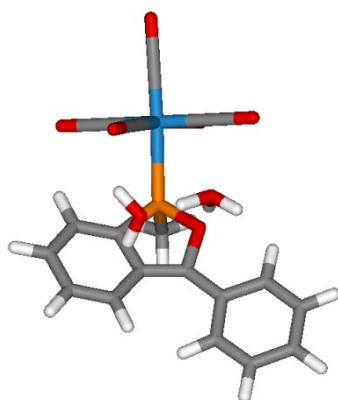
C	-0.285044	0.737114	-0.127911	C	-1.330559	4.477825	-1.553219
O	1.109835	0.716381	-0.054792	C	-2.397996	3.528533	-1.280197
C	-0.813613	1.973031	-0.322676	C	-2.157801	2.332785	-0.698439
C	0.241251	3.073089	-0.289366	H	0.375529	3.419351	0.748747
C	-0.077956	4.266394	-1.128436	H	0.706253	4.989505	-1.315473

H	-1.569925	5.372479	-2.114332	H	2.089849	2.778737	-2.929578
H	-3.400386	3.772394	-1.607316	W	3.915630	2.739946	0.508648
H	-2.957895	1.614855	-0.592264	C	5.633026	3.217077	1.500700
C	-0.910055	-0.578278	-0.036306	O	6.596227	3.482291	2.066493
C	-0.219495	-1.707292	-0.499214	C	4.693287	3.413090	-1.274732
C	-0.810513	-2.961587	-0.454143	O	5.108803	3.777791	-2.278891
C	-2.092443	-3.115586	0.066088	C	4.635032	0.853053	0.094130
C	-2.775427	-2.005293	0.553949	O	5.029103	-0.195762	-0.145113
C	-2.190095	-0.747925	0.508886	C	3.043566	1.998095	2.230097
H	0.777205	-1.590429	-0.900699	O	2.544553	1.541695	3.152792
H	-0.268827	-3.821919	-0.826117	C	3.164745	4.634691	0.875448
H	-2.551040	-4.095307	0.102245	O	2.761043	5.690783	1.044928
H	-3.762912	-2.119558	0.982313	O	0.662911	4.069882	2.882684
H	-2.720680	0.097590	0.924233	H	0.143404	3.262502	3.058400
P	1.793948	2.133900	-0.630454	H	0.027773	4.794807	2.902259
C	1.794912	1.856913	-2.426426	O	-0.707919	1.597694	3.033364
H	2.528750	1.085043	-2.658777	H	-0.079126	0.956800	3.389754
H	0.809922	1.550793	-2.779243	H	-0.802572	1.370818	2.096312



TS(8h'·2H₂O→9h·2H₂O): E = -1741.60418376191 au
 ZPE = 0.31716859 au
 ν = -282.22 cm⁻¹

C	-0.391649	0.805198	-0.308336	H	-3.057514	0.306195	0.125342
O	1.028492	0.802283	-0.026217	P	1.774653	2.150886	-0.644233
C	-0.828519	2.075391	-0.612792	C	1.969363	1.698814	-2.406227
C	0.246648	3.080329	-0.557787	H	2.742772	0.936285	-2.506156
C	0.006247	4.420677	-0.956734	H	1.026616	1.325143	-2.805918
C	-1.262909	4.836925	-1.255984	H	2.275540	2.585122	-2.963920
C	-2.322762	3.881171	-1.260847	W	3.910787	2.863000	0.477840
C	-2.132025	2.560131	-0.966114	C	5.691934	3.420339	1.287776
H	0.165205	3.273864	1.055916	O	6.704545	3.733766	1.731927
H	0.833112	5.120673	-0.987230	C	4.534880	3.623774	-1.334703
H	-1.463708	5.868443	-1.510569	O	4.888769	4.051468	-2.336779
H	-3.317821	4.212405	-1.534194	C	4.655958	1.000544	-0.011381
H	-2.963971	1.877078	-1.050715	O	5.052306	-0.038382	-0.284718
C	-1.033123	-0.449165	-0.040173	C	3.304548	2.130647	2.307914
C	-0.262569	-1.628311	0.086424	O	2.987116	1.738727	3.335987
C	-0.856577	-2.849390	0.367749	C	3.076452	4.680494	0.975591
C	-2.235079	-2.951727	0.535446	O	2.602587	5.682666	1.266216
C	-3.009826	-1.797529	0.431674	O	0.091598	3.248951	2.149664
C	-2.427836	-0.569498	0.159198	H	0.033727	2.246651	2.449532
H	0.807911	-1.572182	-0.050481	H	-0.695821	3.733211	2.443847
H	-0.234621	-3.732597	0.452024	O	0.160297	0.794891	2.694801
H	-2.695545	-3.907043	0.750903	H	0.688354	0.495482	1.929723
H	-4.081963	-1.851301	0.578479	H	-0.682299	0.324293	2.616593

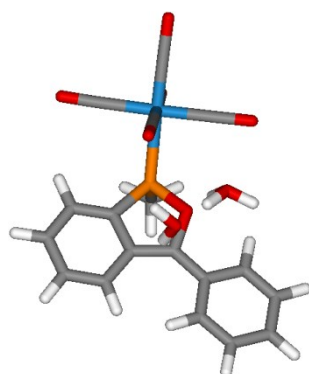


9h·2H₂O:

