

Supporting Information

“Rearrangement and deoxygenation of 3,3-bis(2-pyridyl)oxaphosphirane complexes”

*Melina Klein, Gregor Schnakenburg, Arturo Espinosa Ferao and Rainer Streubel**

Content:

1) Table S1: Energetics of reactions involved in the proposed mechanistic pathway from 3f	2
2) Table S2: Relative energies for products arising from 3g	2
3) Cartesian coordinates and energies for all computed species.	3

1) Table 1. Energetics of reactions involved in the proposed mechanistic pathway from **3f**.^[a]

	3f	3f^N	3f^{PN} ^[b]	TS(3f→7f)	7f	TS(3f→8f)	8f	8f^{CCrot}
B3LYP-D3	0.00	8.87	14.50	24.66	-9.95	32.99	24.46	25.87
PWPB95-D3	0.00	17.29	24.96	31.63	-11.03	38.69	30.71	32.09
SCS-MP2	0.00	17.60	23.62	37.03	-13.30	44.75	34.40	35.75
LPNO-NCEPA1	0.00	10.14	22.92	36.19	-11.94	41.95	32.16	33.57
DLPNO-CCSD(T)	0.00	10.41	13.43	36.43	-11.95	42.31	32.68	34.21

Table 1. Continued

8f^{COrot}	8f^{CC&COrot}	TS(8f^{CC&COrot}→6f)	6f	TS(8f^{COrot}→9f)	9f	TS(9f→10f)	10f	11f	RMSD ^[c]
23.55	22.45	28.28	-4.85	37.16	8.40	67.51	-0.86	-22.56	1.78
29.90	29.04	32.42	-3.50	43.19	8.22	66.44	0.53	-21.59	1.10
36.06	36.09	32.16	-1.03	49.90	9.66	69.18	4.32	-21.25	0.90
33.48	33.38	36.21	-4.12	48.30	6.37	68.97	1.72	-22.64	0.62
34.14	34.27	35.67	-3.05	48.00	7.70	67.26	2.56	-22.06	0.00

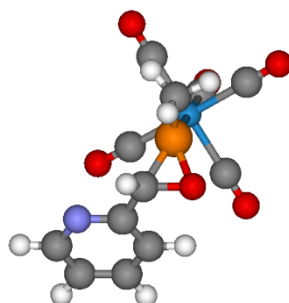
^[a] ZPE-corrected relative energies (to **3f**), in kcal/mol, using the def2-TZVPP basis set, COSMO(THF) solvation and the geometries and zero-point correction at COSMO_{THF}/B3LYP-D3/def2-TZVPecp. ^[b] Most stable van de Waals complex with CO. ^[c] Root mean square deviation of the sixteen data set (removing **3f**) with respect to the reference DLNPO-CCSD(T) level.

2) Table 2. Relative energies for products arising from **3g**.^[a]

	3g	6g	9g	10g	11g	RMSD ^[b]	RMSD ^[c]
B3LYP-D3	0.00	-14.10	3.70	-15.76	-23.90	2.33	1.50
PWPB95-D3	0.00	-12.48	3.63	-13.17	-22.42	1.58	0.94
SCS-MP2	0.00	-8.90	5.27	-8.09	-22.66	0.22	0.72
LPNO-NCEPA1	0.00	-10.03	3.24	-8.56	-23.56	0.44	0.51
DLPNO-CCSD(T)	0.00	-9.13	4.58	-7.95	-23.13	0.00	0.00

^[a] ZPE-corrected relative energies (to **3g**), 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 four data set (removing **3g**), with respect to the reference DLNPO-CCSD(T) level. ^[c] *Idem* for the twenty data set of Table 1 and 2.

3) Cartesian coordinates (Å) and energies (au) for all computed species.

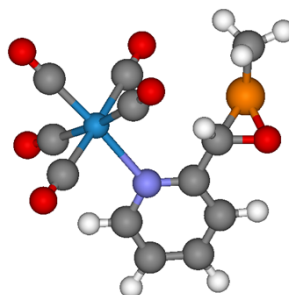


3f:

E = -1374.36527667845 au

ZPE = 0.17966427 au

O	0.003574	0.015325	0.043277	W	2.919919	-0.830594	-2.029224
P	1.670016	0.026349	-0.062718	C	3.981174	-1.537484	-3.617263
C	0.504655	1.386109	-0.000504	O	4.580025	-1.935102	-4.511368
H	0.404177	1.920267	0.939446	C	2.994954	-2.692318	-1.144140
C	0.180924	2.171628	-1.214277	O	3.043630	-3.727653	-0.658068
N	0.628623	3.432676	-1.208411	C	1.143835	-1.349256	-2.952053
C	0.426187	4.171108	-2.299311	O	0.159686	-1.640483	-3.455983
C	-0.226391	3.697546	-3.432679	C	2.869658	1.038197	-2.926703
C	-0.707175	2.395786	-3.420760	O	2.876428	2.059181	-3.439242
C	-0.502954	1.615009	-2.291419	C	4.671178	-0.312957	-1.069076
H	0.803215	5.187443	-2.268756	O	5.641016	-0.031481	-0.529827
H	-0.354814	4.338076	-4.294541	H	3.267776	0.139056	1.718590
H	-1.229972	1.990834	-4.277696	H	1.601241	0.187034	2.358535
H	-0.864818	0.599779	-2.235516	H	2.311316	-1.349724	1.792917
C	2.261368	-0.272654	1.624607				

