

Supporting Information

Computational studies of ring cleavage and deoxygenation reactions of a $\sigma^3\lambda^3$ -oxaphosphirane

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Table of contents

1	Calculated structures	2
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1 Calculated structures

Cartesian coordinates (in Å) and energies (in hartrees) for all computed species. Geometries, zero-point energy correction (ZPE) and Gibbs energy correction (G_{corr}) at the optimization level CPCM(toluene)/PBEh-3c, whereas electronic energies are computed at the CPCM(toluene)/PWPB95-D3/def2-QZVPP level. When explicitly stated, geometries and energy calculations were obtained in the gas phase at the DLPNO-CCSD(T)/def2-QZVPP//RIJCOSX-B3LYP-D4/def2-TZVP level.

1

$E = -1043.114580992$ au

ZPE = 0.25673615 au

$G_{\text{corr}} = 0.18486309$ au

C	1.174117	0.841707	0.132367	H	-2.542972	-0.721693	-1.291305
O	0.818456	2.060333	-0.480999	H	-1.871569	-1.396476	-2.770269
H	1.799392	0.191511	-0.477155	H	-1.074949	-1.700176	-1.228108
P	-0.561319	1.071509	-0.344781	C	1.556836	0.896951	1.561720
C	-0.756256	0.305682	-2.037948	C	2.120503	-0.233708	2.148041
C	-1.545755	1.328223	-2.862963	C	1.348222	2.046869	2.316213
H	-1.801237	0.903125	-3.836639	C	2.454005	-0.192121	3.485497
H	-2.480385	1.616378	-2.377044	H	2.296589	-1.133340	1.572147
H	-0.966342	2.235703	-3.040465	C	1.703395	2.031626	3.650620
C	0.536584	-0.053039	-2.757890	H	0.927666	2.940791	1.876584
H	1.072585	-0.862012	-2.260273	C	2.257996	0.928741	4.270329
H	0.308538	-0.394695	-3.770616	H	2.529806	0.942917	5.316972
H	1.207350	0.802374	-2.847018	F	1.507690	3.134767	4.380022
C	-1.608241	-0.946296	-1.810420	F	2.993307	-1.277304	4.050805

(1→2)[‡]

$E = -1043.064315723$ au

ZPE = 0.22197952 au

$G_{\text{corr}} = 0.18151520$ au

$\nu = -290.94$ cm⁻¹

C	1.423877	0.763830	0.024519	H	-2.242988	0.361820	-0.553235
O	1.535230	2.336785	-1.625049	H	-2.170207	-0.967297	-1.704272
H	2.216515	0.297811	-0.554552	H	-1.017301	-0.896814	-0.374005
P	0.271852	1.766694	-0.932163	C	1.621050	0.822315	1.432056
C	-0.613144	0.502323	-1.998351	C	2.678116	0.084990	1.995358
C	-1.407431	1.316963	-3.021047	C	0.713961	1.496867	2.268068
H	-1.954623	0.647747	-3.689488	C	2.772335	0.001426	3.364994
H	-2.134467	1.974841	-2.541008	H	3.396161	-0.420807	1.363602
H	-0.753558	1.935111	-3.639447	C	0.861636	1.381687	3.629726
C	0.367280	-0.415517	-2.720140	H	-0.069387	2.112608	1.845105
H	0.882382	-1.083036	-2.028121	C	1.879964	0.641295	4.208321
H	-0.165447	-1.039445	-3.442909	H	1.984788	0.580149	5.283590
H	1.120357	0.153007	-3.267280	F	0.006202	2.011086	4.434841
C	-1.559700	-0.290181	-1.101682	F	3.760560	-0.707911	3.909995

2

$E = -1043.128031120$ au

ZPE = 0.22413863 au

$G_{\text{corr}} = 0.18294892$ au

C	2.215855	1.304410	-0.249226	H	-0.426321	-0.294285	0.357571
O	2.020127	1.452818	-2.998960	H	-1.333705	-1.276763	-0.780029
H	3.235587	1.657390	-0.370187	H	0.406364	-1.502119	-0.621333
P	1.442855	1.078311	-1.680562	C	1.738521	1.099599	1.121421
C	-0.209048	0.262313	-1.753707	C	2.470334	0.282765	1.985752
C	-1.301547	1.336917	-1.699775	C	0.594198	1.741318	1.595092
H	-2.273680	0.860141	-1.841479	C	2.030121	0.112175	3.281622
H	-1.326094	1.854445	-0.741592	H	3.362572	-0.223866	1.643046
H	-1.180379	2.081131	-2.487657	C	0.192365	1.528063	2.899347
C	-0.269637	-0.458244	-3.106351	H	0.041439	2.423714	0.963982
H	0.492129	-1.233370	-3.193904	C	0.887112	0.715960	3.773056
H	-1.245179	-0.940042	-3.193704	H	0.560520	0.567798	4.793329
H	-0.155149	0.225716	-3.944808	F	-0.908859	2.144267	3.341280
C	-0.387102	-0.754621	-0.626563	F	2.730613	-0.677593	4.101764

(2→3^t+4)^{MECP}

$E = -1043.083233395$ au

ZPE = 0.22180517 au

$G_{\text{corr}} = 0.18154788$ au

$\nu = -24.30$ cm⁻¹

C	2.279778	0.586080	-0.115212	H	-1.084425	-1.113163	-0.301238
O	2.018074	-1.412831	-2.026570	H	-2.152454	-0.829189	-1.662909
H	3.308452	0.878253	-0.301925	H	-0.764685	-1.902899	-1.841165
P	1.533544	-0.050338	-1.602074	C	1.817646	0.785277	1.212646
C	-0.286180	0.221189	-1.859605	C	2.606942	1.567726	2.084661
C	-0.732371	1.526630	-1.207764	C	0.632238	0.214684	1.714853
H	-1.760939	1.740871	-1.505656	C	2.189441	1.771353	3.377755
H	-0.710081	1.487968	-0.119881	H	3.529099	2.014028	1.736923
H	-0.117781	2.370170	-1.526626	C	0.267983	0.449361	3.019332
C	-0.436167	0.335284	-3.384511	H	0.026184	-0.436808	1.103963
H	-0.069520	-0.555050	-3.896204	C	1.018522	1.229494	3.883993
H	-1.493222	0.450801	-3.633374	H	0.710421	1.399040	4.906608
H	0.097374	1.199486	-3.782067	F	-0.855291	-0.104484	3.484567
C	-1.107274	-0.976771	-1.381107	F	2.938705	2.522184	4.190012

3^t

$E = -468.644867621$ au

ZPE = 0.08824909 au

$G_{\text{corr}} = 0.05582365$ au

C	2.488629	1.182725	-0.025730	H	3.693235	-0.106707	1.994944
H	2.133559	1.659842	-0.924546	C	0.273172	1.403928	2.905180
C	1.990744	1.027936	1.265490	H	0.144122	2.121253	0.897978
C	2.731406	0.321383	2.241403	C	0.982451	0.714984	3.877774
C	0.733823	1.575900	1.622116	H	0.595940	0.594670	4.880450
C	2.210274	0.187489	3.505297	F	-0.913251	1.921325	3.241179

F 2.911356 -0.480844 4.427016

4

$E = -574.343123030$ au

ZPE = 0.12846002 au

$G_{\text{corr}} = 0.09681500$ au

O -0.157384 0.767885 0.319808
P 0.042838 -0.132078 1.490513
C 1.832246 -0.093178 2.002773
C 1.833519 0.356580 3.469460
H 1.192411 -0.268386 4.096219
H 2.846105 0.288488 3.874357
H 1.503723 1.391299 3.580153
C 2.318992 -1.545236 1.912094

H 3.333128 -1.619116 2.312085
H 1.693321 -2.230126 2.489949
H 2.344809 -1.904134 0.881469
C 2.680844 0.828416 1.141733
H 2.674605 0.525365 0.094612
H 2.333063 1.860577 1.187244
H 3.718024 0.812273 1.485702

(1→5)[‡]

$E = -1043.057392633$ au

ZPE = 0.22294622 au

$G_{\text{corr}} = 0.18262245$ au

$\nu = -101.27$ cm⁻¹

C 1.205681 0.063303 0.708757
O 0.291747 0.695190 0.031730
H 1.596147 -0.875216 0.326885
P -0.884631 -0.460241 -0.495887
C -1.026712 0.069421 -2.275914
C -1.371635 1.555213 -2.385637
H -1.504064 1.832824 -3.435555
H -2.297201 1.792980 -1.859618
H -0.581786 2.189060 -1.980808
C 0.256420 -0.230792 -3.052401
H 0.517716 -1.289154 -3.004285
H 0.133167 0.033967 -4.107076
H 1.103396 0.341771 -2.670816
C -2.176989 -0.775219 -2.832480

H -3.115170 -0.583005 -2.307524
H -2.337136 -0.539640 -3.887220
H -1.967910 -1.845317 -2.765198
C 1.702433 0.605940 1.930651
C 2.755884 -0.056523 2.579368
C 1.171893 1.786832 2.471775
C 3.257810 0.481255 3.741163
H 3.169183 -0.971863 2.176183
C 1.724704 2.278078 3.632406
H 0.345044 2.300227 2.001091
C 2.766829 1.651662 4.294926
H 3.175869 2.056346 5.210772
F 1.233626 3.403587 4.156255
F 4.259698 -0.142337 4.365884

5

$E = -1043.068632144$ au

ZPE = 0.22358050 au

$G_{\text{corr}} = 0.18264077$ au

C 0.783656 -0.796915 1.246391
O 0.220850 -0.467753 0.152134
H 0.686310 -1.817635 1.609460
P -0.718270 -1.277477 -0.978445
C -0.981869 0.156848 -2.143752
C -1.738035 1.306228 -1.476697
H -1.950175 2.093823 -2.205832
H -2.689432 0.973270 -1.059423
H -1.160415 1.757868 -0.668874
C 0.333260 0.664970 -2.735386

H 0.886604 -0.133776 -3.231305
H 0.138366 1.446402 -3.475859
H 0.982938 1.095223 -1.971846
C -1.845528 -0.446401 -3.257853
H -2.799783 -0.819270 -2.879235
H -2.066854 0.314772 -4.009345
H -1.340294 -1.270660 -3.766107
C 1.534016 0.166411 1.986528
C 2.134563 -0.243763 3.186364
C 1.683897 1.492853 1.551006

C	2.861898	0.671255	3.913261
H	2.031770	-1.261324	3.540319
C	2.423292	2.357447	2.323491
H	1.233933	1.840808	0.631236

C	3.028957	1.984621	3.512529
H	3.604643	2.687460	4.098918
F	2.569724	3.620968	1.914331
F	3.433443	0.279897	5.055801

(1→6+7^t)^{MECP}

$E = -1043.038008857$ au

ZPE = 0.22268625 au

$G_{\text{corr}} = 0.18234735$ au

$\nu = -207.55$ cm⁻¹

C	1.278542	1.107526	0.049851
O	0.957348	2.240471	-0.502015
H	1.921206	0.422616	-0.530720
P	-0.540878	0.330485	-0.123648
C	-0.779288	0.101490	-1.960454
C	-1.411906	1.359086	-2.564076
H	-1.662065	1.172590	-3.612101
H	-2.333536	1.637771	-2.050752
H	-0.732306	2.208312	-2.524128
C	0.505538	-0.255188	-2.702947
H	0.995721	-1.133500	-2.279136
H	0.269723	-0.484872	-3.745100
H	1.215482	0.571584	-2.705500
C	-1.774559	-1.064896	-2.058094

H	-2.704397	-0.858803	-1.523996
H	-2.031779	-1.235539	-3.106264
H	-1.359106	-1.993775	-1.663911
C	1.608674	1.076075	1.512711
C	2.214879	-0.055590	2.047314
C	1.299441	2.163196	2.320039
C	2.501030	-0.076176	3.396906
H	2.461581	-0.906414	1.424118
C	1.609308	2.089062	3.663137
H	0.833715	3.049041	1.910035
C	2.210354	0.983448	4.235227
H	2.444953	0.950193	5.290533
F	1.320454	3.128974	4.451253
F	3.085883	-1.158820	3.919145

6

$E = -543.998517645$ au

ZPE = 0.09662622 au

$G_{\text{corr}} = 0.06377042$ au

C	1.300919	0.956746	0.128208
O	0.732170	1.852412	-0.439108
H	1.621265	0.046548	-0.410221
C	1.630460	0.963763	1.569584
C	2.290701	-0.136904	2.102612
C	1.283357	2.051941	2.365394
C	2.597943	-0.129438	3.449158

H	2.560205	-0.982664	1.482255
C	1.613733	2.007351	3.701752
H	0.769668	2.907402	1.947377
C	2.271140	0.929770	4.272297
H	2.519031	0.919247	5.325451
F	1.293083	3.036707	4.487908
F	3.231666	-1.177871	3.978250

7^t

$E = -499.041625277$ au

ZPE = 0.12480568 au

$G_{\text{corr}} = 0.09416989$ au

P	-0.623851	1.065791	1.206318
C	-0.105038	-0.258153	-0.001231
C	1.390730	-0.534272	0.173192
H	1.712390	-1.309549	-0.528221
H	1.991944	0.355608	-0.019807
H	1.623347	-0.883216	1.180515
C	-0.906653	-1.531916	0.279748