E = -1741.60944386617 au

ZPE = 0.31959698 au

C	-0.355498	0.731838	-0.422991	H	-3.048856	0.215163	-0.699158
O	1.078344	0.675315	-0.107365	P	1.936312	1.928252	-0.875990
C	-0.703015	2.046656	-0.794830	C	2.224704	1.211378	-2.535601
C	0.435768	2.911441	-1.017513	H	2.964723	0.400512	-2.464661
C	0.310669	4.275464	-1.258971	H	1.281496	0.831894	-2.954113
C	-0.958382	4.865874	-1.314134	H	2.624720	2.009911	-3.179736
C	-2.086940	4.050349	-1.112273	W	3.894018	2.867221	0.398211
C	-1.986968	2.682527	-0.857763	C	5.462799	3.713946	1.400357
H	-0.316336	3.816495	2.109938	O	6.345302	4.199345	1.960400
H	1.204408	4.888590	-1.401640	C	3.984983	4.378732	-1.015446
H	-1.068120	5.935144	-1.502908	O	4.030787	5.214845	-1.804098
H	-3.083712	4.500478	-1.137607	C	5.160533	1.702863	-0.774236
H	-2.899467	2.112648	-0.692638	O	5.831635	1.045290	-1.434271
C	-1.086677	-0.402840	0.037902	C	3.823618	1.329909	1.793586
C	-0.430303	-1.477032	0.715668	O	3.786778	0.475571	2.560574
C	-1.144161	-2.565338	1.219602	C	2.506621	3.930524	1.476465
C	-2.532480	-2.654155	1.068260	O	1.671533	4.492326	2.046082
C	-3.191667	-1.627888	0.373716	O	-0.858720	3.007735	2.097495
C	-2.497775	-0.533849	-0.132939	H	-0.059641	1.894940	2.266202
H	0.656874	-1.464838	0.810712	H	-1.318093	3.006470	1.229690
H	-0.598824	-3.364059	1.731507	O	0.616898	1.050824	2.338992
H	-3.086998	-3.508175	1.463824	H	0.951982	0.861602	1.374772
H	-4.272781	-1.685354	0.215104	H	0.104184	0.260245	2.600179



TS(9h·2H₂O→4h·2H₂O):

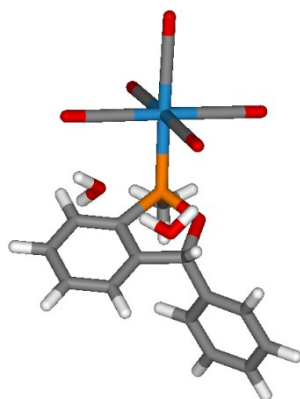
E = -1741.60885729256 au

ZPE = 0.31942253 au

$\nu = -41.92 \text{ cm}^{-1}$

C	-0.459074	1.000759	-0.179749	C	-1.989853	2.782102	-1.211607
O	0.986522	0.918125	0.100159	H	-0.764671	3.366395	2.550756
C	-0.740504	2.217405	-0.828837	H	1.252382	4.826365	-1.892569
C	0.427110	3.001959	-1.130523	H	-0.966442	5.796787	-2.445280
C	0.347569	4.267379	-1.688365	H	-3.010243	4.444723	-2.051345
C	-0.891944	4.809778	-2.010148	H	-2.910138	2.239464	-1.061923
C	-2.041628	4.041461	-1.779661	C	-1.178687	-0.166100	0.194827

C	-0.496786	-1.347064	0.595945	C	5.459871	3.601899	1.522475
C	-1.185210	-2.485061	0.988001	O	6.359639	3.975324	2.130110
C	-2.577213	-2.516350	1.002135	C	3.807305	4.701516	-0.581262
C	-3.267019	-1.367068	0.613591	O	3.801943	5.699122	-1.142708
C	-2.597484	-0.219773	0.224690	C	5.105480	2.134491	-0.998975
H	0.583208	-1.375582	0.554787	O	5.775397	1.699580	-1.818274
H	-0.621422	-3.365047	1.275609	C	3.977587	1.131744	1.485757
H	-3.110365	-3.407400	1.305871	O	4.048766	0.137956	2.050845
H	-4.350778	-1.361238	0.621100	C	2.513053	3.682333	1.804454
H	-3.178952	0.649896	-0.037411	O	1.722589	4.102758	2.522670
P	1.880799	2.023025	-0.788763	O	-0.972580	2.429076	2.431917
C	2.189176	1.076202	-2.314325	H	0.127789	1.531212	2.680008
H	2.902328	0.275644	-2.114723	H	-1.128799	2.281498	1.474629
H	1.254544	0.660855	-2.691988	O	0.947034	0.867593	2.580108
H	2.613877	1.753150	-3.057685	H	1.088644	0.816486	1.536902
W	3.864449	2.915440	0.456985	H	0.707010	-0.010028	2.920148

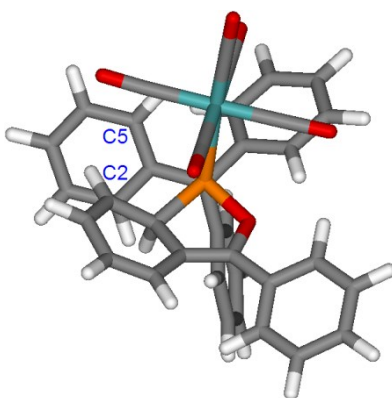


4h·2H₂O:

E = -1741.69683755688 au

ZPE = 0.32122412 au

C	-0.186405	0.582888	0.540044	H	-0.828008	-1.584191	1.998174
O	1.251113	0.460902	0.281004	P	1.928694	1.653700	-0.615002
C	-0.635222	1.867974	-0.105492	C	2.194832	0.910033	-2.254193
C	0.371594	2.559027	-0.774013	H	3.019846	0.199457	-2.197317
C	0.112008	3.776850	-1.396910	H	1.294068	0.406652	-2.603183
C	-1.175603	4.298882	-1.339916	H	2.466015	1.703634	-2.953161
C	-2.185745	3.607700	-0.666146	W	3.895449	2.761237	0.486449
C	-1.921877	2.390441	-0.049580	C	5.465576	3.628517	1.447314
H	-0.121638	4.568573	1.052724	O	6.347644	4.121568	1.995244
H	0.896477	4.315685	-1.911966	C	4.833837	2.975143	-1.333409
H	-1.394403	5.245938	-1.815569	O	5.351010	3.084257	-2.350593
H	-3.182169	4.027153	-0.618840	C	4.753385	0.894626	0.688866
H	-2.706030	1.860066	0.475166	O	5.233348	-0.139645	0.795701
C	-0.891550	-0.660715	0.063402	C	2.893038	2.475934	2.266894
C	-1.284199	-0.811163	-1.266634	O	2.337567	2.282805	3.248900
C	-1.891555	-1.985572	-1.692218	C	3.028877	4.618140	0.258961
C	-2.114360	-3.022596	-0.789667	O	2.562886	5.655784	0.124106
C	-1.730609	-2.877566	0.539264	O	0.135217	4.479310	1.979868
C	-1.123557	-1.699641	0.962199	H	-0.507894	3.032237	2.908629
H	-1.125213	-0.004361	-1.970785	H	0.010219	5.354399	2.366211
H	-2.195185	-2.091457	-2.725991	O	-0.785081	2.255053	3.431658
H	-2.590280	-3.936859	-1.120859	H	0.026191	1.950453	3.853964
H	-1.906436	-3.677791	1.246899	H	-0.290411	0.669154	1.622916



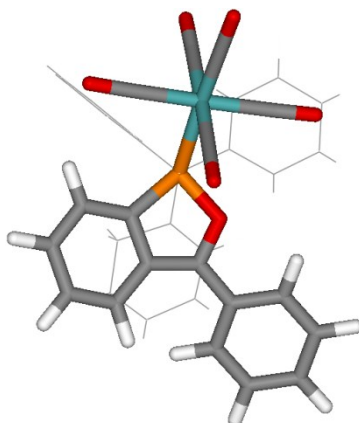
8e: $E = -2281.33735249745$ au
 $ZPE = 0.51842975$ au

C	-0.486574	0.454021	0.476342	H	4.033051	-4.739873	1.281715
O	-0.006009	0.570641	1.769323	H	2.046112	-3.647659	2.249891
C	0.360829	-0.160587	-0.404802	C	1.975919	-0.280620	4.569745
C	1.589829	-0.770664	0.268290	C	1.033741	0.719656	4.865358
C	2.819043	-0.796365	-0.588954	C	1.107721	1.445824	6.054289
C	2.716137	-0.656621	-1.926770	C	2.117245	1.169352	6.983044
C	1.436626	-0.392870	-2.573143	C	3.040607	0.157351	6.712231
C	0.309356	-0.153631	-1.849377	C	2.971688	-0.560878	5.513663
H	1.367590	-1.818552	0.551661	H	0.224477	0.925692	4.161900
H	3.774889	-1.024923	-0.114522	H	0.372612	2.229103	6.255100
H	3.609059	-0.739096	-2.552193	H	2.179789	1.738170	7.913963
H	1.405482	-0.324415	-3.663123	H	3.828113	-0.074950	7.433420
H	-0.608709	0.145450	-2.355638	H	3.702966	-1.346389	5.321082
C	-1.800067	1.065325	0.265317	C	0.628821	-2.052071	3.452757
C	-2.192650	2.169600	1.048366	C	-0.400134	-2.276452	2.526395
C	-3.434871	2.771848	0.847291	C	-1.399290	-3.226658	2.773317
C	-4.310855	2.277058	-0.125838	C	-1.389782	-3.981564	3.946228
C	-3.940112	1.165304	-0.890973	C	-0.364346	-3.776277	4.875666
C	-2.699093	0.558885	-0.694250	C	0.624482	-2.823545	4.630892
H	-1.513069	2.554511	1.808423	H	-0.460017	-1.726957	1.593421
H	-3.722013	3.633377	1.455309	H	-2.189173	-3.370771	2.031799
H	-5.284374	2.748904	-0.279868	H	-2.170849	-4.721957	4.136398
H	-4.627633	0.759287	-1.637103	H	-0.333791	-4.358013	5.800481
H	-2.437091	-0.331949	-1.266649	H	1.411650	-2.679180	5.371605
P	1.665774	0.211966	1.856498	Mo	2.917638	2.402333	1.743365
C	1.815648	-1.080397	3.267552	C	3.759770	4.215430	1.511275
C	3.079878	-1.828826	2.808851	O	4.235203	5.257157	1.371727
C	4.331363	-1.184434	2.799790	C	1.278619	3.267335	2.627230
C	5.457048	-1.800421	2.247206	O	0.370612	3.758395	3.133206
C	5.358241	-3.079434	1.693161	C	2.090845	2.636830	-0.131745
C	4.124810	-3.737205	1.705986	O	1.675412	2.846998	-1.181849
C	2.998871	-3.118552	2.256051	C	4.578331	1.535784	0.896212
H	4.432965	-0.191396	3.231196	O	5.533192	1.093359	0.433727
H	6.412832	-1.271676	2.247546	C	3.792715	2.303383	3.601288
H	6.236814	-3.561335	1.257583	O	4.317780	2.326281	4.622699