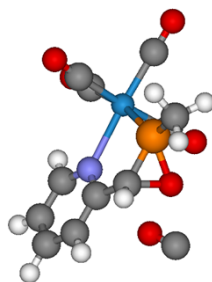


3f^N:

E = -1374.34879277535 au

ZPE = 0.17977585 au

O	0.457910	1.652293	2.551618	W	4.535810	3.364351	0.339302
P	1.420269	0.404304	1.912177	C	6.509789	3.203921	0.519292
C	1.563356	2.216458	1.837750	O	7.657824	3.110433	0.619998
H	2.302153	2.673749	2.483339	C	4.733089	5.420376	0.224469
C	1.227041	2.996747	0.628258	O	4.888576	6.552769	0.166067
N	2.229100	3.605965	-0.044307	C	4.514023	3.519306	2.391431
C	1.893717	4.353180	-1.115361	O	4.617711	3.593427	3.532302
C	0.599479	4.504912	-1.569999	C	4.424589	1.312479	0.443586
C	-0.424103	3.855694	-0.891874	O	4.441983	0.166047	0.488112
C	-0.101727	3.099963	0.220333	C	4.812471	3.182784	-1.700435
H	2.705721	4.844848	-1.629118	O	5.046788	3.068743	-2.815549
H	0.408781	5.118588	-2.438756	H	3.411414	-0.492451	2.944652
H	-1.451909	3.943800	-1.218064	H	2.770049	0.851640	3.929771
H	-0.860319	2.590521	0.794880	H	1.984426	-0.747265	3.954339
C	2.506105	-0.018703	3.329973				



3f^{PN}-CO:

E = -1374.34191277047 au

ZPE = 0.17770519 au

O	1.474910	1.027440	1.825620	W	4.225781	3.031058	1.004718
P	2.674117	1.934812	2.555674	C	5.944372	2.437321	1.786917
C	1.029285	2.415507	2.074586	O	6.943870	2.076468	2.255889
H	0.194655	2.463394	2.763452	C	4.282004	4.666159	2.242123
C	0.929211	3.261803	0.860443	O	4.365279	5.574639	2.942638
N	2.076040	3.613302	0.224822	C	4.284725	1.371820	-0.218015
C	1.969783	4.351701	-0.891318	O	4.373508	0.439304	-0.880864
C	0.758242	4.780727	-1.407638	C	5.206550	4.100263	-0.388798
C	-0.411906	4.435490	-0.749815	O	5.782215	4.716508	-1.179532
C	-0.317078	3.664245	0.399390	H	3.120658	2.301662	4.869706
H	2.892944	4.609548	-1.386486	H	1.729255	1.196300	4.661048
H	0.746979	5.377116	-2.308921	H	3.399537	0.613369	4.411717
H	-1.376304	4.751488	-1.124491	C	0.797147	0.323378	-1.252176
H	-1.202379	3.358834	0.939901	O	1.259551	1.191968	-1.797603
C	2.721665	1.460730	4.299185				

TS(3f-7f):

E = -1374.30520499215 au

ZPE = 0.17764479 au

$\nu = -197.00 \text{ cm}^{-1}$

O	-0.056762	-0.455142	-0.077840	W	2.931525	-1.052714	-2.014835
P	1.440973	-0.108006	-0.203163	C	4.078333	-1.931688	-3.457771
C	1.081067	1.669202	-0.259044	O	4.710532	-2.433617	-4.274513
H	1.252669	2.253142	0.643066	C	2.847748	-2.833761	-0.964230
C	0.439048	2.395123	-1.284456	O	2.817107	-3.812459	-0.372549
N	0.297942	3.731543	-1.044185	C	1.227851	-1.561920	-3.062028
C	-0.233331	4.475525	-1.990898	O	0.279728	-1.831420	-3.644830
C	-0.690729	3.953988	-3.214230	C	3.029213	0.750858	-3.003522
C	-0.582790	2.593315	-3.455544	O	3.081955	1.757096	-3.550340
C	-0.007148	1.799669	-2.480689	C	4.602978	-0.529880	-0.922192
H	-0.321776	5.536856	-1.789121	O	5.524705	-0.241582	-0.306682
H	-1.130817	4.617243	-3.946573	H	3.166504	0.309477	1.461366
H	-0.938796	2.162243	-4.380865	H	1.544083	0.219341	2.203534
H	0.079124	0.733232	-2.609611	H	2.379780	-1.262419	1.687372
C	2.207736	-0.211547	1.452209				

TS(3f-8f):