H	-1.979431	-1.368904	0.165071
H	-0.614862	-2.319751	-0.420730
H	-0.731201	-1.906300	1.289518
C	-0.382770	0.229127	-1.425820
H	0.173359	1.138622	-1.658467
H	-0.083242	-0.535827	-2.148062
H	-1.442523	0.435377	-1.583810

8a

$E = -461.022267902$ au

ZPE = 0.11607989 au

$G_{\text{corr}} = 0.08693548$ au

C	1.300919	0.956746	0.128208
O	0.732170	1.852412	-0.439108
H	1.621265	0.046548	-0.410221
C	1.630460	0.963763	1.569584
C	2.290701	-0.136904	2.102612
C	1.283357	2.051941	2.365394
C	2.597943	-0.129438	3.449158

H	2.560205	-0.982664	1.482255
C	1.613733	2.007351	3.701752
H	0.769668	2.907402	1.947377
C	2.271140	0.929770	4.272297
H	2.519031	0.919247	5.325451
F	1.293083	3.036707	4.487908
F	3.231666	-1.177871	3.978250

8a

$E = -460.482970215$ au (DLPNO-CCSD(T)/def2-QZVPP)

$H_{\text{corr}} = 0.11973385$ au (RIJCOSX-B3LYP-D4/def2-TZVP)

P	0.339400	-0.367942	1.455611
C	1.512684	0.863568	0.725292
H	1.707911	1.655704	1.450286
H	2.463135	0.374989	0.503704
H	1.124892	1.313522	-0.192922
C	0.005527	-1.393717	-0.048691
H	-0.799374	-2.099930	0.162479

H	-0.276783	-0.785240	-0.912434
H	0.896212	-1.971672	-0.301343
C	-1.202291	0.656573	1.468519
H	-1.113614	1.440140	2.223058
H	-1.400656	1.121586	0.498783
H	-2.054134	0.030223	1.739231

8b

$E = -686.732341649$ au

ZPE = 0.13207335 au

$G_{\text{corr}} = 0.09699264$ au

P	-2.012496	-1.582695	2.153619
O	-3.175141	-2.456487	1.397194
O	-2.850564	-1.316951	3.550084
O	-2.187212	-0.191037	1.337237
C	-2.134172	-0.815828	4.664592
H	-2.056290	0.273240	4.634425
H	-2.673405	-1.097575	5.567753
H	-1.122111	-1.227785	4.728240

C	-3.320459	-3.818321	1.758176
H	-3.868672	-4.317629	0.961215
H	-2.355265	-4.321385	1.875310
H	-3.880449	-3.929025	2.688912
C	-3.446053	0.426778	1.088350
H	-3.983378	-0.080915	0.287090
H	-4.077528	0.446832	1.977676
H	-3.246446	1.451589	0.781296

8c

$E = -744.941349766$ au

ZPE = 0.25673615 au

$G_{\text{corr}} = 0.21797186$ au

P	-2.345139	-1.121286	1.906503
N	-3.384969	-2.156990	1.041593
N	-3.213821	0.193715	2.552564
N	-2.214551	-2.069423	3.366447
C	-3.345137	-2.080625	-0.398745
H	-3.448545	-3.076205	-0.841472
H	-4.142679	-1.452517	-0.815223
H	-2.391463	-1.668375	-0.728659
C	-4.607808	-2.717687	1.564866

H	-5.487998	-2.109046	1.323404
H	-4.775872	-3.715913	1.148736
H	-4.548109	-2.817479	2.646693
C	-4.402425	0.075892	3.362878
H	-4.405311	-0.871546	3.897842
H	-4.434984	0.877151	4.107762
H	-5.324039	0.139927	2.771314
C	-3.084267	1.465327	1.883224
H	-3.913952	1.672091	1.195575

H	-3.050541	2.283124	2.609877
H	-2.159721	1.495843	1.306554
C	-1.667138	-3.398250	3.161302
H	-1.753330	-3.971218	4.087087
H	-2.216430	-3.931421	2.388922

H	-0.604985	-3.392815	2.876437
C	-1.519439	-1.395334	4.448030
H	-0.447174	-1.249060	4.252594
H	-1.958046	-0.420096	4.645817
H	-1.606371	-1.990570	5.359568

8c

$E = -744.079261772$ au (DLPNO-CCSD(T)/def2-QZVPP)
 $H_{\text{corr}} = 0.26385146$ au (RIJCOSX-B3LYP-D4/def2-TZVP)

P	-1.864908	-1.290888	-0.788254
N	-1.924233	-0.270280	-2.201239
C	-2.954169	0.762568	-2.164458
H	-2.723935	1.566501	-1.447635
H	-3.043470	1.215945	-3.155250
H	-3.915941	0.334466	-1.893512
C	-0.640176	0.299320	-2.595815
H	-0.287382	1.075327	-1.898265
H	0.120935	-0.474808	-2.651757
H	-0.739830	0.759536	-3.582439
N	-0.758743	-2.440098	-1.384043
C	-0.832819	-3.077389	-2.685240
H	-1.382555	-2.445401	-3.379244
H	0.174328	-3.232055	-3.089304

H	-1.324559	-4.058800	-2.637881
C	0.040474	-3.165485	-0.416098
H	0.048187	-2.628402	0.532700
H	-0.344122	-4.179037	-0.232593
H	1.075239	-3.262749	-0.765052
N	-3.451789	-1.900352	-0.879148
C	-4.078002	-2.330034	0.355702
H	-3.552403	-1.895699	1.206491
H	-5.123604	-2.002167	0.393068
H	-4.069253	-3.423481	0.469823
C	-4.082661	-2.424165	-2.075847
H	-4.021683	-3.519815	-2.129636
H	-5.144206	-2.151304	-2.095574
H	-3.609333	-2.004993	-2.960991

9a

$E = -536.307667240$ au
 $ZPE = 0.12055391$ au
 $G_{\text{corr}} = 0.09014405$ au

O	1.029999	1.053809	-1.267726
P	1.313755	2.512457	-1.079633
C	-0.014164	3.599913	-1.671207
H	-0.179429	3.429264	-2.734815
H	-0.938371	3.369619	-1.141611
H	0.224234	4.652152	-1.518391
C	2.803170	3.087632	-1.943775

H	3.669920	2.530938	-1.588040
H	2.698079	2.907284	-3.013408
H	2.980157	4.150877	-1.783770
C	1.569049	2.992489	0.652508
H	0.679854	2.749616	1.233906
H	2.409211	2.435046	1.066104
H	1.772713	4.058259	0.752805

9a

$E = -535.689460055$ au (DLPNO-CCSD(T)/def2-QZVPP)
 $H_{\text{corr}} = 0.12527931$ au (RIJCOSX-B3LYP-D4/def2-TZVP)

O	-0.535299	0.932895	-1.508657
P	-1.491213	0.412218	-2.516170
C	-0.876453	-1.030926	-3.433878
H	-1.599811	-1.385976	-4.169773
H	0.049961	-0.758973	-3.941121
H	-0.658353	-1.832624	-2.727258
C	-1.936846	1.622718	-3.796184

H	-2.638516	1.210525	-4.523194
H	-2.384628	2.494348	-3.317262
H	-1.030053	1.942125	-4.311196
C	-3.078979	-0.127440	-1.815416
H	-3.757042	-0.503109	-2.583612
H	-2.893924	-0.913899	-1.082761
H	-3.545557	0.715428	-1.304152

9b

$E = -762.030277664$ au

ZPE = 0.13782029 au

G_{corr} = 0.10173255 au

O -0.705365 -2.061201 2.269904
P -2.092928 -1.587058 2.162968
O -3.138270 -2.504048 1.385615
O -2.851077 -1.374825 3.559887
O -2.202665 -0.210927 1.375058
C -2.140217 -0.832340 4.671979
H -1.785917 0.179115 4.466703
H -2.837618 -0.795896 5.505007
H -1.289921 -1.457464 4.942725

C -3.286749 -3.879179 1.737743
H -3.935232 -4.329644 0.990995
H -2.326942 -4.396001 1.732992
H -3.748429 -3.985916 2.719879
C -3.445519 0.441827 1.126537
H -4.031571 -0.099555 0.384281
H -4.035195 0.552225 2.037378
H -3.210523 1.430083 0.739646

9c

E = -820.242345602 au

ZPE = 0.26251204 au

G_{corr} = 0.22247675 au

N -3.347453 -2.162711 1.049589
N -3.175459 0.185426 2.561720
N -2.113027 -2.061133 3.341789
C -3.329922 -2.057768 -0.394627
H -3.487932 -3.044511 -0.837115
H -4.115109 -1.394230 -0.775052
H -2.370084 -1.684301 -0.738958
C -4.574546 -2.718277 1.575826
H -5.448320 -2.094226 1.355986
H -4.753390 -3.701905 1.134079
H -4.514113 -2.850782 2.653841
C -4.364207 0.063399 3.376136
H -4.358834 -0.866782 3.940036
H -4.403533 0.884021 4.097085
H -5.286025 0.099721 2.784423

C -3.079476 1.448844 1.860567
H -3.906342 1.600439 1.157162
H -3.102275 2.271316 2.579891
H -2.145893 1.510432 1.309267
C -1.658286 -3.433079 3.191490
H -1.925861 -4.003908 4.082895
H -2.126950 -3.908097 2.333913
H -0.572232 -3.497896 3.065042
C -1.500291 -1.411160 4.488041
H -0.407466 -1.391093 4.417319
H -1.850769 -0.387662 4.590205
H -1.766759 -1.952560 5.397931
P -2.361603 -1.150379 1.954515
O -1.181189 -0.722271 1.154799

9c

E = -819.304598933 au (DLPNO-CCSD(T)/def2-QZVPP)

H_{corr} = 0.27075042 au (RIJCOSX-B3LYP-D4/def2-TZVP)

O -1.490062 -0.873052 0.096942
P -1.882982 -1.445268 -1.206529
N -1.960606 -0.448832 -2.548278
C -3.032355 0.540648 -2.617913
H -2.763509 1.465752 -2.093970
H -3.232167 0.786366 -3.664548
H -3.941275 0.147174 -2.171417
C -0.712733 0.056134 -3.114294
H -0.377391 0.967890 -2.605477
H 0.071856 -0.690465 -3.029157
H -0.862497 0.290418 -4.171850
N -0.772425 -2.594327 -1.694682
C -0.888021 -3.334766 -2.937173
H -1.458871 -2.767186 -3.668449

H 0.108064 -3.516686 -3.353851
H -1.372190 -4.310221 -2.797453
C 0.082489 -3.223383 -0.698782
H 0.133293 -2.593730 0.185051
H -0.290161 -4.214836 -0.408963
H 1.091652 -3.349603 -1.104582
N -3.441008 -2.043581 -1.130331
C -4.008244 -2.380416 0.167121
H -3.466982 -1.852626 0.947301
H -5.061104 -2.081363 0.199272
H -3.958480 -3.459113 0.366521
C -4.112933 -2.664815 -2.256190
H -4.028323 -3.759314 -2.239353
H -5.178881 -2.415235 -2.235034

H -3.701786 -2.300663 -3.194862

1-8a^(o)

$E = -1504.14327329712$ au

ZPE = 0.34160604 au

$G_{\text{corr}} = 0.29155060$ au

C 0.762984 -0.729537 0.977877
H 1.103118 -1.681686 0.568685
P -0.496737 0.204110 0.056183
C -0.734706 -0.810970 -1.507232
C -1.716341 -0.030687 -2.387291
H -1.953067 -0.608709 -3.283841
H -2.657009 0.167795 -1.868711
H -1.298919 0.927121 -2.697328
C 0.560177 -1.062327 -2.268387
H 1.289409 -1.627424 -1.686632
H 0.345658 -1.643916 -3.168859
H 1.029730 -0.128955 -2.579154
C -1.388958 -2.130963 -1.087072
H -2.277004 -1.971562 -0.470372
H -1.708391 -2.686077 -1.972636
H -0.705314 -2.768711 -0.525831
C 0.842096 -0.638899 2.451634
C 0.675253 -1.798781 3.205403
C 1.060412 0.579537 3.087313
C 0.719215 -1.711418 4.580874
H 0.512435 -2.756638 2.727764

C 1.096935 0.607185 4.467204
H 1.206390 1.490856 2.524087
C 0.929146 -0.519382 5.248651
H 0.964580 -0.472150 6.328430
F 1.309018 1.776547 5.080747
F 0.557029 -2.824600 5.304344
P 0.624984 2.962929 -1.608292
O 1.179436 0.402138 0.241204
C 0.179363 4.390462 -2.691090
H 0.093625 4.058452 -3.725942
H -0.788969 4.793002 -2.393236
H 0.918050 5.193017 -2.644121
C 2.359717 2.667593 -2.160260
H 2.820378 1.921096 -1.514232
H 2.363750 2.275646 -3.177704
H 2.963253 3.576950 -2.136086
C 0.935166 3.849001 -0.021594
H -0.007276 4.199038 0.399456
H 1.384843 3.161893 0.694150
H 1.600686 4.704746 -0.149251