TS(8e-10e): $E = -2281.28945061759$ au
 $ZPE = 0.51268952$ au
 $\nu = -1075.64$ cm⁻¹

C	0.000908	0.385580	0.243464	H	2.452067	-1.065546	0.601015
O	0.175853	0.917451	1.516034	H	4.507959	0.952938	0.444370
C	1.187646	0.298627	-0.469411	H	4.783282	0.752012	-2.003770
C	2.370771	0.412381	0.399997	H	2.838300	0.166418	-3.460830
C	3.655651	0.703225	-0.189706	H	0.570975	-0.039856	-2.544920
C	3.806532	0.583333	-1.544316	C	-1.362187	0.029452	-0.083626
C	2.682043	0.256129	-2.382913	C	-2.434466	0.572187	0.663301
C	1.415439	0.122715	-1.873978	C	-3.748497	0.198505	0.393192

C	-4.028680	-0.730556	-0.618941	H	4.141907	0.498343	2.862992
C	-2.975935	-1.292177	-1.348296	H	6.338708	-0.233458	3.662258
C	-1.655167	-0.928667	-1.079913	H	6.586493	-2.416780	4.854902
H	-2.218013	1.295878	1.450507	H	4.571528	-3.857929	5.205287
H	-4.564200	0.635723	0.974749	H	2.355420	-3.118041	4.381842
H	-5.060907	-1.022643	-0.827412	C	0.726707	-0.549266	4.242254
H	-3.182139	-2.035238	-2.123138	C	-0.642569	-0.270432	4.053938
H	-0.844090	-1.410907	-1.623838	C	-1.462990	0.095140	5.122627
P	1.760909	0.865301	2.060979	C	-0.938688	0.217955	6.411446
C	1.664148	-0.890767	3.079209	C	0.420974	-0.026419	6.613727
C	1.222576	-1.907660	2.068925	C	1.238019	-0.404650	5.545332
C	2.218570	-2.255615	1.061452	H	-1.075656	-0.296582	3.059621
C	1.828550	-3.126505	-0.016855	H	-2.519229	0.304602	4.936698
C	0.533818	-3.582604	-0.128340	H	-1.579628	0.514133	7.245486
C	-0.413927	-3.266836	0.871606	H	0.859333	0.081725	7.609066
C	-0.067900	-2.443276	1.940950	H	2.294664	-0.576650	5.737394
H	3.260288	-2.354912	1.395733	Mo	2.307435	3.068628	3.137750
H	2.585321	-3.420623	-0.748226	C	2.574485	4.936483	3.844218
H	0.246939	-4.226019	-0.964093	O	2.711550	6.011850	4.237521
H	-1.423685	-3.677577	0.815694	C	0.390167	3.073794	3.908627
H	-0.820282	-2.230743	2.696325	O	-0.673822	3.121110	4.332781
C	3.074823	-1.250262	3.565972	C	1.600324	3.824656	1.357838
C	4.212184	-0.461809	3.370269	O	1.208465	4.230410	0.358035
C	5.469531	-0.874213	3.829439	C	4.211808	3.077768	2.388806
C	5.607362	-2.092434	4.494220	O	5.289692	3.083649	1.984346
C	4.477937	-2.898401	4.690603	C	3.037326	2.299347	4.901578
C	3.230440	-2.481787	4.229153	O	3.480126	1.917359	5.890313



10e:

$E = -2281.30844748768$ au

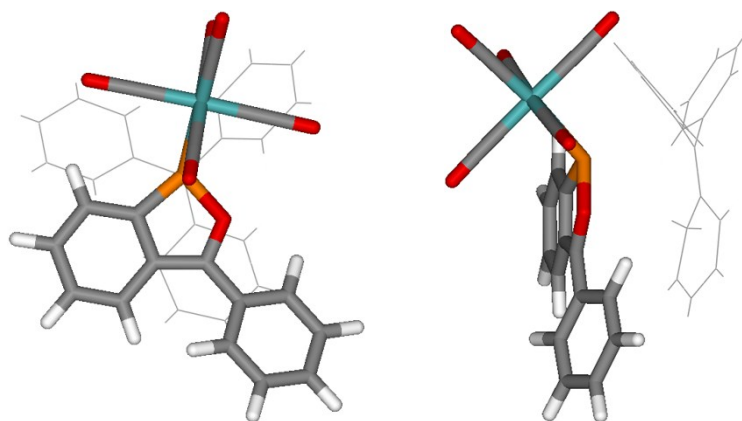
$ZPE = 0.51859161$ au

C	0.081871	0.298242	0.326555	H	-4.501526	0.513644	0.882357
O	0.186322	1.072072	1.459173	H	-4.917396	-1.244483	-0.846400
C	1.311556	0.304643	-0.411377	H	-2.981292	-2.290672	-2.026492
C	2.394946	0.787589	0.388553	H	-0.675309	-1.610776	-1.483986
C	3.685933	0.935120	-0.144972	P	1.757656	1.103794	2.040550
C	3.912671	0.596510	-1.473096	C	1.606802	-0.776043	2.921132
C	2.852186	0.101392	-2.268459	C	1.094886	-1.730334	1.896902
C	1.572387	-0.048788	-1.757954	C	2.116665	-2.311571	0.947887
H	2.747872	-1.508470	0.528022	C	1.565604	-3.182868	-0.130665
H	4.504537	1.313749	0.468346	C	0.302056	-3.662372	-0.081954
H	4.907922	0.717292	-1.906193	C	-0.571176	-3.286461	1.000842
H	3.041520	-0.152560	-3.314345	C	-0.173496	-2.362632	1.943615
H	0.771812	-0.413709	-2.400694	H	2.854915	-2.908955	1.524817
C	-1.254289	-0.106794	-0.027984	H	2.244341	-3.472349	-0.937646
C	-2.363570	0.458973	0.650670	H	-0.069283	-4.335702	-0.859173
C	-3.661188	0.054253	0.355582	H	-1.560635	-3.740966	1.077691
C	-3.896464	-0.929230	-0.617347	H	-0.875467	-2.101782	2.731222
C	-2.812830	-1.509873	-1.280288	C	3.016564	-1.178799	3.369063
C	-1.505613	-1.117857	-0.983911	C	4.166283	-0.406047	3.187546
H	-2.187858	1.236541	1.394780	C	5.416701	-0.841856	3.643222

C	5.537586	-2.073053	4.287047	H	-2.511292	0.439138	4.907771
C	4.396895	-2.866323	4.468460	H	-1.527621	0.532594	7.206548
C	3.156333	-2.423497	4.012811	H	0.907631	0.032915	7.505553
H	4.114335	0.563498	2.696505	H	2.293204	-0.580609	5.584506
H	6.293913	-0.208094	3.491785	Mo	2.294287	3.203651	3.295340
H	6.511477	-2.415731	4.644994	C	2.626886	4.982481	4.180860
H	4.475361	-3.834422	4.969406	O	2.808056	6.006160	4.679368
H	2.270860	-3.046659	4.161125	C	0.402692	3.176790	4.129022
C	0.703870	-0.451731	4.117443	O	-0.645047	3.224887	4.591194
C	-0.661835	-0.133634	3.968556	C	1.534388	4.150601	1.632868
C	-1.456618	0.200966	5.066036	O	1.111425	4.672913	0.702151
C	-0.908054	0.258085	6.349320	C	4.174509	3.272310	2.492295
C	0.449160	-0.023365	6.514946	O	5.241462	3.315821	2.061653
C	1.238959	-0.374396	5.416824	C	3.088290	2.257537	4.942241
H	-1.115653	-0.118062	2.983641	O	3.581221	1.784332	5.865458

TS(10e-11e-12): $E = -2281.30469897761$ au
 $ZPE = 0.51628019$ au
 $v = -101.74$ cm⁻¹

C	0.065336	0.331578	0.269218	H	-1.679118	-3.607134	1.036655
O	0.170741	1.008378	1.449884	H	-0.914911	-2.096447	2.780324
C	1.308608	0.301263	-0.426626	C	3.059041	-1.254375	3.402505
C	2.384937	0.767708	0.402408	C	4.148171	-0.387166	3.276029
C	3.697936	0.874146	-0.101450	C	5.430637	-0.759270	3.696526
C	3.947837	0.525796	-1.417874	C	5.647777	-2.019200	4.254955
C	2.892998	0.056006	-2.244522	C	4.569620	-2.903092	4.389387
C	1.600580	-0.060752	-1.770246	C	3.296104	-2.523476	3.967095
H	2.715855	-1.568130	0.609093	H	4.018492	0.610062	2.861086
H	4.508782	1.235290	0.532656	H	6.257398	-0.053128	3.586432
H	4.956381	0.619090	-1.826587	H	6.647364	-2.312234	4.585186
H	3.105715	-0.204876	-3.284083	H	4.721691	-3.892255	4.828564
H	0.810097	-0.406291	-2.435181	H	2.458580	-3.216302	4.082844
C	-1.271452	-0.070944	-0.093903	C	0.759871	-0.545175	4.207920
C	-2.376268	0.453303	0.623052	C	-0.585822	-0.142284	4.071418
C	-3.675048	0.057072	0.320837	C	-1.346952	0.241089	5.176214
C	-3.914398	-0.877007	-0.697807	C	-0.784508	0.258465	6.455146
C	-2.833954	-1.419065	-1.398621	C	0.553185	-0.111257	6.608803
C	-1.526688	-1.034122	-1.096045	C	1.310827	-0.505756	5.503376
H	-2.197341	1.191709	1.405392	H	-1.041850	-0.092529	3.087758
H	-4.512055	0.483668	0.879343	H	-2.384481	0.550275	5.028499
H	-4.935851	-1.185581	-0.933421	H	-1.377870	0.569818	7.318347
H	-3.005775	-2.163346	-2.180377	H	1.021593	-0.087189	7.596066
H	-0.700050	-1.502280	-1.624922	H	2.353614	-0.774689	5.658396
P	1.741775	1.102310	2.028538	Mo	2.199490	3.247352	3.247683
C	1.617932	-0.932162	3.017700	C	2.475921	5.064055	4.067589
C	1.096148	-1.829829	2.000848	O	2.623928	6.113425	4.522706
C	2.083121	-2.386281	0.999837	C	0.267054	3.235695	3.978032
C	1.488007	-3.175720	-0.118190	O	-0.806124	3.280515	4.378896
C	0.199124	-3.582532	-0.100208	C	1.533729	4.110079	1.501460
C	-0.663159	-3.210012	0.994213	O	1.166012	4.573956	0.517791
C	-0.223906	-2.361209	1.983683	C	4.117839	3.278873	2.537754
H	2.825236	-3.027608	1.519825	O	5.202790	3.292619	2.152717
H	2.153375	-3.461559	-0.937615	C	2.900988	2.363764	4.972495
H	-0.203433	-4.193866	-0.912177	O	3.342074	1.925739	5.937993