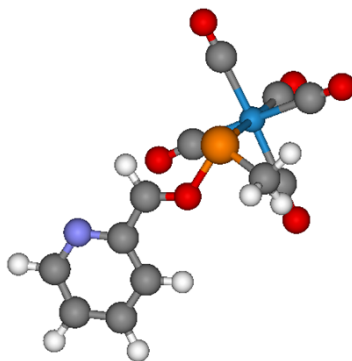
E = -1374.29577407424 au

ZPE = 0.17757991 au

$\nu = -202.88 \text{ cm}^{-1}$

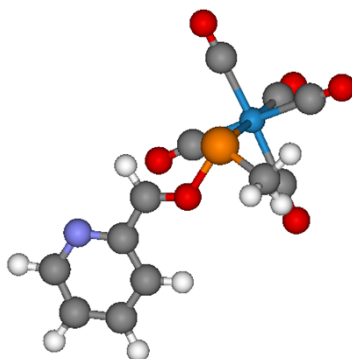
O	0.658977	0.542397	-0.267459	C	-0.847496	4.080408	-3.408714
P	2.379858	0.226280	0.167614	C	-0.798623	2.704431	-3.572960
C	0.625463	1.841019	-0.248120	C	-0.306841	1.931208	-2.532690
H	0.943726	2.384776	0.635553	H	-0.439623	5.714032	-2.057442
C	0.105610	2.578188	-1.361865	H	-1.215036	4.724282	-4.196104
N	0.055390	3.918464	-1.195654	H	-1.129152	2.243400	-4.493749
C	-0.409105	4.640023	-2.201252	H	-0.241359	0.856497	-2.607560

C	2.044456	-0.848634	1.612793	C	3.185944	0.745607	-2.984131
W	3.256896	-1.022928	-1.921577	O	3.149706	1.735010	-3.562288
C	4.015649	-2.019905	-3.500733	C	5.154008	-0.539020	-1.269133
O	4.440118	-2.600685	-4.402044	O	6.207149	-0.269350	-0.906908
C	3.302600	-2.746761	-0.791771	H	2.999829	-1.264933	1.940277
O	3.318781	-3.699585	-0.155502	H	1.615262	-0.276844	2.436564
C	1.341544	-1.483089	-2.515940	H	1.372493	-1.665875	1.342602
O	0.272230	-1.736714	-2.843975				



8f: E = -1374.31222370385 au
ZPE = 0.17868481 au

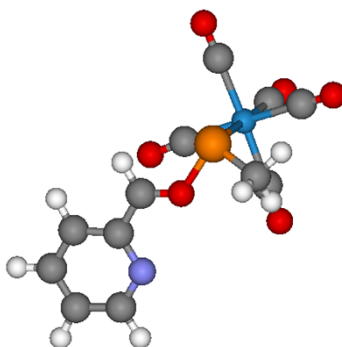
O	1.217338	0.955048	-0.551775	W	3.659241	-1.222534	-1.693669
P	2.476026	-0.049133	0.306512	C	4.637247	-2.165644	-3.190474
C	1.387147	2.139860	-0.923694	O	5.185198	-2.707424	-4.048630
H	2.310361	2.665246	-0.678132	C	3.875759	-2.855529	-0.449807
C	0.382912	2.847493	-1.677946	O	3.974665	-3.752903	0.257019
N	0.709101	4.120654	-1.973019	C	1.835217	-1.944223	-2.312798
C	-0.164325	4.829083	-2.672880	O	0.803131	-2.327239	-2.636788
C	-1.388975	4.314044	-3.108067	C	3.307305	0.478835	-2.776293
C	-1.719447	3.002176	-2.796818	O	3.034471	1.468282	-3.296459
C	-0.816685	2.245610	-2.066514	C	5.416754	-0.417567	-0.974751
H	0.112402	5.851117	-2.904419	O	6.380394	0.046649	-0.562399
H	-2.061503	4.937959	-3.680858	H	1.779981	-1.969350	1.537348
H	-2.659426	2.575754	-3.119671	H	0.571845	-0.691528	1.707644
H	-1.021221	1.217757	-1.802081	H	0.614822	-1.696585	0.232701
C	1.218718	-1.204207	0.994557				



8f: E = -1374.31222370385 au
ZPE = 0.17868481 au

O	1.217338	0.955048	-0.551775	H	2.310361	2.665246	-0.678132
P	2.476026	-0.049133	0.306512	C	0.382912	2.847493	-1.677946
C	1.387147	2.139860	-0.923694	N	0.709101	4.120654	-1.973019

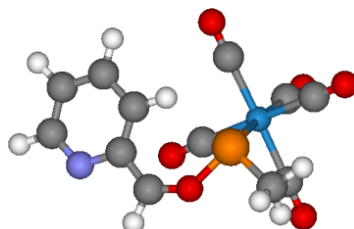
C	-0.164325	4.829083	-2.672880	C	3.875759	-2.855529	-0.449807
C	-1.388975	4.314044	-3.108067	O	3.974665	-3.752903	0.257019
C	-1.719447	3.002176	-2.796818	C	1.835217	-1.944223	-2.312798
C	-0.816685	2.245610	-2.066514	O	0.803131	-2.327239	-2.636788
H	0.112402	5.851117	-2.904419	C	3.307305	0.478835	-2.776293
H	-2.061503	4.937959	-3.680858	O	3.034471	1.468282	-3.296459
H	-2.659426	2.575754	-3.119671	C	5.416754	-0.417567	-0.974751
H	-1.021221	1.217757	-1.802081	O	6.380394	0.046649	-0.562399
C	1.218718	-1.204207	0.994557	H	1.779981	-1.969350	1.537348
W	3.659241	-1.222534	-1.693669	H	0.571845	-0.691528	1.707644
C	4.637247	-2.165644	-3.190474	H	0.614822	-1.696585	0.232701
O	5.185198	-2.707424	-4.048630				



8f^{CCrot}:

E = -1374.3100379266 au
ZPE = 0.17894491 au

O	0.023730	-0.035671	0.035134	W	2.327698	-0.043698	-2.534486
P	1.841150	0.027515	0.024752	C	2.766906	-0.111611	-4.505047
C	-0.721146	0.970293	0.026610	O	3.008726	-0.162319	-5.631959
H	-0.277142	1.963856	0.096444	C	3.937820	-1.246616	-2.063010
C	-2.154964	0.858086	-0.080663	O	4.816050	-1.923404	-1.771116
N	-2.694318	-0.371321	-0.185596	C	1.129855	-1.714197	-2.663339
C	-4.009168	-0.448060	-0.298788	O	0.453794	-2.639137	-2.710033
C	-4.849087	0.674221	-0.315744	C	0.662425	1.118021	-2.779245
C	-4.288440	1.935202	-0.203679	O	-0.303818	1.743704	-2.803964
C	-2.908331	2.034397	-0.083688	C	3.485783	1.644367	-2.289335
H	-4.432054	-1.442736	-0.383822	O	4.119897	2.588912	-2.143583
H	-5.917859	0.543871	-0.417456	H	3.068060	-1.905833	0.703037
H	-4.905864	2.823011	-0.212045	H	1.628613	-1.734217	1.713111
H	-2.419325	2.995670	0.000564	H	1.497380	-2.431920	0.075530
C	1.998188	-1.682614	0.688307				

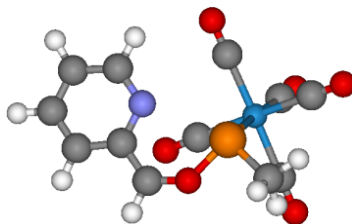


8f^{COrot}:

E = -1374.31031878941 au
ZPE = 0.17910915 au

O	0.146231	-0.074236	0.596894	C	-0.223274	2.309097	0.333770
P	1.849863	-0.407019	0.341513	N	-1.282882	3.153336	0.297877
C	-0.596613	0.950947	0.599030	C	-1.049378	4.427390	0.046303
H	-1.638727	0.762669	0.842927	C	0.235919	4.945501	-0.168217

C	1.320938	4.090456	-0.097863	O	4.923685	-1.967299	-1.540227
C	1.095701	2.742488	0.151843	C	1.201426	-1.903400	-2.459432
H	-1.912223	5.083066	0.014444	O	0.564461	-2.846050	-2.595459
H	0.363742	5.998949	-0.376465	C	0.655007	0.924466	-2.618187
H	2.328201	4.456810	-0.241366	O	-0.291065	1.533622	-2.840260
H	1.920303	2.053375	0.226109	C	3.437766	1.523581	-1.975212
C	1.698100	-2.182224	0.789087	O	4.052954	2.486216	-1.861981
W	2.334437	-0.198194	-2.221904	H	2.689841	-2.619469	0.650330
C	2.800764	-0.234303	-4.179684	H	1.421988	-2.289728	1.838323
O	3.061386	-0.273365	-5.302185	H	0.989686	-2.724944	0.163941
C	3.999933	-1.333822	-1.784365				



8f^{CC&COrot}:

E = -1374.30999553445 au

ZPE = 0.17899084 au

O	0.151850	-0.008765	0.679666	W	2.305487	-0.627823	-2.100380
P	1.862818	-0.285113	0.461173	C	2.718618	-1.023216	-4.025288
C	-0.613554	0.991382	0.528855	O	2.948820	-1.269112	-5.129925
H	-1.642648	0.828663	0.835869	C	3.992258	-1.655412	-1.512173
C	-0.210257	2.278541	0.059971	O	4.927630	-2.234695	-1.186756
N	1.090686	2.449557	-0.247503	C	1.191118	-2.353470	-1.988017
C	1.475753	3.656548	-0.640959	O	0.562299	-3.311218	-1.927463
C	0.598558	4.733685	-0.767135	C	0.595316	0.393734	-2.613113
C	-0.744790	4.553788	-0.451942	O	-0.374992	0.947013	-2.876521
C	-1.161649	3.307039	-0.023122	C	3.389025	1.126636	-2.156965
H	2.525231	3.775473	-0.880843	O	3.993916	2.100251	-2.199442
H	0.967737	5.690193	-1.111226	H	2.806331	-2.355136	1.200047
H	-1.448086	5.370786	-0.539549	H	1.529759	-1.852541	2.316108
H	-2.192879	3.117244	0.243193	H	1.111563	-2.638833	0.772843
C	1.795216	-1.944691	1.261846				

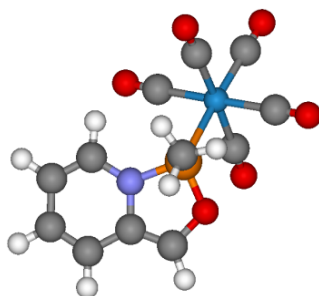
TS(8f^{CC&COrot}-6f):