1-8a^(c)

$E = -1504.14702495122$ au

ZPE = 0.34202034 au

$G_{\text{corr}} = 0.29322646$ au

P -1.270515 -0.370571 -0.038401
C -1.280322 -0.688115 -1.883390
C -2.449220 0.140211 -2.429285
H -2.589584 -0.072157 -3.492081
H -3.389361 -0.091644 -1.923799
H -2.267695 1.210956 -2.326634
C 0.001353 -0.322744 -2.619373
H 0.840627 -0.946693 -2.309655
H -0.136236 -0.473341 -3.693312
H 0.274017 0.723354 -2.472505
C -1.583819 -2.178226 -2.055640
H -2.495749 -2.474939 -1.531994
H -1.728312 -2.407010 -3.114279
H -0.770708 -2.801958 -1.682482
C 0.823884 0.141541 1.786230
C 1.857941 -0.742624 2.088574
C 0.211479 0.875077 2.796701

C 2.249155 -0.880523 3.403071
H 2.343746 -1.317579 1.310975
C 0.648892 0.700077 4.094855
H -0.585388 1.572876 2.578902
C 1.662926 -0.174063 4.437158
H 1.987411 -0.293744 5.461884
F 0.067663 1.406269 5.070635
F 3.232277 -1.740525 3.697967
O -0.614203 1.207278 0.081528
P -0.415602 -3.349527 1.406816
C 0.371799 0.243095 0.382321
H 1.168319 0.156395 -0.355025
C -1.714108 -4.568030 0.917682
H -2.610294 -4.038401 0.593192
H -1.364655 -5.167696 0.076909
H -1.985090 -5.238679 1.735329
C 0.827323 -4.494679 2.152676

H	1.287982	-5.101556	1.372993
H	1.619144	-3.920400	2.633914
H	0.384102	-5.161287	2.894941
C	-1.185218	-2.673677	2.940101

H	-0.467802	-2.049457	3.472366
H	-2.034985	-2.043904	2.677546
H	-1.524994	-3.464169	3.611895

(1+8a→9a+10^E)[‡]

$E = -1504.093607517$ au

ZPE = 0.33924491 au

$G_{\text{corr}} = 0.29023614$ au

$\nu = -523.82$ cm⁻¹

C	0.423178	-0.843722	0.774605
H	0.907065	-1.696912	0.313381
P	-0.681447	0.159895	-0.167514
C	-1.070720	-0.865711	-1.682506
C	-1.672086	0.101853	-2.705923
H	-1.991569	-0.441678	-3.598803
H	-2.543354	0.625560	-2.307331
H	-0.945926	0.855202	-3.019378
C	0.128515	-1.573374	-2.300594
H	0.546088	-2.337796	-1.644621
H	-0.174638	-2.077656	-3.222087
H	0.924783	-0.872948	-2.552174
C	-2.131112	-1.879278	-1.247212
H	-2.991328	-1.395724	-0.777934
H	-2.502199	-2.432341	-2.113721
H	-1.730276	-2.605652	-0.538125
C	0.778233	-0.569759	2.139313
C	1.788008	-1.330592	2.753369
C	0.152718	0.440449	2.891502
C	2.137064	-1.070549	4.059046
H	2.292970	-2.115839	2.205994

C	0.548638	0.657654	4.190704
H	-0.646697	1.034582	2.467321
C	1.541288	-0.077486	4.815960
H	1.831258	0.111094	5.840275
F	-0.055983	1.623539	4.895251
F	3.100685	-1.806323	4.628420
P	1.016356	2.688390	-1.140621
O	0.846275	0.760946	-0.421290
C	0.696967	3.969168	-2.441432
H	1.047878	3.606657	-3.406973
H	-0.373958	4.153169	-2.518876
H	1.201261	4.912249	-2.215192
C	2.840523	2.697678	-1.061491
H	3.173948	2.110459	-0.207822
H	3.255181	2.250113	-1.964360
H	3.229569	3.712211	-0.967472
C	0.520050	3.574617	0.378140
H	-0.557760	3.734213	0.382078
H	0.778781	2.976156	1.250864
H	1.015921	4.543208	0.456079

10^E

$E = -967.877901761$ au

ZPE = 0.21973792 au

$G_{\text{corr}} = 0.17963941$ au

C	0.034874	-0.813024	0.886851
H	0.256116	-1.840117	0.608022
P	-0.695615	0.216038	-0.207823
C	-0.926351	-0.847701	-1.742425
C	-1.599834	0.056492	-2.778760
H	-1.767506	-0.495297	-3.706691
H	-2.568567	0.420279	-2.431120
H	-0.985652	0.926590	-3.018247
C	0.423523	-1.322092	-2.280907
H	0.930306	-1.992366	-1.585913
H	0.278739	-1.867201	-3.217682
H	1.095461	-0.487050	-2.485934
C	-1.832092	-2.042505	-1.443809

H	-2.796678	-1.730366	-1.040110
H	-2.024315	-2.601584	-2.363655
H	-1.380940	-2.731554	-0.729110
C	0.430500	-0.471200	2.248300
C	1.031205	-1.456994	3.035976
C	0.230713	0.803835	2.791523
C	1.413444	-1.154524	4.327617
H	1.198696	-2.451540	2.643594
C	0.630714	1.051070	4.084143
H	-0.230910	1.593585	2.212643
C	1.228186	0.093080	4.886763
H	1.533749	0.313510	5.900475
F	0.437999	2.270034	4.598378

F 1.987007 -2.107378 5.069659

(1→11a^{ery})[‡]

$E = -1504.110621222$ au

ZPE = 0.34017433 au

$G_{\text{corr}} = 0.29196073$ au

$\nu = -505.44$ cm⁻¹

P	-1.102749	0.204254	-0.026801	C	2.073725	0.038279	4.379779
C	-1.519921	-0.563771	-1.691778	H	2.528257	0.237047	5.340873
C	-2.004990	0.622993	-2.531522	F	-0.002180	0.776659	5.149502
H	-2.345478	0.279282	-3.511717	F	4.106741	-0.711681	3.510107
H	-2.841388	1.143318	-2.058126	O	0.248671	1.028892	-0.228568
H	-1.207675	1.350205	-2.692452	P	-0.367165	-3.063228	1.393552
C	-0.346674	-1.234077	-2.392624	C	0.284372	-0.783448	0.579832
H	-0.046694	-2.159244	-1.895282	H	0.948439	-1.199184	-0.165641
H	-0.612581	-1.495292	-3.420683	C	-0.565035	-4.549648	0.335753
H	0.520358	-0.572540	-2.435431	H	-1.249657	-4.342434	-0.485601
C	-2.669211	-1.547502	-1.492140	H	0.398489	-4.823053	-0.092995
H	-3.512842	-1.087916	-0.972211	H	-0.949571	-5.397437	0.904753
H	-3.035449	-1.914082	-2.454817	C	0.666523	-3.690352	2.769353
H	-2.361560	-2.420737	-0.912898	H	1.671961	-3.908504	2.411364
C	0.895766	-0.465859	1.887088	H	0.744649	-2.932027	3.547921
C	2.250718	-0.722397	2.085788	H	0.242266	-4.596536	3.204401
C	0.127985	0.047872	2.931161	C	-2.007917	-2.885670	2.184887
C	2.806775	-0.463893	3.321553	H	-1.967719	-2.095105	2.933557
H	2.862699	-1.115142	1.284497	H	-2.756456	-2.606078	1.444730
C	0.733775	0.287088	4.147021	H	-2.320735	-3.810631	2.671053
H	-0.922341	0.270792	2.792069				

11a^{ery}

$E = -1504.182913368$ au

ZPE = 0.34259198 au

$G_{\text{corr}} = 0.29502754$ au

P	-2.021861	-1.026526	0.237687	C	0.765660	-0.473009	2.153924
C	-1.212312	-0.170668	-1.250367	C	3.150463	-1.298790	1.041195
C	-2.394820	0.552134	-1.908731	H	2.014111	-2.734336	-0.059105
H	-2.061944	1.100777	-2.794603	C	1.964936	0.117892	2.494698
H	-3.173468	-0.146622	-2.223190	H	-0.171123	-0.076640	2.522397
H	-2.851018	1.271549	-1.225918	C	3.180128	-0.269173	1.961668
C	-0.158428	0.863176	-0.872632	H	4.105415	0.213316	2.245675
H	0.774891	0.404797	-0.547898	F	1.958135	1.121801	3.379112
H	0.074672	1.503395	-1.729428	F	4.306454	-1.704125	0.501291
H	-0.513912	1.502585	-0.063760	O	-2.159528	0.017726	1.362093
C	-0.655340	-1.202013	-2.225158	P	-1.140987	-3.231806	2.104514
H	-1.365207	-2.015684	-2.402272	C	-0.498751	-2.171208	0.802210
H	-0.440810	-0.744058	-3.195128	H	-0.317002	-2.857627	-0.032125
H	0.278636	-1.641543	-1.868540	C	0.141834	-4.346937	2.715180
C	0.772290	-1.513324	1.222406	H	0.523608	-4.958169	1.898715
C	1.982995	-1.931361	0.666383	H	0.964510	-3.769614	3.134290

H	-0.263870	-4.998317	3.488425
C	-1.775099	-2.309953	3.514345
H	-0.951540	-1.842955	4.051681
H	-2.445436	-1.528146	3.160259
H	-2.295560	-2.990687	4.186618

C	-2.472016	-4.243856	1.432788
H	-3.259985	-3.594391	1.055640
H	-2.094266	-4.848011	0.609064
H	-2.868273	-4.900386	2.205906

(11a^{ery}→12a^{ery})[‡]

$E = -1504.174182490$ au

ZPE = 0.34299528 au

$G_{\text{corr}} = 0.29627187$ au

$\nu = -95.88$ cm⁻¹

O	-0.104518	-0.772998	-0.423828
P	-0.064783	-0.211883	1.046397
C	1.840066	-0.063347	1.083375
P	2.190226	-0.092323	-0.719561
C	-0.285227	-1.683890	2.208758
C	0.206777	-1.283204	3.596364
H	-0.242736	-0.343235	3.926228
H	-0.050939	-2.046839	4.335789
H	1.291516	-1.155910	3.629090
C	-1.795564	-1.932295	2.250878
H	-2.032627	-2.763423	2.921171
H	-2.337213	-1.053763	2.607904
H	-2.185355	-2.183026	1.262184
C	0.410971	-2.947094	1.719847
H	0.111630	-3.189473	0.699589
H	1.500376	-2.859998	1.738887
H	0.156089	-3.799870	2.355876
H	2.301195	-0.990282	1.442152
C	2.447998	1.096825	1.800952
C	3.594762	0.920727	2.573293
C	4.146232	2.007704	3.221640

C	3.611405	3.278271	3.135948
C	2.470494	3.419805	2.369505
C	1.874482	2.364336	1.708855
H	4.053803	-0.054871	2.669455
F	5.246537	1.828791	3.960443
H	4.056467	4.118256	3.651794
F	1.918997	4.633749	2.273574
H	0.951494	2.518407	1.165410
C	3.951164	0.407512	-0.794949
H	4.301790	0.369848	-1.826530
H	4.087807	1.421297	-0.421432
H	4.567200	-0.263374	-0.196438
C	1.391433	1.171897	-1.741925
H	1.015480	1.973682	-1.108548
H	2.116966	1.593662	-2.435813
H	0.552390	0.741961	-2.277453
C	2.236486	-1.733541	-1.487123
H	3.130794	-1.831834	-2.100877
H	2.255975	-2.493303	-0.708104
H	1.345053	-1.889488	-2.084539

12a^{ery}

$E = -1504.173710380$ au

ZPE = 0.34405062 au

$G_{\text{corr}} = 0.29740026$ au

O	-0.005628	-0.106060	0.273279
P	0.190300	0.035851	1.878437
C	2.020226	-0.322905	1.551463
P	1.817678	-0.478011	-0.302624
C	-0.619924	-1.479377	2.643938
C	-0.070369	-1.668609	4.057168
H	-0.048055	-0.727817	4.613469
H	-0.704788	-2.360648	4.617514
H	0.939422	-2.078226	4.057454
C	-2.097176	-1.069910	2.735969
H	-2.679329	-1.870742	3.200048
H	-2.233614	-0.169189	3.337363

H	-2.526494	-0.880313	1.749785
C	-0.528568	-2.767420	1.839776
H	-0.908563	-2.631649	0.827228
H	0.489583	-3.147761	1.779988
H	-1.130785	-3.548589	2.312719
H	2.499721	0.661484	1.630850
C	2.843322	-1.270764	2.354180
C	2.987158	-2.618226	2.032135
C	3.710546	-3.442448	2.870773
C	4.306697	-2.995395	4.032934
C	4.157361	-1.652831	4.323154
C	3.452997	-0.787040	3.512730