11e-12:

$E = -2281.31428496599$ au

$ZPE = 0.51667202$ au

C	0.132326	0.338475	-0.030816	H	-2.406764	-2.956628	2.068148
O	0.078834	0.868230	1.184317	H	-0.929708	-2.361173	3.911986
C	1.467435	0.093028	-0.455819	C	3.162845	-1.511252	3.577707
C	2.414205	0.498439	0.551299	C	3.766988	-0.305609	4.000864
C	3.800947	0.291657	0.351395	C	5.134510	-0.081649	3.851105
C	4.231957	-0.294753	-0.821826	C	5.952853	-1.073487	3.296714
C	3.301935	-0.723849	-1.809562	C	5.384549	-2.292668	2.918748
C	1.946017	-0.544717	-1.635572	C	4.010016	-2.508480	3.057146
H	2.344225	-2.220719	1.101877	C	3.146461	0.466126	4.450457
H	4.515385	0.580150	1.123898	H	5.563401	0.873257	4.164452
H	5.300349	-0.451127	-0.989369	H	7.025061	-0.901054	3.174754
H	3.669998	-1.216831	-2.712091	H	6.014398	-3.088014	2.511790
H	1.250752	-0.920762	-2.384374	H	3.600724	-3.478940	2.780338
C	-1.152523	0.062233	-0.661254	C	1.062758	-1.023212	4.875766
C	-2.297585	-0.066878	0.155012	C	-0.018856	-0.130083	4.748615
C	-3.536561	-0.364536	-0.407116	C	-0.560737	0.512479	5.863149
C	-3.661947	-0.527617	-1.792201	C	-0.032003	0.275627	7.135449
C	-2.538867	-0.372725	-2.612950	C	1.044009	-0.606810	7.280401
C	-1.294491	-0.076716	-2.056912	C	1.588188	-1.243149	6.162787
H	-2.195807	0.045038	1.234156	H	-0.429849	0.073677	3.759386
H	-4.410642	-0.476111	0.239106	H	-1.389340	1.212867	5.731274
H	-4.634098	-0.763612	-2.231953	H	-0.448833	0.783726	8.008611
H	-2.634132	-0.472572	-3.696871	H	1.467171	-0.796182	8.270420
H	-0.441861	0.080348	-2.716020	H	2.437172	-1.920399	6.283995
P	1.582574	1.042049	2.002362	Mo	1.782049	3.388754	2.934462
C	1.688376	-1.669900	3.684410	C	1.905998	5.306421	3.503019
C	0.922068	-2.311974	2.733420	O	1.974730	6.419218	3.804856
C	1.493503	-2.840407	1.426594	C	-0.244972	3.337302	3.299367
C	0.497440	-2.980954	0.309708	O	-1.370337	3.273336	3.521962
C	-0.829728	-2.994915	0.533765	C	1.454946	3.949893	0.980363
C	-1.336147	-2.832618	1.886493	O	1.267555	4.228737	-0.117839
C	-0.509327	-2.506706	2.916388	C	3.805593	3.298572	2.601956
H	1.931853	-3.847024	1.587033	O	4.939371	3.219391	2.423298
H	0.898485	-3.131943	-0.695812	C	2.093606	2.787598	4.878080
H	-1.537389	-3.129112	-0.287540	O	2.282181	2.498209	5.974555

TS(8e-11e-12):

$E = -2281.28046186946$ au

$ZPE = 0.51326185$ au

$\nu = -833.08$ cm⁻¹

C	-0.340557	0.467323	0.430522	H	2.096455	-1.797120	0.799704
O	0.212477	0.930953	1.604147	H	4.055798	-0.440446	-0.168301
C	0.591804	-0.126349	-0.411770	H	3.777248	-0.925409	-2.568904
C	1.899345	-0.320138	0.231742	H	1.492198	-1.031725	-3.588766
C	3.060668	-0.469707	-0.610221	H	-0.498921	-0.422906	-2.295052
C	2.901835	-0.752705	-1.938747	C	-1.777349	0.655227	0.316524
C	1.588809	-0.800176	-2.525215	C	-2.415420	1.648129	1.093023
C	0.469908	-0.485176	-1.799297	C	-3.794089	1.836000	1.011740