E = -1374.30669842459 au

ZPE = 0.17793534 au

$\nu = -169.48 \text{ cm}^{-1}$

O	-0.108029	-0.148512	0.414287	W	2.250102	-0.598056	-2.277295
P	1.537748	-0.015394	0.102191	C	2.683694	-1.253166	-4.137961
C	-0.997325	0.821983	0.272160	O	2.920249	-1.644062	-5.195296
H	-1.999610	0.588808	0.597466	C	3.911976	-1.535893	-1.508380
C	-0.504574	2.081136	-0.029648	O	4.833115	-2.057927	-1.068224
N	0.825140	2.059080	-0.336406	C	1.138730	-2.308629	-1.974677
C	1.497937	3.218612	-0.442754	O	0.522528	-3.257115	-1.795604
C	0.866691	4.433873	-0.354192	C	0.566414	0.400177	-2.938644
C	-0.521133	4.474216	-0.069311	O	-0.373541	0.957243	-3.279261
C	-1.208646	3.307997	0.111117	C	3.369031	1.111653	-2.579538
H	2.557070	3.139279	-0.653738	O	3.994016	2.053032	-2.771329
H	1.422505	5.344926	-0.526695	H	3.069243	-1.439832	1.313673
H	-1.024635	5.427228	0.024125	H	1.658743	-1.066191	2.328057
H	-2.253539	3.296215	0.390900	H	1.534166	-2.293497	1.043257
C	1.983071	-1.336677	1.322972				



6f:

E = -1374.36971495548 au
ZPE = 0.17924935 au

O	-0.164951	-0.044184	-0.338865	W	2.581585	-1.339171	-2.120910
P	1.471942	-0.114817	-0.270369	C	3.430244	-2.397275	-3.648553
C	-0.655065	1.212380	0.088227	O	3.906833	-2.990721	-4.506212
H	-1.718225	1.284096	0.223992	C	4.198739	-1.737935	-0.907760
C	0.306384	2.150921	0.157190	O	5.096391	-1.952062	-0.229258
N	1.585258	1.609147	-0.160695	C	1.641288	-3.051272	-1.447469
C	2.714760	2.390229	-0.205573	O	1.124632	-4.002264	-1.076048
C	2.652326	3.713520	0.051617	C	0.932303	-0.879253	-3.286018
C	1.381967	4.302547	0.400232	O	0.017871	-0.614025	-3.917670
C	0.255907	3.556360	0.459115	C	3.522872	0.356532	-2.827095
H	3.634643	1.878601	-0.449319	O	4.050809	1.284180	-3.239771
H	3.547474	4.314486	0.001112	H	2.869693	-0.489667	1.646778
H	1.336975	5.361795	0.617415	H	1.209552	-0.060602	2.140624
H	-0.700321	3.989962	0.718290	H	1.579088	-1.701183	1.536368
C	1.808872	-0.639508	1.437271				

TS(8f^{COrot}-9f):

E = -1374.28744053474 au
ZPE = 0.17832161 au
 $\nu = -92.85 \text{ cm}^{-1}$

O	-0.474461	0.788280	-0.786477	W	1.139064	-0.200160	-3.716260
P	1.155666	0.790745	-1.395758	C	1.046488	-1.040526	-5.565608
C	-0.977711	1.718848	-0.025447	O	0.978471	-1.536030	-6.601859
H	-2.059363	1.714754	0.046353	C	2.253938	1.391964	-4.416102
C	-0.241438	2.803034	0.444648	O	2.871367	2.281736	-4.790847
N	-0.997379	3.924127	0.682631	C	2.871104	-1.224197	-3.277520
C	-0.395750	5.082061	0.681288	O	3.832484	-1.792029	-3.016389
C	0.996614	5.237662	0.432234	C	0.049615	-1.740178	-2.880852
C	1.782221	4.125406	0.302808	O	-0.536545	-2.581862	-2.370729
C	1.186547	2.845627	0.366233	C	-0.585442	0.874640	-4.077797
H	-1.008448	5.956794	0.871672	O	-1.537264	1.483779	-4.265832
H	1.424040	6.231118	0.407783	H	3.005567	-0.305939	-0.352421
H	2.856380	4.212082	0.206539	H	1.794274	0.074256	0.886975
H	1.792713	2.021233	0.688425	H	1.549926	-1.304151	-0.202459
C	1.936199	-0.287106	-0.132073				



9f:

E = -1374.35278864655 au

ZPE = 0.1794402 au

O	-0.114229	0.060847	0.106279	W	1.032624	0.313136	-3.231699
P	1.233887	0.598123	-0.759137	C	0.858107	0.057329	-5.244807
C	-0.911431	1.127282	0.456324	O	0.761946	-0.090058	-6.379212
H	-1.923776	0.879329	0.736911	C	2.697123	1.493913	-3.506342
C	-0.350884	2.341680	0.363532	O	3.630465	2.142293	-3.658253
N	-1.042672	3.531778	0.515647	C	2.243323	-1.350646	-3.124846
C	-0.523585	4.575946	-0.035886	O	2.915302	-2.276715	-3.067887
C	0.698119	4.564654	-0.836043	C	-0.634486	-0.868362	-2.895585
C	1.481557	3.481736	-0.870517	O	-1.557890	-1.510722	-2.693336
C	1.123345	2.301927	-0.023424	C	-0.214879	1.960043	-3.339173
H	-1.060728	5.513670	0.071016	O	-0.926102	2.851252	-3.435192
H	0.951152	5.457342	-1.392818	H	3.526160	0.163146	-0.281562
H	2.400502	3.469554	-1.441464	H	2.531466	-0.029945	1.188680
H	1.755624	2.302723	0.876562	H	2.543350	-1.293723	-0.072080
C	2.585483	-0.221561	0.117472				