H	2.551013	-3.039034	1.137106
F	3.840819	-4.732795	2.544541
H	4.866935	-3.659010	4.677291
F	4.726593	-1.176398	5.434924
H	3.365610	0.256018	3.788298
C	3.634345	-0.790498	-0.666191
H	3.807104	-0.784560	-1.743921
H	4.256158	-0.009674	-0.223606
H	3.984999	-1.747396	-0.281134

C	1.710915	1.091885	-1.233209
H	1.743675	1.923759	-0.529377
H	2.533494	1.199177	-1.936365
H	0.761708	1.146746	-1.759808
C	1.170436	-1.922327	-1.212244
H	1.875368	-2.240464	-1.977852
H	1.005700	-2.753505	-0.529240
H	0.212532	-1.674585	-1.661891

12a^{ery-eq}

$E = -1504.160783617$ au

ZPE = 0.34418321 au

$G_{\text{corr}} = 0.29753074$ au

O	-0.027142	-0.234598	0.387732
P	0.016742	-0.249670	2.081626
C	1.841861	-0.294207	1.842173
P	1.544372	-0.499628	-0.194982
C	-0.762511	-1.906657	2.481066
C	-0.446846	-2.218162	3.945101
H	-0.705032	-1.380344	4.597188
H	-1.031140	-3.079407	4.278407
H	0.604774	-2.450130	4.110206
C	-2.269053	-1.631415	2.352673
H	-2.833272	-2.526734	2.626698
H	-2.593312	-0.821616	3.008093
H	-2.548338	-1.367026	1.330914
C	-0.420588	-3.074620	1.565489
H	-0.654966	-2.850801	0.523982
H	0.624197	-3.372836	1.616010
H	-1.011166	-3.950157	1.847857
H	2.054552	0.780040	1.901122
C	2.905575	-0.953488	2.631436
C	2.944351	-2.325172	2.897286
C	3.999570	-2.860351	3.604983

C	5.056229	-2.104440	4.075154
C	5.005038	-0.752800	3.797981
C	3.968124	-0.170077	3.098978
H	2.166914	-2.985401	2.547328
F	4.006883	-4.177642	3.845137
H	5.874090	-2.545584	4.628022
F	6.005390	0.023525	4.231731
H	3.980709	0.898263	2.924425
C	2.450948	-2.082474	-0.394509
H	2.832193	-2.149407	-1.412807
H	3.276983	-2.168317	0.305946
H	1.776966	-2.923959	-0.239912
C	2.731962	0.853876	-0.544138
H	3.610099	0.767639	0.094234
H	3.037089	0.849519	-1.589506
H	2.249812	1.809797	-0.333995
C	0.779156	-0.534722	-1.910668
H	1.552204	-0.662103	-2.669447
H	0.071347	-1.359215	-2.007782
H	0.244356	0.391244	-2.124183

(12a^{ery-eq}→9a+10^z)[‡]

$E = -1504.156601973$ au

ZPE = 0.34305029 au

$G_{\text{corr}} = 0.29651851$ au

$\nu = -182.24$ cm⁻¹

O	0.046350	-0.515152	0.253959
P	0.033136	-0.272645	1.982259
C	1.816162	-0.231692	2.070836
P	1.537182	-0.507912	-0.371881
C	-0.807435	-1.870417	2.490099
C	-0.580139	-2.038056	3.994010
H	-0.870130	-1.138489	4.542121
H	-1.193040	-2.859053	4.374141

H	0.456538	-2.254212	4.247745
C	-2.302021	-1.598714	2.255829
H	-2.890124	-2.463328	2.575015
H	-2.650816	-0.732517	2.819571
H	-2.523641	-1.422320	1.201568
C	-0.439785	-3.125647	1.705006
H	-0.674849	-3.015860	0.646164
H	0.609258	-3.401805	1.780424

H	-1.018776	-3.974374	2.078524
H	2.043370	0.832441	2.160496
C	2.869829	-0.981646	2.726290
C	2.834147	-2.344337	3.065469
C	3.939767	-2.956015	3.615329
C	5.132547	-2.306187	3.866207
C	5.154652	-0.963347	3.532428
C	4.079400	-0.301468	2.988066
H	1.952015	-2.940142	2.903082
F	3.855329	-4.260105	3.921788
H	5.985204	-2.808844	4.300147
F	6.284777	-0.275815	3.757633
H	4.166969	0.754891	2.766445

C	2.644541	-1.939639	-0.259753
H	2.917173	-2.278402	-1.259096
H	3.539743	-1.690032	0.302849
H	2.144558	-2.758196	0.255099
C	2.464560	1.049795	-0.491192
H	3.337964	1.024922	0.154928
H	2.771770	1.227285	-1.522403
H	1.823612	1.872193	-0.175496
C	0.945679	-0.678754	-2.103368
H	1.791604	-0.686828	-2.790944
H	0.391391	-1.608450	-2.230717
H	0.290653	0.149617	-2.371626

13a

$E = -929.782842843$ au

ZPE = 0.20968654 au

$G_{\text{corr}} = 0.17009287$ au

C	0.000000	0.000000	0.000000
P	0.000000	0.000000	1.746701
H	1.032826	0.000000	-0.343765
C	-0.865011	-0.928865	-0.724324
C	-0.314459	-1.813881	-1.661205
C	-1.138104	-2.667426	-2.362760
C	-2.508215	-2.713593	-2.182921
C	-3.028613	-1.827747	-1.258764
C	-2.254637	-0.938376	-0.543549
H	0.754042	-1.838010	-1.832127
F	-0.588100	-3.505169	-3.252071
H	-3.136530	-3.394337	-2.740216
F	-4.354132	-1.822849	-1.064661

H	-2.737137	-0.222769	0.107521
C	0.300112	-1.641400	2.465505
H	0.297795	-1.600174	3.554589
H	-0.478973	-2.328473	2.136199
H	1.261582	-2.021532	2.123531
C	-1.527398	0.571353	2.525720
H	-2.351524	-0.101351	2.297297
H	-1.385929	0.584639	3.606321
H	-1.761462	1.577130	2.184293
C	1.329308	1.080905	2.302126
H	1.399777	1.062290	3.388573
H	2.276339	0.749199	1.879027
H	1.115065	2.094325	1.965126

12a^{thr}

$E = -1504.181222394$ au

ZPE = 0.34352329 au

$G_{\text{corr}} = 0.29642118$ au

O	0.108076	-0.591742	-0.336405
P	-0.020742	-0.151728	1.223569
C	1.844223	-0.000483	1.231614
P	1.981236	-0.148481	-0.636802
C	-0.297029	-1.737992	2.191994
C	0.095683	-1.443139	3.638992
H	-0.412174	-0.555812	4.024568
H	-0.174300	-2.281250	4.286684
H	1.170555	-1.281006	3.748253
C	-1.800751	-2.016184	2.112214
H	-2.058123	-2.900966	2.700692
H	-2.386879	-1.179767	2.497898
H	-2.119682	-2.200056	1.084305

C	0.462907	-2.944119	1.656859
H	0.211091	-3.144105	0.615330
H	1.546364	-2.825522	1.727102
H	0.208682	-3.836443	2.235581
H	2.321403	-0.910161	1.612227
C	2.487700	1.186877	1.863626
C	3.667402	1.038442	2.589712
C	4.260588	2.151304	3.151767
C	3.732730	3.421224	3.027587
C	2.556952	3.535706	2.310359
C	1.922492	2.454783	1.733200
H	4.123805	0.064696	2.712163
F	5.393656	1.997881	3.845458

H	4.209565	4.281705	3.476906
F	2.011550	4.749231	2.178235
H	0.983432	2.597825	1.214380
C	3.809023	0.267311	-0.723128
H	4.159865	0.207962	-1.754915
H	4.014550	1.273970	-0.358763
H	4.402049	-0.429575	-0.127344
C	1.398152	1.209889	-1.704385

H	0.988097	2.008086	-1.086163
H	2.210111	1.621016	-2.299965
H	0.600420	0.853660	-2.350929
C	2.132077	-1.773230	-1.458284
H	2.986470	-1.790547	-2.131796
H	2.282563	-2.537438	-0.695758
H	1.221303	-2.014360	-1.998404

(12a^{thr}→12a^{thr-eq})[‡]

$E = -1504.173193069$ au

ZPE = 0.34350630 au

$G_{\text{corr}} = 0.29762389$ au

$\nu = -62.54$ cm⁻¹

O	-0.250868	-0.323456	-0.528614
P	-0.419281	0.189922	1.058373
C	1.412069	0.175809	1.111639
P	1.454014	-0.301274	-0.855254
C	-0.885358	-1.395115	1.943306
C	-0.627474	-1.145597	3.429660
H	-1.141719	-0.250539	3.787340
H	-0.989733	-1.988880	4.022678
H	0.435979	-1.025614	3.646718
C	-2.384355	-1.595871	1.704620
H	-2.739834	-2.477228	2.244782
H	-2.966670	-0.739195	2.048819
H	-2.606201	-1.747034	0.646579
C	-0.130121	-2.630376	1.465385
H	-0.297204	-2.823121	0.405096
H	0.946100	-2.561959	1.635123
H	-0.476562	-3.510871	2.012732
C	2.153513	1.386898	1.543174
C	3.425390	1.256472	2.104983
C	4.134528	2.386412	2.460784
C	3.640022	3.664354	2.294069

C	2.373594	3.765421	1.747721
C	1.625395	2.669944	1.373824
H	3.858055	0.278570	2.274028
F	5.352381	2.239830	2.996276
H	4.207228	4.538297	2.583604
F	1.855271	4.987540	1.578216
H	0.633297	2.814428	0.965350
C	3.117052	-1.119418	-0.632651
H	3.622116	-1.264820	-1.587604
H	3.755035	-0.527122	0.021829
H	2.979582	-2.100390	-0.173381
C	1.873338	1.294150	-1.624619
H	2.626484	1.830068	-1.052620
H	2.257257	1.117278	-2.628470
H	0.985016	1.919448	-1.703250
C	1.044686	-1.336165	-2.359225
H	1.899743	-1.380316	-3.033454
H	0.802666	-2.356993	-2.058599
H	0.189337	-0.935122	-2.900387
H	1.801768	-0.690374	1.652305

12a^{thr-eq}

$E = -1504.173776738$ au

ZPE = 0.34367892 au

$G_{\text{corr}} = 0.29707313$ au

O	-0.175208	-0.467377	-0.536433
P	-0.367680	0.131590	1.045844
C	1.443076	0.194118	1.129184
P	1.450720	-0.342019	-0.926192
C	-0.838440	-1.419830	1.980725
C	-0.676219	-1.073844	3.461963
H	-1.243779	-0.182018	3.737464
H	-1.040021	-1.896558	4.082266
H	0.368243	-0.898222	3.727174

C	-2.313838	-1.685060	1.668723
H	-2.674508	-2.540337	2.246010
H	-2.940887	-0.827762	1.920079
H	-2.467475	-1.913109	0.612483
C	-0.017732	-2.655342	1.630078
H	-0.092723	-2.908120	0.571660
H	1.037542	-2.543281	1.883648
H	-0.386581	-3.515521	2.194801
C	2.132993	1.427133	1.553297

C	3.449427	1.348211	2.021287
C	4.131403	2.502376	2.346806
C	3.572571	3.761113	2.241086
C	2.266421	3.811480	1.789498
C	1.540796	2.690591	1.448690
H	3.937745	0.388421	2.134929
F	5.391636	2.402123	2.789407
H	4.120699	4.654676	2.505912
F	1.683204	5.012286	1.681433
H	0.517232	2.798178	1.112685
C	2.864311	-1.479138	-0.612717
H	3.342167	-1.783906	-1.542985

H	3.593991	-1.000823	0.038190
H	2.497175	-2.374777	-0.110323
C	2.090306	1.262486	-1.512947
H	2.923286	1.605218	-0.904540
H	2.408336	1.183712	-2.551007
H	1.300274	2.011461	-1.454259
C	1.025618	-1.067514	-2.600053
H	1.908485	-1.082388	-3.240368
H	0.664613	-2.092434	-2.500939
H	0.250962	-0.485996	-3.099972
H	1.867395	-0.661804	1.658295

(12a^{thr}→11a^{thr})[‡]

$E = -1504.182009216$ au
 $ZPE = 0.34270660$ au
 $G_{\text{corr}} = 0.29527658$ au
 $\nu = -90.86$ cm⁻¹

O	-0.104518	-0.772998	-0.423828
P	-0.064783	-0.211883	1.046397
C	1.840066	-0.063347	1.083375
P	2.190226	-0.092323	-0.719561
C	-0.285227	-1.683890	2.208758
C	0.206777	-1.283204	3.596364
H	-0.242736	-0.343235	3.926228
H	-0.050939	-2.046839	4.335789
H	1.291516	-1.155910	3.629090
C	-1.795564	-1.932295	2.250878
H	-2.032627	-2.763423	2.921171
H	-2.337213	-1.053763	2.607904
H	-2.185355	-2.183026	1.262184
C	0.410971	-2.947094	1.719847
H	0.111630	-3.189473	0.699589
H	1.500376	-2.859998	1.738887
H	0.156089	-3.799870	2.355876
H	2.301195	-0.990282	1.442152
C	2.447998	1.096825	1.800952
C	3.594762	0.920727	2.573293
C	4.146232	2.007704	3.221640