C	-4.569155	1.038651	0.160509	H	0.601824	1.215721	4.237279
C	-3.950691	0.039458	-0.600439	H	0.899907	2.363470	6.403189
C	-2.572528	-0.156967	-0.521128	H	2.542917	1.481061	8.071701
H	-1.812980	2.271332	1.755478	H	3.870416	-0.561312	7.525481
H	-4.269307	2.613023	1.616202	H	3.585802	-1.687347	5.344089
H	-5.649899	1.188105	0.097467	C	0.467493	-1.684965	3.374084
H	-4.549507	-0.604038	-1.250184	C	-0.307793	-2.010538	2.247192
H	-2.115900	-0.971722	-1.083425	C	-1.555757	-2.625218	2.368707
P	1.833950	0.520373	1.848569	C	-2.060249	-2.957785	3.627093
C	1.838586	-0.999707	3.294375	C	-1.296036	-2.666024	4.759903
C	2.939055	-1.780048	2.685604	C	-0.057199	-2.032562	4.634767
C	4.282555	-1.373525	2.796804	H	0.043775	-1.783495	1.247528
C	5.284789	-1.936077	2.006974	H	-2.134250	-2.837238	1.466404
C	4.978560	-2.927818	1.046019	H	-3.036235	-3.439506	3.724436
C	3.672308	-3.319402	0.859963	H	-1.665686	-2.925748	5.755231
C	2.597351	-2.683409	1.592364	H	0.508441	-1.811025	5.538732
H	4.556675	-0.606000	3.519308	Mo	3.233174	2.611382	2.067327
H	6.317599	-1.606451	2.138013	C	4.185478	4.381362	2.022287
H	5.780860	-3.382400	0.459791	O	4.714208	5.406332	1.985124
H	3.419720	-4.089443	0.127306	C	1.620345	3.505064	2.984879
H	1.689743	-3.285874	1.714602	O	0.726267	4.005424	3.504139
C	2.121345	-0.278956	4.601862	C	2.446912	3.005252	0.206499
C	1.352335	0.847973	4.939208	O	2.017515	3.220675	-0.836509
C	1.502842	1.482098	6.171662	C	4.869768	1.722019	1.209854
C	2.419221	0.986250	7.105322	O	5.816850	1.260266	0.748037
C	3.165481	-0.153461	6.796810	C	4.092876	2.221720	3.898631
C	3.014778	-0.782982	5.556705	O	4.652933	2.055705	4.887080

11e (level B): $E = -1549.31452582279$ au
 $ZPE = 0.22567912$ au

C	0.152105	0.166079	0.486418	H	-1.983083	1.105156	1.790699
O	0.395871	0.312328	1.764080	H	-4.376149	0.800556	1.188873
C	1.318815	0.265546	-0.327981	H	-4.995873	-0.529939	-0.829315
C	2.488485	0.462142	0.476656	H	-3.213778	-1.572442	-2.228381
C	3.747865	0.598743	-0.145721	H	-0.832134	-1.285499	-1.626648
C	3.824060	0.576594	-1.528433	P	2.083366	0.512717	2.213735
C	2.662675	0.420752	-2.328871	Mo	2.179962	3.002079	2.969585
C	1.421050	0.267973	-1.745066	C	2.225925	4.919231	3.527283
H	4.649186	0.742513	0.453425	O	2.247657	6.031515	3.842996
H	4.794713	0.698240	-2.015804	C	0.237968	2.819649	3.625494
H	2.754093	0.433340	-3.416997	O	-0.855092	2.714890	3.966947
H	0.530636	0.175065	-2.366273	C	1.468090	3.483279	1.104285
C	-1.243417	-0.038398	0.105163	O	1.060201	3.718566	0.055213
C	-2.257874	0.522801	0.909711	C	4.103489	3.131921	2.262834
C	-3.597526	0.350797	0.568745	O	5.176586	3.205106	1.854024
C	-3.944170	-0.394505	-0.565386	C	2.877670	2.407133	4.811549
C	-2.944788	-0.972998	-1.355692	O	3.263577	2.079244	5.843543
C	-1.600615	-0.797308	-1.027289				

12 (level B): $E = -731.969326563749$ au
 $ZPE = 0.28942785$ au

H	-0.003193	-0.014078	0.004402	H	3.420974	2.617568	-0.310022
C	2.704124	0.004029	-0.037182	C	2.269198	-1.366317	0.340372
C	1.863923	1.088630	-0.026566	C	2.638615	-2.463602	-0.465517
C	0.379761	0.977888	0.292202	C	2.245653	-3.761980	-0.139626
C	-0.472418	2.065489	-0.307022	C	1.488375	-4.000215	1.013893
C	0.058296	3.228408	-0.730404	C	1.133174	-2.926836	1.836458
C	1.498009	3.446116	-0.647845	C	1.517511	-1.625260	1.502128
C	2.345130	2.435298	-0.325079	H	3.235450	-2.286827	-1.363223
H	0.227614	1.022810	1.391225	H	2.533098	-4.593831	-0.788115
H	-1.554201	1.901161	-0.326927	H	1.183204	-5.017480	1.272373
H	-0.578543	4.027462	-1.119837	H	0.556744	-3.102913	2.748534
H	1.895865	4.439196	-0.874179	H	1.252864	-0.802381	2.167718

C	4.125088	0.109872	-0.474847	H	3.687768	1.054334	-2.369617
C	4.475305	0.673498	-1.715923	H	6.058920	1.168564	-3.098136
C	5.809926	0.731991	-2.127315	H	7.866153	0.271558	-1.626441
C	6.822179	0.226283	-1.305461	H	7.272286	-0.747955	0.575134
C	6.488205	-0.346893	-0.072501	H	4.897969	-0.868310	1.292268
C	5.153928	-0.411619	0.333089				