TS(9f-10f):

E = -1374.25219527685 au

ZPE = 0.17376621 au

$\nu = -1589.27 \text{ cm}^{-1}$

O	-0.463148	0.243915	-0.308400	W	1.124588	0.119741	-3.481005
P	0.983339	0.661412	-1.050978	C	1.264485	-0.326416	-5.464710
C	-0.829311	1.181830	0.674895	O	1.347209	-0.578942	-6.581319
H	-1.543189	0.836153	1.404562	C	2.782423	1.333958	-3.600742
C	-0.181390	2.333111	0.561715	O	3.698999	2.020327	-3.654356
N	0.061694	3.445072	1.426551	C	2.326888	-1.495268	-3.025323
C	0.072495	4.627601	0.768576	O	2.993568	-2.389468	-2.767735
C	0.348737	4.730424	-0.594447	C	-0.559580	-1.072546	-3.285864
C	0.892534	3.601781	-1.195957	O	-1.491217	-1.722649	-3.164494
C	0.850584	2.389498	-0.482149	C	-0.086347	1.736524	-3.898228
H	0.039826	5.516810	1.389039	O	-0.753487	2.639055	-4.124554
H	0.366758	5.694859	-1.080586	H	3.205626	0.302761	-0.242731
H	1.421415	3.680142	-2.137205	H	2.030813	0.253883	1.097113
H	1.386475	2.973866	0.899894	H	2.196556	-1.139112	-0.006818
C	2.221530	-0.052350	0.068414				



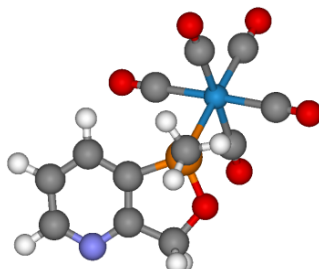
10f:

E = -1374.36150329052 au

ZPE = 0.179974 au

O	-0.213009	0.066974	-0.189169	H	-0.335621	5.538526	1.244083
P	1.045564	0.643225	-1.098782	H	1.257026	5.701019	-0.652021
C	-0.715040	1.044910	0.707215	H	1.966475	3.575667	-1.826041
H	-1.456853	0.689534	1.400957	H	-1.188564	3.489570	1.884390
C	-0.227742	2.280423	0.487879	C	2.513802	0.169447	-0.128093
N	-0.533579	3.484370	1.119359	W	1.038848	0.042718	-3.526140
C	-0.008403	4.668809	0.692606	C	1.035912	-0.412531	-5.510655
C	0.862810	4.744545	-0.346121	O	1.034512	-0.667425	-6.631151
C	1.257828	3.530790	-1.008221	C	2.745170	1.172117	-3.736174
C	0.750359	2.351488	-0.589921	O	3.696512	1.806039	-3.831424

C	2.185450	-1.619019	-3.106516	O	-0.744619	2.654866	-4.069984
O	2.821886	-2.540412	-2.864370	H	3.383970	0.664243	-0.563624
C	-0.675343	-1.075907	-3.209303	H	2.400113	0.475548	0.911885
O	-1.619395	-1.689917	-3.012986	H	2.655069	-0.910030	-0.186935
C	-0.112543	1.719305	-3.881507				

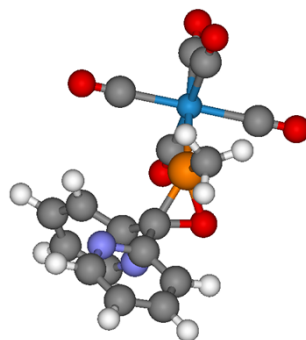


11f:

E = -1374.40164884963 au

ZPE = 0.1808779 au

O	-0.103260	-0.049035	-0.287280	W	2.561087	-1.401925	-2.144882
P	1.538247	-0.133880	-0.246711	C	3.357909	-2.442297	-3.705214
C	-0.666727	1.244063	0.017499	O	3.805767	-3.026560	-4.586701
H	-1.145336	1.212652	0.999795	C	4.198059	-1.841150	-0.974576
C	0.459084	2.241140	-0.006516	O	5.105781	-2.076826	-0.315460
N	0.248890	3.548595	0.103546	C	1.603748	-3.094849	-1.449426
C	1.331521	4.334785	0.070834	O	1.074178	-4.029978	-1.054578
C	2.631344	3.853982	-0.068531	C	0.889318	-0.908811	-3.259898
C	2.836407	2.484657	-0.177182	O	-0.038817	-0.621968	-3.863206
C	1.719502	1.661698	-0.142746	C	3.486917	0.316874	-2.805293
H	1.152708	5.400353	0.157642	O	3.992986	1.277771	-3.169418
H	3.462214	4.545423	-0.093406	H	3.001692	-0.564043	1.609830
H	3.834920	2.081436	-0.285585	H	1.376586	-0.114247	2.180702
H	-1.423236	1.466866	-0.735047	H	1.687609	-1.751359	1.537085
C	1.930628	-0.692952	1.441271				