C	3.611405	3.278271	3.135948
C	2.470494	3.419805	2.369505
C	1.874482	2.364336	1.708855
H	4.053803	-0.054871	2.669455
F	5.246537	1.828791	3.960443
H	4.056467	4.118256	3.651794
F	1.918997	4.633749	2.273574
H	0.951494	2.518407	1.165410
C	3.951164	0.407512	-0.794949
H	4.301790	0.369848	-1.826530
H	4.087807	1.421297	-0.421432
H	4.567200	-0.263374	-0.196438
C	1.391433	1.171897	-1.741925
H	1.015480	1.973682	-1.108548
H	2.116966	1.593662	-2.435813
H	0.552390	0.741961	-2.277453
C	2.236486	-1.733541	-1.487123
H	3.130794	-1.831834	-2.100877
H	2.255975	-2.493303	-0.708104
H	1.345053	-1.889488	-2.084539

11a^{thr}

$E = -1504.186351326$ au
 $ZPE = 0.34262257$ au
 $G_{\text{corr}} = 0.29506335$ au

O	-0.379699	-0.953816	-0.457043
P	-0.109496	-0.273067	0.908114
C	1.861479	-0.138174	0.936057
P	2.397585	-0.038728	-0.784447
C	-0.267473	-1.630814	2.220061

C	0.326926	-1.157580	3.542086
H	-0.040558	-0.165305	3.815988
H	0.061182	-1.841173	4.354002
H	1.417183	-1.104982	3.513219
C	-1.778875	-1.820223	2.382488

H	-1.993655	-2.595600	3.123614
H	-2.264933	-0.900491	2.716071
H	-2.245409	-2.119792	1.442274
C	0.351266	-2.949506	1.774794
H	-0.030311	-3.248568	0.798012
H	1.441026	-2.898302	1.705392
H	0.120041	-3.748396	2.485868
H	2.303048	-1.076807	1.288092
C	2.389264	1.002195	1.745576
C	3.472731	0.810649	2.602451
C	3.953357	1.878312	3.332978
C	3.412123	3.146764	3.247722
C	2.338364	3.304391	2.393308
C	1.811361	2.267658	1.648332
H	3.934559	-0.163247	2.703073
F	4.991652	1.683597	4.153473

H	3.802999	3.971804	3.827549
F	1.783076	4.516376	2.291232
H	0.932877	2.429143	1.037640
C	4.128189	0.490331	-0.839010
H	4.480777	0.490804	-1.870142
H	4.232417	1.494213	-0.430613
H	4.747446	-0.188960	-0.255065
C	1.482655	1.162648	-1.768002
H	1.543068	2.146675	-1.305687
H	1.926240	1.217864	-2.761710
H	0.445381	0.846664	-1.837064
C	2.326275	-1.663538	-1.553088
H	2.665403	-1.600384	-2.586234
H	2.971446	-2.350977	-1.007441
H	1.294102	-2.004195	-1.505684

(12a^{thr-eq}→9a+10²)[‡]

$E = -1504.172372280$ au

ZPE = 0.34285187 au

$G_{\text{corr}} = 0.29661256$ au

$\nu = -149.58$ cm⁻¹

O	0.397977	-0.786921	-0.193423
P	0.184218	-0.212236	1.438859
C	1.910193	0.135822	1.623468
P	1.863256	-0.404775	-0.767719
C	-0.118143	-1.851184	2.289400
C	-0.106774	-1.531187	3.785874
H	-0.820996	-0.744876	4.040697
H	-0.380097	-2.419337	4.360879
H	0.879206	-1.206628	4.122639
C	-1.512215	-2.328294	1.874621
H	-1.775078	-3.241813	2.414585
H	-2.276783	-1.581509	2.096257
H	-1.562625	-2.551637	0.807739
C	0.904417	-2.937532	1.978445
H	0.921220	-3.189864	0.917310
H	1.913659	-2.657760	2.284021
H	0.650120	-3.851143	2.522411
H	2.522214	-0.670358	2.025334
C	2.392824	1.446191	2.018892
C	3.726737	1.590631	2.441154
C	4.226286	2.838734	2.741683

C	3.477363	3.997642	2.657079
C	2.164496	3.832604	2.250380
C	1.611473	2.612919	1.934949
H	4.366636	0.722086	2.536715
F	5.504547	2.939581	3.138095
H	3.886806	4.967678	2.901171
F	1.393918	4.927732	2.160404
H	0.572362	2.561496	1.634688
C	3.369034	-1.363401	-0.410651
H	3.854303	-1.662333	-1.340513
H	4.053808	-0.774786	0.194255
H	3.105110	-2.262500	0.143908
C	2.246424	1.330268	-1.123220
H	3.058247	1.687277	-0.495656
H	2.513538	1.444613	-2.173566
H	1.370599	1.945861	-0.920780
C	1.493164	-1.033069	-2.456492
H	2.348220	-0.873715	-3.113606
H	1.273320	-2.100421	-2.432779
H	0.632108	-0.516393	-2.879275

(1+8b→9b+10^F)[‡]

$E = -1729.799395226$ au

ZPE = 0.35526107 au

$G_{\text{corr}} = 0.30152195$ au

$\nu = -493.65$ cm⁻¹

C	-0.021249	-1.686031	0.817675
H	0.413129	-2.540543	0.311236
P	-1.189675	-0.665971	-0.025854
C	-1.684404	-1.661797	-1.526494
C	-2.282549	-0.657093	-2.515606
H	-2.670559	-1.178459	-3.394075
H	-3.106154	-0.091771	-2.074777
H	-1.533261	0.058871	-2.860931
C	-0.551916	-2.424733	-2.202805
H	-0.154324	-3.223964	-1.576563
H	-0.920773	-2.894916	-3.118067
H	0.272835	-1.767404	-2.478385
C	-2.772037	-2.626476	-1.047519
H	-3.594046	-2.104613	-0.552171
H	-3.194872	-3.166372	-1.898168
H	-2.378976	-3.367878	-0.349488
C	0.443196	-1.438736	2.153940
C	1.431539	-2.277211	2.695192
C	-0.059639	-0.390832	2.943323
C	1.877762	-2.057893	3.979166
H	1.842242	-3.090967	2.112001
C	0.429701	-0.217092	4.215679

H	-0.817224	0.281087	2.562601
C	1.400560	-1.032456	4.774110
H	1.766077	-0.874289	5.779391
F	-0.051064	0.785928	4.960877
F	2.816696	-2.867272	4.484228
P	0.544948	1.779584	-0.883861
O	0.315729	-0.048100	-0.429017
O	0.457788	3.192599	-1.765823
O	0.173399	2.289874	0.603061
O	2.163073	1.733625	-0.805476
C	0.595862	3.546497	1.117532
H	1.664377	3.710839	0.976377
H	0.048698	4.374841	0.665120
H	0.384669	3.532034	2.184733
C	-0.810688	3.595394	-2.247514
H	-0.654304	4.268082	-3.089310
H	-1.411177	2.747694	-2.593509
H	-1.384585	4.125004	-1.482820
C	2.892155	1.190530	-1.895151
H	2.837934	1.832848	-2.776345
H	3.931701	1.115792	-1.583432
H	2.539405	0.191749	-2.163080

(1→11b^{ery})[‡]

$E = -1729.813710065$ au

ZPE = 0.35665716 au

$G_{\text{corr}} = 0.30418131$ au

$\nu = -518.77$ cm⁻¹

C	0.955869	-0.354605	-0.101831
H	0.848521	-1.429979	-0.178322
P	1.207413	0.540557	-1.681020
C	0.204598	-0.424350	-2.948844
C	1.031181	-0.264878	-4.231433
H	0.513648	-0.735250	-5.071501
H	1.185063	0.785872	-4.490211
H	2.011954	-0.733576	-4.139276
C	0.048273	-1.905063	-2.633865
H	-0.634738	-2.074024	-1.799101
H	-0.364178	-2.439567	-3.494183
H	1.008363	-2.363896	-2.391104
C	-1.154388	0.243369	-3.142223
H	-1.055521	1.317783	-3.312328
H	-1.665213	-0.181005	-4.010992
H	-1.808571	0.101878	-2.282395
C	1.706596	0.126762	1.084866
C	2.252547	-0.797511	1.970669
C	1.835295	1.491532	1.332569
C	2.917801	-0.336396	3.088585
H	2.169437	-1.860118	1.785211
C	2.510830	1.897821	2.464401

H	1.424909	2.222791	0.648267
C	3.059929	1.009144	3.369964
H	3.587385	1.351013	4.250187
F	2.634283	3.206008	2.708258
F	3.445358	-1.222318	3.938743
P	-1.209335	0.001280	0.799410
O	2.503916	-0.333716	-1.398376
O	-2.459579	-0.798808	0.152602
O	-1.744032	0.078879	2.335349
O	-1.428830	1.468777	0.193420
C	-0.940877	0.641685	3.370187
H	-0.733376	1.697413	3.189305
H	-1.506242	0.551176	4.294683
H	0.004581	0.110089	3.485432
C	-2.634242	-2.181409	0.447622
H	-3.290517	-2.594343	-0.314172
H	-1.688508	-2.729313	0.422499
H	-3.092641	-2.316364	1.427292
C	-2.679116	2.162287	0.216776
H	-3.339932	1.785978	-0.562891
H	-3.176242	2.074723	1.182974
H	-2.461673	3.209670	0.024797

11b^{ery-ap} $E = -1729.871617560$ au

ZPE = 0.35858015 au

 $G_{\text{corr}} = 0.30694530$ au

C	-0.543750	-1.851813	1.429872	H	0.128916	0.705642	2.109531
H	-0.503466	-2.935278	1.292294	C	2.327934	-0.567585	4.361740
P	0.269110	-1.068851	-0.342665	H	3.052290	-0.245447	5.097289
C	-0.749233	-1.987068	-1.665794	F	1.764337	1.642136	3.863450
C	0.088121	-1.770869	-2.933804	F	2.835031	-2.811363	4.761284
H	-0.425139	-2.197214	-3.800809	P	-2.170415	-1.439701	1.892793
H	0.247235	-0.708686	-3.140817	O	1.594594	-1.815550	-0.281987
H	1.067042	-2.241991	-2.852625	O	-3.263165	-2.358443	1.220996
C	-0.869893	-3.482236	-1.408829	O	-2.559764	-1.551958	3.427985
H	-1.574784	-3.707663	-0.606018	O	-2.463915	0.023867	1.400594
H	-1.227303	-4.010677	-2.298339	C	-1.967963	-0.854890	4.533530
H	0.099580	-3.905386	-1.139119	H	-1.796118	0.194960	4.300555
C	-2.110133	-1.332290	-1.876668	H	-2.676387	-0.929110	5.354124
H	-2.018053	-0.247197	-1.968684	H	-1.027795	-1.321165	4.819271
H	-2.576318	-1.698424	-2.796575	C	-3.480780	-3.726353	1.596143
H	-2.809944	-1.538087	-1.068588	H	-4.091702	-4.165525	0.813825
C	0.451754	-1.406134	2.450628	H	-2.543018	-4.278076	1.664327
C	1.201843	-2.344446	3.153266	H	-4.006297	-3.779014	2.547547
C	0.654654	-0.045672	2.684399	C	-3.735396	0.674493	1.550257
C	2.119747	-1.905852	4.085580	H	-4.451623	0.264754	0.840988
H	1.077211	-3.403425	2.971773	H	-4.122940	0.573879	2.563479
C	1.580373	0.337239	3.633849	H	-3.568452	1.724429	1.331879

11b^{ery-sc} $E = -1729.878575728$ au

ZPE = 0.35862130 au

 $G_{\text{corr}} = 0.30564898$ au

C	-1.291026	-1.678271	1.451404	C	0.626189	-0.235773	2.179153
H	-1.587867	-2.730107	1.430923	C	1.898585	-2.420526	3.285313
P	-1.358869	-1.069344	-0.529702	H	0.215121	-3.577323	2.664992
C	-0.259937	-2.450508	-1.239321	C	1.859492	-0.123646	2.789329
C	-0.463965	-2.280852	-2.751420	H	0.175520	0.621364	1.700828
H	0.136474	-3.011683	-3.300841	C	2.528528	-1.192558	3.353516
H	-1.507849	-2.425427	-3.040275	H	3.495963	-1.074588	3.822099
H	-0.161826	-1.286587	-3.085844	F	2.444706	1.078567	2.834697
C	1.216978	-2.263883	-0.919205	F	2.511484	-3.483038	3.822942
H	1.444199	-2.476014	0.124730	P	-2.605222	-0.827102	2.229857
H	1.831647	-2.931836	-1.531003	O	-0.538189	0.214208	-0.570355
H	1.528499	-1.239201	-1.121447	O	-4.012717	-1.486403	1.952786
C	-0.755403	-3.832056	-0.830047	O	-2.551606	-0.762765	3.808654
H	-1.845087	-3.911386	-0.904607	O	-2.586700	0.674644	1.786113
H	-0.333930	-4.605400	-1.478591	C	-2.490474	-1.942748	4.621391
H	-0.467990	-4.088874	0.191621	H	-2.377990	-1.604762	5.646925
C	0.017582	-1.489505	2.132503	H	-3.406180	-2.525162	4.530693
C	0.663928	-2.592426	2.697182	H	-1.631275	-2.557399	4.353844