12 (level A): $E = -732.244133942917$ au
 $ZPE = 0.28878824$ au

H	0.015734	-0.016021	0.052953	C	1.556740	-1.621180	1.512079
C	2.701600	0.006654	-0.038978	H	3.162263	-2.268345	-1.394471
C	1.870031	1.083428	-0.017379	H	2.465409	-4.557894	-0.819800
C	0.391703	0.976101	0.306966	H	1.196080	-4.986802	1.268591
C	-0.455618	2.037631	-0.336920	H	0.637330	-3.093887	2.769817
C	0.071539	3.189654	-0.765038	H	1.318705	-0.807241	2.183078
C	1.501377	3.423762	-0.647024	C	4.119034	0.111778	-0.471676
C	2.345442	2.428462	-0.307553	C	4.472429	0.687785	-1.696449
H	0.243844	1.064637	1.394150	C	5.800833	0.745212	-2.102500
H	-1.523563	1.859970	-0.384384	C	6.803963	0.226485	-1.290377
H	-0.555385	3.966029	-1.186599	C	6.466468	-0.356912	-0.071726
H	1.889514	4.410820	-0.866656	C	5.138072	-0.420699	0.327286
H	3.409737	2.616531	-0.276410	H	3.695786	1.078649	-2.340565
C	2.266350	-1.360168	0.334954	H	6.050667	1.188926	-3.058318
C	2.598366	-2.445747	-0.487634	H	7.838696	0.269552	-1.606095
C	2.209128	-3.737200	-0.161351	H	7.239768	-0.765994	0.566649
C	1.495216	-3.978954	1.009845	H	4.881917	-0.885444	1.271159
C	1.177782	-2.915922	1.848387				

13 (level B): $E = -732.014223959441$ au
 $ZPE = 0.29098534$ au

C	-0.080184	-0.170667	0.095640	H	0.927911	-2.505359	-1.041472
C	-0.014187	-0.151157	1.620345	H	3.195266	-2.879444	-1.973034
C	0.931221	-0.896275	2.338508	H	4.858910	-1.017901	-2.016667
C	0.929705	-0.893523	3.738148	H	4.222664	1.225213	-1.116539
C	-0.015539	-0.140164	4.440123	H	1.954563	1.588248	-0.172200
C	-0.961233	0.611044	3.732028	C	-1.163377	-1.111582	-0.421842
C	-0.958510	0.602580	2.335310	C	-1.510457	-2.290837	0.252410
H	1.678702	-1.482544	1.800031	C	-2.473824	-3.158462	-0.273622
H	1.674774	-1.481395	4.280969	C	-3.109414	-2.856151	-1.481574
H	-0.014147	-0.134250	5.533266	C	-2.774000	-1.678915	-2.160278
H	-1.702446	1.207826	4.270433	C	-1.808963	-0.816948	-1.632924
H	-1.703376	1.187199	1.787365	H	-1.025796	-2.532998	1.200367
C	1.282912	-0.433249	-0.539044	H	-2.730288	-4.073439	0.266952
C	1.648488	-1.685256	-1.051306	H	-3.865528	-3.531425	-1.890405
C	2.928698	-1.895516	-1.577954	H	-3.268174	-1.430186	-3.103216
C	3.860629	-0.854556	-1.602658	H	-1.548339	0.099714	-2.169930
C	3.503416	0.401934	-1.097884	H	-0.375441	0.844310	-0.215235
C	2.226443	0.606743	-0.571601				

13 (level A): $E = -732.287794868867$ au
 $ZPE = 0.2900941$ au

C	-0.066219	-0.174519	0.112093	H	1.781802	-1.342115	4.277641
C	-0.003893	-0.172886	1.634581	H	-0.007421	-0.160863	5.522147
C	0.996990	-0.827742	2.347755	H	-1.795043	1.019237	4.268871
C	0.994989	-0.826712	3.740801	H	-1.792438	1.002432	1.804150
C	-0.007635	-0.165436	4.439454	C	1.286054	-0.448645	-0.529521
C	-1.011037	0.496426	3.735127	C	1.665236	-1.716616	-0.964826
C	-1.006530	0.489549	2.346682	C	2.932445	-1.935933	-1.498093
H	1.786604	-1.341872	1.816560	C	3.838237	-0.886952	-1.607271

C	3.465973	0.385781	-1.182696	C	-3.111979	-2.787329	-1.500687
C	2.200602	0.599075	-0.650208	C	-2.747402	-1.621661	-2.169189
H	0.967717	-2.540364	-0.891215	C	-1.778148	-0.784175	-1.630305
H	3.209086	-2.928677	-1.830982	H	-1.073858	-2.507317	1.192478
H	4.822962	-1.056623	-2.024093	H	-2.780735	-4.003713	0.239075
H	4.160223	1.212485	-1.269066	H	-3.868309	-3.440929	-1.916643
H	1.917512	1.591201	-0.317643	H	-3.220364	-1.363694	-3.108650
C	-1.158035	-1.091772	-0.418491	H	-1.496343	0.120670	-2.156495
C	-1.534917	-2.257366	0.246004	H	-0.342854	0.841140	-0.183583
C	-2.502189	-3.101475	-0.291256				