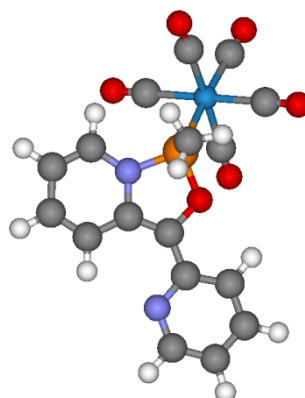
3g:

E = -1621.01443283695 au

ZPE = 0.24806815 au

C	0.028960	-0.000155	-0.018378	H	-3.189190	3.118394	1.252119
O	1.487222	0.014865	0.018422	H	-2.184312	0.833905	1.325379
C	-0.604499	1.362285	-0.029039	C	-0.551543	-0.984871	-0.984384
N	-0.022500	2.279296	-0.802044	C	0.243778	-1.596585	-1.948966
C	-0.563174	3.499019	-0.838952	C	-0.354056	-2.489866	-2.828978
C	-1.698650	3.851244	-0.119674	C	-1.714114	-2.741372	-2.711299
C	-2.304106	2.885923	0.674345	C	-2.422958	-2.080426	-1.713538
C	-1.747510	1.616167	0.722592	N	-1.862142	-1.217443	-0.866131
H	-0.065016	4.226037	-1.470809	H	1.298944	-1.372443	-2.002428
H	-2.092804	4.856463	-0.182409	H	0.235239	-2.979212	-3.593757

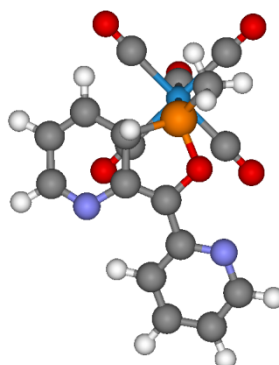
H	-2.219348	-3.431190	-3.373542	O	1.964361	2.305540	6.256969
H	-3.486714	-2.252071	-1.590368	C	1.360579	-1.052794	4.590263
P	0.885169	-0.530213	1.474670	O	1.396485	-2.046964	5.157823
C	1.027526	-2.336349	1.461587	C	-0.736224	0.868114	3.968228
H	0.831602	-2.758585	0.478792	O	-1.854722	0.942506	4.197144
H	2.035341	-2.603736	1.783687	C	1.199120	2.542522	2.559191
H	0.316412	-2.735676	2.186752	O	1.159735	3.558365	2.038852
W	1.287843	0.735629	3.570951	C	3.310806	0.605276	3.159160
C	1.712519	1.739343	5.291500	O	4.429729	0.532863	2.934928



6g:

E = -1621.02951613828 au
ZPE = 0.24860081 au

O	-0.113530	0.114615	-0.306618	H	-4.224422	3.951353	0.391960
P	1.498899	-0.007474	-0.112834	H	-5.820807	2.056192	0.223767
C	-0.604926	1.430369	-0.092568	H	-4.891457	-0.252292	-0.119406
C	0.411297	2.346001	-0.087965	H	-2.431548	-0.542207	-0.266634
N	1.671432	1.722679	-0.225110	C	1.722869	-0.285826	1.667351
C	2.838949	2.433659	-0.293789	H	2.776849	-0.148413	1.916241
C	2.829011	3.785050	-0.229967	H	1.114055	0.409560	2.245678
C	1.575047	4.460996	-0.071220	H	1.440493	-1.312903	1.902370
C	0.406017	3.773443	0.002657	W	2.640582	-1.520045	-1.694517
H	3.743954	1.851701	-0.394580	C	3.492996	-2.849836	-2.996335
H	3.755915	4.334369	-0.294051	O	3.957270	-3.603018	-3.724609
H	1.563390	5.541481	-0.011316	C	4.239289	-1.653496	-0.403065
H	-0.548446	4.261403	0.118468	O	5.113700	-1.711694	0.334513
C	-2.029832	1.565300	-0.011446	C	1.713700	-3.081812	-0.712352
N	-2.537213	2.805307	0.168920	O	1.198752	-3.944396	-0.164449
C	-3.858672	2.939628	0.245899	C	0.984898	-1.309545	-2.921878
C	-4.756108	1.882052	0.151701	O	0.061167	-1.177101	-3.580188
C	-4.234380	0.604628	-0.037510	C	3.559955	0.044447	-2.686909
C	-2.865013	0.435877	-0.120330	O	4.068212	0.907321	-3.239640

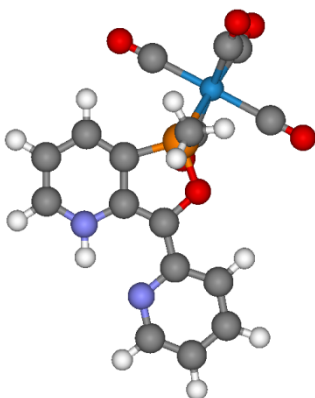


9g:

E = -1621.0073770927 au

ZPE = 0.2483066 au

O	-0.010314	0.018058	0.193323	H	-4.422451	-0.490515	-0.783078
P	1.663752	-0.024162	0.099101	H	-5.437104	1.587900	-1.688764
C	-0.458577	1.321042	0.043010	H	-4.022797	3.656969	-1.793659
C	0.474045	2.256772	0.362556	H	-1.671292	3.535891	-0.982738
N	0.327197	3.617021	0.196629	C	2.070585	-1.223500	1.386801
C	1.402387	4.330024	0.137011	W	2.534947	-0.295337	-2.227452
C	2.754360	3.792959	0.208484	C	3.194386	-0.521153	-4.141925
C	2.952723	2.515698	0.551141	O	3.565622	-0.649645	-5.221063
C	1.779383	1.652706	0.875197	C	4.378867	0.437821	-1.678003
H	1.278637	5.400747	0.004951	O	5.414137	0.832647	-1.382741
H	3.583904	4.458302	0.009385	C	3.173634	-2.194157	-1.749328
H	3.950193	2.111607	0.663086	O	3.530592	-3.246696	-1.470910
H	1.729502	1.498991	1.964068	C	0.674297	-1.034651	-2.763675
C	-1.828295	1.457062	-0.451467	O	-0.353977	-1.435008	-3.059548
N	-2.586172	0.348465	-0.403410	C	1.872906	1.613913	-2.667238
C	-3.840936	0.423666	-0.839816	O	1.507092	2.663055	-2.942929
C	-4.411424	1.586460	-1.345500	H	3.153003	-1.216954	1.527488
C	-3.625164	2.730545	-1.399393	H	1.572023	-0.974276	2.322873
C	-2.315610	2.671937	-0.950810	H	1.771558	-2.219230	1.059754

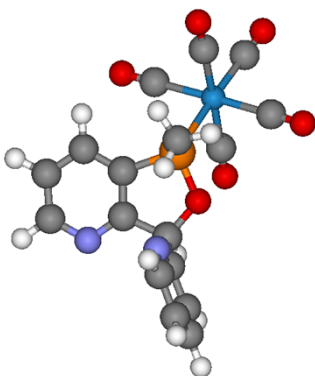


10g:

E = -1621.02860527714 au

ZPE = 0.24957081 au

O	-0.066555	0.214084	0.032573	H	3.700276	0.009850	-4.215966
P	-0.023584	0.136619	1.686781	H	1.826827	0.507608	-5.767107
C	1.211954	0.093504	-0.565827	H	-0.468087	0.828959	-4.799924
C	2.183277	-0.224535	0.343428	H	-0.771465	0.640157	-2.339943
N	3.514941	-0.473351	0.092854	C	-0.010145	1.884521	2.193122
C	4.369396	-0.828302	1.086286	H	0.209354	1.928749	3.261600
C	3.954707	-0.946147	2.379336	H	0.747905	2.438453	1.639198
C	2.585707	-0.684183	2.696727	H	-0.995090	2.318008	2.017201
C	1.730511	-0.322874	1.705214	W	-1.747059	-1.400651	2.640465
H	5.389019	-1.009629	0.778896	C	-3.155619	-2.696561	3.337393
H	4.658086	-1.230251	3.146580	O	-3.948943	-3.429154	3.729566
H	2.250580	-0.770084	3.721808	C	-2.344619	0.029915	3.998273
H	3.800761	-0.397619	-0.880681	O	-2.668502	0.828724	4.753209
C	1.316043	0.224589	-1.980406	C	-3.078021	-0.640365	1.250214
N	2.555222	0.051760	-2.512447	O	-3.810127	-0.214879	0.480497
C	2.695573	0.156723	-3.832692	C	-1.067077	-2.777915	1.256276
C	1.649780	0.434296	-4.703124	O	-0.668030	-3.524775	0.486694
C	0.377090	0.612229	-4.158413	C	-0.394813	-2.127219	4.015288
C	0.200364	0.509497	-2.793195	O	0.355840	-2.532916	4.780544



11g:

E = -1621.0536753407 au
ZPE = 0.25044533 au

O	-0.096308	0.287645	-0.281024	H	-1.136792	1.878878	4.208012
P	1.519754	0.048585	-0.076255	H	-3.577042	2.329797	4.092233
C	-0.556636	1.660914	-0.229752	H	-4.660034	2.491413	1.839736
C	0.679911	2.528648	-0.206214	H	-3.238394	2.174309	-0.188691
N	0.599896	3.852617	-0.258466	C	1.724721	-0.393099	1.674588
C	1.755933	4.524804	-0.226052	H	2.789604	-0.360494	1.913873
C	3.002925	3.909581	-0.141103	H	1.171884	0.307638	2.298897
C	3.070240	2.523374	-0.090365	H	1.363870	-1.410187	1.831677
C	1.874610	1.818799	-0.122866	W	2.496269	-1.518220	-1.770183
H	1.683540	5.605394	-0.271182	C	3.214137	-2.825804	-3.157421
H	3.900867	4.511446	-0.118716	O	3.612850	-3.567405	-3.939224
H	4.024561	2.016841	-0.027805	C	3.843186	-2.220632	-0.378358
H	-1.124238	1.836292	-1.144589	O	4.593275	-2.604192	0.398656
C	-1.453911	1.870443	0.968186	C	1.109882	-2.906731	-1.123642
N	-0.872706	1.792019	2.168983	O	0.343830	-3.671541	-0.750461
C	-1.636067	1.952175	3.247860	C	1.123954	-0.748845	-3.112343
C	-3.003449	2.205431	3.183676	O	0.357836	-0.308034	-3.839027
C	-3.600108	2.293913	1.934828	C	3.865205	-0.097594	-2.369905
C	-2.810656	2.119801	0.803551	O	4.624954	0.694098	-2.699514