C	-4.574718	-1.800560	0.666439
H	-5.608406	-2.076372	0.854641
H	-4.529393	-0.946202	-0.004329
H	-4.044342	-2.632776	0.208866

C	-3.439476	1.687809	2.340586
H	-4.475730	1.355057	2.388487
H	-3.095893	1.967964	3.334042
H	-3.366807	2.541410	1.674358

12b^{ery}

$E = -1729.900572728$ au

ZPE = 0.36161342 au

$G_{\text{corr}} = 0.31175631$ au

O	0.473558	0.137496	0.212513
P	0.701232	0.177945	1.860707
C	2.378665	-0.537157	1.418176
P	1.916262	-0.605792	-0.394410
C	-0.397373	-1.168004	2.552809
C	0.097044	-1.453948	3.972803
H	0.249681	-0.537605	4.548948
H	-0.644465	-2.052057	4.508165
H	1.033416	-2.011896	3.977466
C	-1.780124	-0.505198	2.625542
H	-2.496592	-1.193819	3.080687
H	-1.767779	0.405357	3.227583
H	-2.157628	-0.247414	1.634009
C	-0.510823	-2.455097	1.748662
H	-0.863735	-2.271427	0.735793
H	0.432991	-2.992495	1.689170
H	-1.228904	-3.122011	2.234193
H	3.039836	0.336878	1.483493
C	3.042095	-1.649704	2.157057
C	2.982913	-2.978244	1.746222
C	3.585375	-3.948759	2.522267
C	4.256304	-3.667854	3.695482

C	4.309022	-2.339483	4.071448
C	3.726931	-1.332065	3.331212
H	2.483801	-3.270502	0.834452
F	3.519809	-5.222242	2.118528
H	4.721186	-4.445938	4.285419
F	4.955594	-2.022091	5.198134
H	3.795439	-0.306674	3.671685
O	2.312757	0.671859	-1.305246
C	1.594650	1.890294	-1.426734
H	1.510057	2.419563	-0.477386
H	2.168201	2.506505	-2.117368
H	0.596614	1.741795	-1.836043
O	3.298353	-1.405237	-0.882450
C	4.593809	-0.885845	-0.722444
H	4.801347	-0.078395	-1.428181
H	4.787882	-0.512186	0.288379
H	5.300352	-1.695120	-0.907294
O	0.977196	-1.723632	-1.077913
C	1.367437	-2.708165	-2.026117
H	2.001177	-3.477072	-1.585854
H	0.442782	-3.170439	-2.367273
H	1.881114	-2.276651	-2.884132

(12b^{ery}→12b^{ery2})[‡]

$E = -1729.891440978$ au

ZPE = 0.36088602 au

$G_{\text{corr}} = 0.31151784$ au

$\nu = -100.60$ cm⁻¹

O	0.598326	0.029188	0.170693
P	0.729592	0.078420	1.825521
C	2.441312	-0.614800	1.478784
P	2.088058	-0.738626	-0.344715
C	-0.374969	-1.275193	2.492705
C	0.047887	-1.494450	3.947777
H	0.141979	-0.553909	4.496794
H	-0.704587	-2.095846	4.463801
H	0.998378	-2.022862	4.024036
C	-1.775260	-0.646998	2.465275
H	-2.498451	-1.336109	2.908908
H	-1.818590	0.286411	3.029883

H	-2.104254	-0.438069	1.445346
C	-0.412864	-2.596062	1.738852
H	-0.728240	-2.464357	0.705872
H	0.549024	-3.103934	1.738871
H	-1.130822	-3.265345	2.221513
H	3.073591	0.280830	1.549267
C	3.104915	-1.688306	2.274612
C	3.121254	-3.025027	1.886835
C	3.713247	-3.954426	2.719620
C	4.299473	-3.624627	3.925313
C	4.277346	-2.288782	4.276284
C	3.702688	-1.319922	3.480968

H	2.693416	-3.352759	0.950658
F	3.723123	-5.237295	2.341553
H	4.757481	-4.372353	4.558345
F	4.840663	-1.924459	5.433366
H	3.709526	-0.286308	3.803068
O	2.384973	0.446875	-1.406358
C	1.610267	1.611163	-1.657222
H	1.509991	2.240565	-0.773905
H	2.152211	2.165582	-2.421777
H	0.616578	1.374572	-2.034564

O	3.548663	-1.451958	-0.745367
C	4.785350	-0.814282	-0.551266
H	5.569712	-1.541663	-0.761147
H	4.924040	0.039224	-1.219879
H	4.935116	-0.467823	0.477628
O	1.310508	-2.042177	-0.896230
C	0.864759	-2.097131	-2.242686
H	1.689163	-1.986532	-2.949235
H	0.414001	-3.076554	-2.385168
H	0.108889	-1.336413	-2.450471

12b^{ery2}

$E = -1729.896995659$ au

ZPE = 0.36137890 au

$G_{\text{corr}} = 0.31106718$ au

O	0.654498	-0.090675	0.003589
P	0.759787	0.037187	1.658615
C	2.488285	-0.631267	1.376870
P	2.187356	-0.795886	-0.464540
C	-0.327426	-1.315296	2.354760
C	-0.051498	-1.332343	3.861174
H	-0.128165	-0.336960	4.304838
H	-0.782978	-1.970004	4.363528
H	0.938975	-1.727046	4.091721
C	-1.754086	-0.808494	2.107303
H	-2.473259	-1.484026	2.577269
H	-1.916023	0.187366	2.525028
H	-1.989488	-0.767212	1.042036
C	-0.189866	-2.717846	1.780156
H	-0.361644	-2.745712	0.706264
H	0.784093	-3.156380	1.981431
H	-0.936876	-3.371501	2.239026
H	3.113689	0.269245	1.444925
C	3.135385	-1.678292	2.222840
C	3.240759	-3.012517	1.839631
C	3.829563	-3.912456	2.706674
C	4.326736	-3.555793	3.944147

C	4.214629	-2.223726	4.292212
C	3.639633	-1.283513	3.463228
H	2.882256	-3.360634	0.881832
F	3.924986	-5.192553	2.331635
H	4.784279	-4.280423	4.603802
F	4.688384	-1.833510	5.480470
H	3.577978	-0.250938	3.783088
O	2.587758	0.472383	-1.385356
C	1.888380	1.700750	-1.517116
H	1.751353	2.207761	-0.561427
H	2.507809	2.328744	-2.155256
H	0.915106	1.574500	-1.988769
O	3.629783	-1.551792	-0.807437
C	4.878738	-0.978936	-0.511871
H	5.637653	-1.742125	-0.683383
H	5.100989	-0.124130	-1.155224
H	4.977717	-0.655913	0.529762
O	1.478382	-2.029744	-1.229325
C	0.214641	-1.957898	-1.871426
H	0.167714	-1.133701	-2.584818
H	0.104057	-2.891778	-2.418855
H	-0.612577	-1.859443	-1.170895

12b^{ery3}

$E = -1729.895481697$ au

ZPE = 0.36152989 au

$G_{\text{corr}} = 0.31174800$ au

O	0.240041	0.298827	0.548823
P	0.556881	0.184276	2.177426
C	2.232028	-0.411007	1.572465
P	1.657979	-0.314250	-0.208182
C	-0.453379	-1.268429	2.788282
C	0.134275	-1.685034	4.138441
H	0.301669	-0.828398	4.796589

H	-0.558959	-2.355775	4.652103
H	1.081567	-2.213221	4.030035
C	-1.846211	-0.662317	3.013339
H	-2.514504	-1.418214	3.433819
H	-1.820458	0.179880	3.707362
H	-2.291632	-0.313770	2.079386
C	-0.586450	-2.466634	1.859612

H	-1.002252	-2.186771	0.893564
H	0.362875	-2.969495	1.690582
H	-1.260730	-3.200302	2.310460
H	2.869955	0.473798	1.695135
C	2.959737	-1.573795	2.156572
C	2.895989	-2.857989	1.623123
C	3.565312	-3.884704	2.259208
C	4.304732	-3.703153	3.410679
C	4.357081	-2.416720	3.911927
C	3.712162	-1.355735	3.311608
H	2.342434	-3.072858	0.721373
F	3.497225	-5.113449	1.735796
H	4.819730	-4.523512	3.891618
F	5.068278	-2.195344	5.022083
H	3.785604	-0.366660	3.745436

O	1.785529	1.115492	-0.967476
C	2.419928	1.316793	-2.221121
H	2.136267	0.567160	-2.960229
H	2.081825	2.288461	-2.576699
H	3.507068	1.341609	-2.145952
O	3.066229	-0.969967	-0.860497
C	4.354048	-0.519418	-0.511874
H	4.993237	-0.580622	-1.394378
H	4.378748	0.517375	-0.161157
H	4.794388	-1.145657	0.267997
O	0.750616	-1.420791	-0.949102
C	1.145191	-2.372321	-1.928007
H	1.849905	-3.104951	-1.536458
H	0.232933	-2.888788	-2.220596
H	1.580568	-1.906145	-2.810954

(12b^{ery}→9b+10²)[‡]

$E = -1729.867430302$ au

ZPE = 0.35981861 au

$G_{\text{corr}} = 0.30943702$ au

$\nu = -235.05$ cm⁻¹

O	0.444537	-1.054240	0.133553
P	0.655012	-0.160863	1.661751
C	2.373335	-0.502465	1.766862
P	1.767600	-0.914693	-0.706768
C	-0.493057	-1.173143	2.741864
C	-0.138786	-0.735325	4.166017
H	-0.160525	0.351326	4.281517
H	-0.862329	-1.150144	4.871933
H	0.852496	-1.084592	4.459142
C	-1.903671	-0.681548	2.391688
H	-2.632482	-1.126845	3.074007
H	-1.991629	0.403151	2.473089
H	-2.189492	-0.965095	1.377125
C	-0.462572	-2.693500	2.639618
H	-0.564828	-3.042635	1.611696
H	0.448517	-3.113817	3.057120
H	-1.300411	-3.108005	3.207443
H	2.899702	0.434140	1.946988
C	3.058114	-1.634565	2.384492
C	2.746496	-2.973307	2.102324
C	3.480322	-3.986792	2.677695
C	4.552795	-3.768447	3.523068

C	4.857282	-2.443775	3.774905
C	4.148575	-1.392423	3.236717
H	1.948813	-3.231198	1.421497
F	3.153330	-5.256569	2.390678
H	5.117120	-4.581808	3.957303
F	5.890857	-2.175548	4.587595
H	4.431272	-0.376628	3.482502
O	2.269276	0.556633	-1.045921
C	1.342006	1.612893	-1.324627
H	0.808551	1.903299	-0.419187
H	1.932233	2.452115	-1.681309
H	0.625810	1.325155	-2.094352
O	3.034089	-1.858873	-0.736358
C	4.371970	-1.497702	-0.387049
H	4.905072	-1.229979	-1.298230
H	4.400973	-0.666542	0.312966
H	4.832922	-2.367736	0.071690
O	1.069286	-1.425004	-2.064795
C	1.810275	-1.621199	-3.261738
H	2.385645	-2.546118	-3.226133
H	1.086415	-1.689282	-4.070735
H	2.486547	-0.790835	-3.475484

13b

$E = -1155.507011633$ au

ZPE = 0.22720701 au

$G_{\text{corr}} = 0.18338628$ au

C	0.002794	-0.078242	-0.021959
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P	0.022200	0.024773	1.638212
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H	0.945079	0.173802	-0.491753
C	-1.118326	-0.362039	-0.876140
C	-0.895180	-0.461038	-2.263596
C	-1.939179	-0.736189	-3.115222
C	-3.241767	-0.932636	-2.690621
C	-3.441427	-0.828806	-1.327450
C	-2.439548	-0.549306	-0.423968
H	0.100227	-0.325377	-2.665921
F	-1.686071	-0.823105	-4.429617
H	-4.047474	-1.148317	-3.377690
F	-4.686577	-1.002258	-0.857527
H	-2.703209	-0.470633	0.622373
O	-0.418500	1.363372	2.407455
C	-1.520926	2.135641	1.936337

H	-2.468296	1.693099	2.246247
H	-1.431867	3.125237	2.377150
H	-1.504843	2.227342	0.848795
O	-0.930371	-1.016393	2.394677
C	-0.879880	-2.405272	2.051476
H	0.122150	-2.810937	2.192593
H	-1.566524	-2.914977	2.722213
H	-1.193520	-2.570368	1.021236
O	1.520271	-0.158035	2.131556
C	1.964890	0.219853	3.437180
H	1.311239	-0.171923	4.216760
H	2.955063	-0.210554	3.560175
H	2.029503	1.302684	3.531035

12b^{thr}

$E = -1729.903547810$ au

ZPE = 0.36104625 au

$G_{\text{corr}} = 0.31039527$ au

O	-0.048111	0.181746	0.183905
P	0.015547	-0.000808	1.841220
C	1.856874	0.016449	1.587861
P	1.620736	0.418659	-0.222181
C	-0.367034	-1.807612	2.135741
C	0.112930	-2.098582	3.559037
H	-0.312030	-1.402608	4.286074
H	-0.187977	-3.105625	3.857377
H	1.200600	-2.045152	3.644253
C	-1.892139	-1.929970	2.067429
H	-2.199549	-2.951151	2.306576
H	-2.385909	-1.261358	2.775200
H	-2.268579	-1.698828	1.069259
C	0.262106	-2.779186	1.144837
H	-0.046082	-2.571318	0.121398
H	1.352750	-2.769628	1.176872
H	-0.050067	-3.798934	1.385383
H	2.298877	-0.981543	1.656507
C	2.694729	0.987580	2.351610
C	3.963457	0.615383	2.785702
C	4.735577	1.528710	3.474158
C	4.306277	2.811462	3.752544

C	3.042967	3.150337	3.307667
C	2.230515	2.273796	2.618341
H	4.348643	-0.375733	2.586015
F	5.952965	1.160881	3.891019
H	4.924717	3.513246	4.295336
F	2.591163	4.383902	3.561635
H	1.241207	2.590993	2.314231
O	1.390583	1.944110	-0.701926
C	0.143367	2.584976	-0.924914
H	-0.415493	2.729338	-0.000806
H	0.381369	3.560686	-1.345073
H	-0.481263	2.041932	-1.632874
O	3.271041	0.571090	-0.399765
C	3.961558	1.444304	-1.262024
H	4.979543	1.065465	-1.364422
H	3.528279	1.512497	-2.263531
H	4.013005	2.453989	-0.848839
O	1.422164	-0.725905	-1.352290
C	2.430910	-1.260475	-2.193392
H	3.277184	-1.654907	-1.632542
H	1.963981	-2.078452	-2.739482
H	2.795519	-0.532730	-2.919231

12b^{thr2}

$E = -1729.901868137$ au

ZPE = 0.36106467 au

$G_{\text{corr}} = 0.31017812$ au

O	0.697449	0.178074	-0.427345
P	0.366296	0.222628	1.211479
C	2.201944	0.010727	1.386520

P	2.427282	0.410017	-0.436349
C	-0.319192	-1.468971	1.615036
C	-0.153777	-1.609323	3.130407

H	-0.594481	-0.768570	3.671179
H	-0.652091	-2.517162	3.478061
H	0.895731	-1.679764	3.424552
C	-1.807345	-1.425214	1.257410
H	-2.292320	-2.361726	1.543824
H	-2.324504	-0.613659	1.772443
H	-1.959297	-1.291213	0.184721
C	0.341061	-2.636223	0.893829
H	0.215596	-2.567592	-0.185820
H	1.407674	-2.724325	1.105578
H	-0.119783	-3.573989	1.214377
H	2.450851	-1.045250	1.530059
C	2.968738	0.840098	2.358132
C	3.969597	0.256495	3.129909
C	4.675781	1.037577	4.023669
C	4.428489	2.384379	4.194199
C	3.422597	2.931880	3.419720
C	2.689723	2.196690	2.512313
H	4.200429	-0.796867	3.037744

F	5.636706	0.466864	4.758982
H	4.989008	2.980879	4.901011
F	3.150314	4.233137	3.564949
H	1.903433	2.678814	1.946954
O	2.357767	1.970512	-0.825828
C	1.196354	2.707987	-1.173988
H	0.488544	2.788233	-0.347995
H	1.546240	3.707184	-1.425891
H	0.680890	2.291482	-2.038445
O	4.077063	0.582515	-0.318882
C	4.923062	-0.522371	-0.133422
H	5.839813	-0.166941	0.338274
H	4.502649	-1.296678	0.519436
H	5.183825	-0.999477	-1.081349
O	2.617882	-0.631832	-1.661352
C	1.615839	-1.152754	-2.519242
H	1.039968	-0.366442	-3.006891
H	2.143677	-1.718751	-3.285106
H	0.929027	-1.820452	-2.003202

12b^{thr3}

$E = -1729.896716762$ au

ZPE = 0.36049674 au

$G_{\text{corr}} = 0.31129049$ au

O	-0.021447	0.183224	0.093392
P	0.072158	0.015083	1.750914
C	1.908277	-0.028187	1.447990
P	1.612867	0.392305	-0.363788
C	-0.352903	-1.782900	2.048230
C	0.150482	-2.097798	3.458014
H	-0.236922	-1.394500	4.198783
H	-0.172560	-3.097631	3.757374
H	1.241101	-2.076963	3.519579
C	-1.882289	-1.860242	2.014205
H	-2.213745	-2.873457	2.255090
H	-2.339842	-1.181919	2.736887
H	-2.274492	-1.612026	1.026350
C	0.224152	-2.764153	1.035287
H	-0.098123	-2.537695	0.020077
H	1.315388	-2.791591	1.044480
H	-0.113890	-3.776115	1.273272
H	2.301394	-1.045419	1.523897
C	2.777718	0.901751	2.227025
C	3.891988	0.408797	2.900767
C	4.677743	1.275251	3.636584
C	4.404904	2.624014	3.736359

C	3.285901	3.082691	3.065565
C	2.467626	2.258048	2.322233
H	4.145355	-0.642942	2.861862
F	5.743804	0.789232	4.278885
H	5.029667	3.288942	4.316528
F	2.987855	4.381823	3.148091
H	1.590926	2.671118	1.840840
O	1.296318	1.930489	-0.720819
C	2.195465	2.910895	-1.216858
H	2.608512	2.641913	-2.188597
H	1.606621	3.819712	-1.328972
H	3.015741	3.104493	-0.527230
O	3.246923	0.581732	-0.728984
C	4.211565	-0.403740	-0.467020
H	4.883978	-0.482702	-1.324205
H	4.811425	-0.136180	0.405986
H	3.792329	-1.401161	-0.290883
O	1.335309	-0.694262	-1.540628
C	2.085925	-0.827652	-2.733474
H	3.009374	-1.389377	-2.587840
H	1.456621	-1.387339	-3.423733
H	2.329016	0.130716	-3.192884

(12b^{thr}→11b^{thr-sc})[‡]

$E = -1729.884236635$ au

ZPE = 0.35876830 au

S24

$G_{\text{corr}} = 0.30704703 \text{ au}$
 $\nu = -88.01 \text{ cm}^{-1}$

O	-0.026762	0.100335	-0.580223	C	3.322661	2.423324	3.621729
P	0.206529	0.321455	0.943250	C	2.668927	1.937342	2.507449
C	2.150939	0.042580	0.954611	H	3.865263	-1.239281	2.642586
P	2.663256	0.790688	-0.589499	F	5.128720	-0.450400	4.741922
C	-0.331585	-1.275459	1.800947	H	4.657604	2.050972	5.272953
C	0.174751	-1.286716	3.239751	F	3.133653	3.698901	3.973030
H	-0.036149	-0.343064	3.748869	H	1.996848	2.578528	1.952969
H	-0.308099	-2.083825	3.812706	O	2.007646	2.188277	-0.843903
H	1.251267	-1.454812	3.298360	C	1.115900	2.538694	-1.917505
C	-1.861811	-1.186153	1.802839	H	0.247639	1.887120	-1.898007
H	-2.296050	-2.060564	2.295686	H	0.824104	3.567968	-1.732418
H	-2.212423	-0.299459	2.336018	H	1.634169	2.475787	-2.872804
H	-2.261556	-1.143601	0.788016	O	4.181682	1.254459	-0.482135
C	0.088192	-2.538453	1.061512	C	5.240533	0.308824	-0.327718
H	-0.227291	-2.506707	0.018270	H	6.146863	0.882416	-0.156468
H	1.169682	-2.696178	1.082498	H	5.079144	-0.347329	0.528183
H	-0.363580	-3.423195	1.519766	H	5.361717	-0.291352	-1.229316
H	2.346973	-1.030105	0.858492	O	2.647571	-0.137116	-1.854721
C	2.869038	0.609280	2.136115	C	1.996457	-1.402258	-2.068192
C	3.706285	-0.200001	2.901493	H	0.923176	-1.286079	-1.974031
C	4.327879	0.334096	4.012143	H	2.282293	-1.713950	-3.068624
C	4.161408	1.648833	4.400217	H	2.354753	-2.137541	-1.348187

11b^{thr-sc}

$E = -1729.884375027 \text{ au}$
 $\text{ZPE} = 0.35877571 \text{ au}$
 $G_{\text{corr}} = 0.30721810 \text{ au}$

O	-0.052570	0.091281	-0.584246	C	4.147839	1.633009	4.399945
P	0.202220	0.320753	0.933359	C	3.308539	2.408946	3.623618
C	2.151967	0.039287	0.939651	C	2.658984	1.926922	2.505069
P	2.675348	0.795862	-0.594629	H	3.865058	-1.246555	2.626005
C	-0.330461	-1.270099	1.806740	F	5.121101	-0.464963	4.732565
C	0.182721	-1.272454	3.243174	H	4.640810	2.032141	5.275881
H	-0.020396	-0.323578	3.745720	F	3.114604	3.682015	3.981208
H	-0.302132	-2.062176	3.824632	H	1.985854	2.568788	1.952672
H	1.258336	-1.446511	3.298336	O	2.011116	2.189296	-0.847313
C	-1.860661	-1.179095	1.816370	C	1.119177	2.535246	-1.922957
H	-2.292844	-2.049786	2.317540	H	0.257276	1.875007	-1.908906
H	-2.207457	-0.288604	2.345757	H	0.816180	3.560552	-1.734106
H	-2.265949	-1.142791	0.803572	H	1.641512	2.481912	-2.876546
C	0.083705	-2.539254	1.074668	O	4.191292	1.263033	-0.483358
H	-0.244471	-2.519301	0.035050	C	5.252430	0.319381	-0.328055
H	1.165663	-2.694563	1.084142	H	6.158284	0.895394	-0.162893
H	-0.360988	-3.420315	1.546806	H	5.094261	-0.332322	0.531718
H	2.348024	-1.033150	0.840401	H	5.371303	-0.284769	-1.227290
C	2.864152	0.601517	2.127107	O	2.652955	-0.127612	-1.862656
C	3.702358	-0.209156	2.890101	C	2.013798	-1.403562	-2.057536
C	4.319457	0.320877	4.005119	H	0.955171	-1.320338	-1.835885

H 2.185872 -1.663746 -3.097915

H 2.478486 -2.154587 -1.419042

(12b^{thr}→9b+10^Z)[‡]

$E = -1729.876775566$ au

ZPE = 0.35900660 au

$G_{\text{corr}} = 0.30835960$ au

$\nu = -247.33$ cm⁻¹

O 0.301280 -0.217576 -0.035691
P 0.314173 -0.031004 1.748867
C 2.053595 0.096796 1.900408
P 1.684936 0.073353 -0.692048
C -0.128220 -1.797895 2.173128
C 0.028127 -1.872928 3.694871
H -0.549121 -1.098009 4.204851
H -0.332039 -2.838751 4.057411
H 1.069639 -1.766956 4.001056
C -1.596235 -2.013662 1.797863
H -1.923580 -3.007497 2.114518
H -2.247550 -1.282026 2.279154
H -1.754479 -1.944165 0.720595
C 0.732086 -2.864608 1.506784
H 0.582604 -2.887604 0.426950
H 1.795671 -2.730919 1.706645
H 0.454079 -3.851230 1.886878
H 2.615611 -0.817635 2.072758
C 2.639930 1.266745 2.519079
C 3.900854 1.173322 3.139170
C 4.496428 2.294456 3.670613
C 3.917553 3.550546 3.643821

C 2.673621 3.619367 3.040102
C 2.033618 2.537045 2.481828
H 4.406769 0.217957 3.201525
F 5.701814 2.167795 4.249904
H 4.400211 4.418315 4.070493
F 2.068295 4.817382 2.988837
H 1.065069 2.675968 2.018490
O 2.241785 1.548327 -0.658354
C 3.605961 1.907681 -0.403801
H 4.178931 1.841572 -1.328447
H 3.595621 2.933570 -0.048829
H 4.054444 1.274955 0.357098
O 2.870204 -0.981675 -0.620980
C 2.911155 -2.172725 -1.422176
H 3.226563 -1.950999 -2.440573
H 3.644846 -2.822725 -0.954381
H 1.950635 -2.684179 -1.444943
O 1.166753 -0.051512 -2.210011
C 1.903524 0.492872 -3.298761
H 2.970115 0.259984 -3.249945
H 1.500112 0.049720 -4.205985
H 1.782829 1.574834 -3.350144

(1+8c→9c+10^F)[‡]

$E = -1788.011968497$ au

ZPE = 0.48014922 au

$G_{\text{corr}} = 0.42297731$ au

$\nu = -525.60$ cm⁻¹

C -0.008163 -2.421331 0.926957
H -0.200406 -3.154453 0.152728
P -1.055634 -1.010007 1.069373
C -2.610980 -1.513109 0.150836
C -3.379546 -0.226443 -0.154402
H -4.353125 -0.458558 -0.593937
H -3.554314 0.368170 0.744827
H -2.838431 0.399289 -0.867130
C -2.387432 -2.282070 -1.144655
H -1.925794 -3.255665 -0.979391
H -3.346409 -2.465178 -1.637080
H -1.761977 -1.726404 -1.843411
C -3.410813 -2.361109 1.143410
H -3.574101 -1.838940 2.089208

H -4.394037 -2.598516 0.729189
H -2.908841 -3.303940 1.366767
C 1.136508 -2.665735 1.762174
C 2.014582 -3.714067 1.437096
C 1.411070 -1.898316 2.907888
C 3.110313 -3.956631 2.233957
H 1.836826 -4.327296 0.563263
C 2.525683 -2.183127 3.661101
H 0.750852 -1.094150 3.206990
C 3.406191 -3.208249 3.359095
H 4.273645 -3.414370 3.970514
F 2.775694 -1.440512 4.748344
F 3.935699 -4.960671 1.908179
P 0.201022 1.436047 -0.754184

O	0.092063	-0.652202	-0.076872	H	-0.892648	2.529067	-3.171728
N	1.030802	1.184217	-2.196346	H	-2.392761	2.109313	-2.333837
N	-0.801117	2.805937	-1.088168	C	-1.615211	3.274359	0.019043
N	1.249229	2.154843	0.350318	H	-1.054402	3.249678	0.951325
C	1.856862	2.195966	-2.816068	H	-1.917942	4.308104	-0.160530
H	2.153054	2.958589	-2.101054	H	-2.525535	2.679348	0.159868
H	2.770525	1.741843	-3.208682	C	1.636451	3.551654	0.359786
H	1.351434	2.697042	-3.649922	H	1.028170	4.133993	-0.326463
C	0.702391	0.076219	-3.064381	H	1.514596	3.970770	1.363011
H	1.615663	-0.406805	-3.422255	H	2.688490	3.674613	0.079286
H	0.121879	-0.670229	-2.529307	C	2.090476	1.340709	1.202728
H	0.128326	0.393553	-3.942765	H	2.026476	1.683711	2.239243
C	-1.535799	2.795437	-2.335862	H	1.793323	0.298565	1.174575
H	-1.923419	3.797560	-2.530134	H	3.140540	1.399485	0.897488

(1→11c^{ery})[‡]

$E = -1788.029049112$ au

ZPE = 0.48165524 au

$G_{\text{corr}} = 0.42629572$ au

$\nu = -474.68$ cm⁻¹

H	1.418058	-1.311856	-0.154218	N	-2.000539	-1.190978	0.289904
P	1.787486	0.195316	-2.114392	N	-1.605284	1.524503	0.100897
C	1.024604	-1.187060	-3.133861	N	-1.085155	0.293513	2.308492
C	1.659330	-1.013182	-4.519543	C	-1.499034	-2.529176	0.077220
H	1.261274	-1.757415	-5.214287	H	-1.666607	-3.178822	0.944265
H	1.454474	-0.026155	-4.939787	H	-1.982590	-2.994078	-0.785966
H	2.743210	-1.142679	-4.485896	H	-0.428738	-2.513789	-0.113682
C	1.349672	-2.581196	-2.616455	C	-3.401792	-1.152421	0.648581
H	0.865588	-2.798418	-1.664483	H	-3.986054	-1.698060	-0.096268
H	1.003446	-3.338203	-3.325527	H	-3.598650	-1.608493	1.625735
H	2.422627	-2.714673	-2.480796	H	-3.777767	-0.134158	0.672039
C	-0.481528	-0.962315	-3.237208	C	-2.738126	2.186563	0.718142
H	-0.714284	0.029232	-3.632732	H	-2.952341	1.766178	1.697008
H	-0.930432	-1.693410	-3.915461	H	-2.525332	3.251608	0.846385
H	-0.982408	-1.056746	-2.272004	H	-3.638989	2.102308	0.100910
C	2.030255	0.603852	0.678266	C	-1.322468	2.019653	-1.226998
C	2.602581	0.011214	1.801539	H	-2.121359	1.783320	-1.937923
C	2.023456	1.991575	0.553579	H	-1.205574	3.106221	-1.202820
C	3.168256	0.817087	2.767603	H	-0.395950	1.603893	-1.617933
H	2.628416	-1.065315	1.906704	C	-0.947446	-0.883101	3.141430
C	2.598339	2.750594	1.550377	H	-1.397844	-0.688461	4.117169
H	1.594902	2.470807	-0.316844	H	-1.468124	-1.738158	2.715046
C	3.180358	2.195928	2.675286	H	0.097174	-1.170590	3.313344
H	3.630838	2.811490	3.442134	C	-0.524608	1.472555	2.941628
F	2.592215	4.082730	1.433152	H	0.509492	1.326103	3.267745
F	3.728209	0.246830	3.839952	H	-0.543240	2.326519	2.269729
P	-0.924625	0.075339	0.611614	H	-1.115567	1.727906	3.825316
O	3.130123	-0.389983	-1.495475				

11c^{ery-sc}

$E = -1788.107964611$ au

ZPE = 0.48511921 au

$G_{\text{corr}} = 0.43041575$ au

C	-1.230929	-1.965164	1.243002	O	-0.971461	-0.236941	-0.983731
H	-1.386393	-3.035054	1.401406	N	-3.962021	-2.146940	1.755340
P	-1.443595	-1.677752	-0.733312	N	-3.118322	0.317124	1.294362
C	-0.072935	-2.830341	-1.369182	N	-2.381712	-0.772171	3.542417
C	-0.362450	-2.886663	-2.875450	C	-3.934670	-3.445229	1.107665
H	0.370003	-3.522289	-3.381738	H	-3.653398	-4.250720	1.791813
H	-1.355232	-3.292671	-3.083220	H	-4.931824	-3.662655	0.723373
H	-0.308627	-1.894585	-3.327919	H	-3.263163	-3.438193	0.251740
C	1.335559	-2.285153	-1.167013	C	-5.157198	-1.865652	2.531053
H	1.664999	-2.356532	-0.131594	H	-6.043055	-2.024815	1.914252
H	2.053680	-2.842753	-1.776930	H	-5.232571	-2.507845	3.412873
H	1.388675	-1.236410	-1.460187	H	-5.181891	-0.828929	2.861861
C	-0.220219	-4.231482	-0.787733	C	-4.006695	0.398623	0.143152
H	-1.256879	-4.580227	-0.830318	H	-4.577949	-0.516265	0.019908
H	0.382175	-4.951314	-1.349793	H	-4.705818	1.224112	0.294118
H	0.110856	-4.283559	0.251103	H	-3.432408	0.573912	-0.766568
C	0.087880	-1.567208	1.805572	C	-2.301716	1.512970	1.441180
C	0.857879	-2.520223	2.479269	H	-1.726223	1.687298	0.531417
C	0.611873	-0.288820	1.615203	H	-2.949209	2.373467	1.622997
C	2.109062	-2.179100	2.945651	H	-1.611837	1.430345	2.277357
H	0.488476	-3.526720	2.631228	C	-1.822460	-1.800418	4.401978
C	1.866963	-0.000007	2.109002	H	-2.580264	-2.177252	5.094638
H	0.087785	0.436744	1.013120	H	-1.449889	-2.646627	3.831683
C	2.648797	-0.917750	2.783693	H	-0.988513	-1.403381	4.982652
H	3.630912	-0.664646	3.158927	C	-3.056982	0.277137	4.284121
F	2.363508	1.229393	1.917999	H	-2.330188	0.854066	4.859653
F	2.831968	-3.104244	3.591935	H	-3.584576	0.959163	3.624749
P	-2.668440	-1.132010	1.947207	H	-3.784366	-0.145608	4.983212

(11c^{ery-sc}→12c^{ery})[‡]

$E = -1788.081590178$ au

ZPE = 0.48587197 au

$G_{\text{corr}} = 0.43288075$ au

$\nu = -171.78$ cm⁻¹

O	-0.419625	-0.229795	-0.191100	C	-1.360662	-2.569526	1.863423
P	-0.130295	0.041380	1.339512	H	-1.870736	-2.516631	0.901047
C	1.685555	-0.538335	1.137263	H	-0.451648	-3.156205	1.743192
P	1.855917	-0.579526	-0.703150	H	-2.011573	-3.128627	2.543016
C	-1.091689	-1.179944	2.420641	H	2.283255	0.353034	1.367983
C	-0.415049	-1.261295	3.787464	C	2.315613	-1.674629	1.871096
H	-0.116758	-0.273782	4.150702	C	2.093011	-3.008642	1.534689
H	-1.101810	-1.683818	4.526540	C	2.666386	-4.003352	2.298290
H	0.473724	-1.891454	3.771581	C	3.461300	-3.745930	3.398574
C	-2.442573	-0.466515	2.582528	C	3.671467	-2.415944	3.705532
H	-3.108506	-1.058400	3.217181	C	3.127747	-1.384106	2.968222
H	-2.329794	0.516549	3.043213	H	1.494790	-3.283668	0.678451
H	-2.942070	-0.326765	1.620986	F	2.448207	-5.279073	1.958351

H	3.898538	-4.542723	3.984587
F	4.441767	-2.120014	4.758108
H	3.324493	-0.358805	3.253799
C	1.000250	2.068131	-0.876054
H	0.870191	2.063021	0.203727
H	1.515928	2.996526	-1.130637
H	0.011880	2.078761	-1.336143
C	4.132752	-2.185343	-0.837226
H	4.943018	-2.254072	-1.569347
H	4.558611	-2.399622	0.148387
H	3.414124	-2.967347	-1.059749
C	1.859734	-2.086802	-2.950163
H	1.981008	-3.158482	-3.120526
H	1.185225	-1.697631	-3.718343
H	2.831185	-1.623591	-3.081114

N	1.829133	0.970374	-1.338133
N	3.535768	-0.863399	-0.891192
N	1.311245	-1.869721	-1.615469
C	2.282489	1.159861	-2.706270
H	2.692307	2.166103	-2.808014
H	3.075860	0.464860	-2.965643
H	1.470252	1.054303	-3.432279
C	4.472357	0.135631	-0.413762
H	4.062966	1.138682	-0.493476
H	4.761829	-0.037145	0.630682
H	5.385055	0.100690	-1.014025
C	0.041650	-2.557965	-1.472966
H	-0.750395	-2.100558	-2.068176
H	0.185697	-3.584090	-1.819799
H	-0.290958	-2.590142	-0.447357

12c^{ery}

$E = -1788.087910623$ au

ZPE = 0.48678509 au

$G_{\text{corr}} = 0.43395676$ au

O	-0.048146	-0.377411	-0.153601
P	0.073718	0.056891	1.444463
C	1.837735	-0.522203	1.264013
P	1.661276	-0.581204	-0.639649
C	-0.989534	-1.114274	2.456215
C	-0.386207	-1.135927	3.862408
H	-0.142417	-0.131792	4.220369
H	-1.104082	-1.562638	4.567393
H	0.521148	-1.737048	3.910877
C	-2.351337	-0.406465	2.511436
H	-3.043779	-0.979244	3.134195
H	-2.273343	0.596164	2.934715
H	-2.800019	-0.315056	1.519889
C	-1.207004	-2.527869	1.939145
H	-1.698366	-2.524756	0.966729
H	-0.282827	-3.095015	1.860429
H	-1.860875	-3.071517	2.627123
H	2.478892	0.338984	1.471481
C	2.409063	-1.697954	1.979691
C	2.180210	-3.008862	1.566913
C	2.713525	-4.050980	2.296274
C	3.476576	-3.862012	3.432153
C	3.698339	-2.552830	3.812541
C	3.191646	-1.476391	3.113747
H	1.619953	-3.225416	0.667852
F	2.488691	-5.304452	1.884381
H	3.885709	-4.694427	3.988243
F	4.440080	-2.324095	4.902305

H	3.395433	-0.469553	3.454997
C	0.651573	1.951619	-1.222381
H	0.283337	2.046375	-0.204358
H	1.073127	2.923101	-1.488550
H	-0.200680	1.770264	-1.883559
C	4.016491	-2.172484	-0.913660
H	4.812006	-2.197679	-1.668909
H	4.478015	-2.439101	0.045443
H	3.308171	-2.957846	-1.157830
C	1.795659	-2.010536	-2.968774
H	1.966707	-3.062296	-3.212876
H	1.113555	-1.601653	-3.722630
H	2.743214	-1.493659	-3.060101
N	1.705542	0.959393	-1.359999
N	3.396428	-0.866500	-0.876819
N	1.225251	-1.890185	-1.635650
C	2.502428	1.242534	-2.542203
H	2.961372	2.231300	-2.457787
H	3.296934	0.518571	-2.677105
H	1.883025	1.242667	-3.445981
C	4.327721	0.093978	-0.329181
H	3.893827	1.089532	-0.263004
H	4.681147	-0.186830	0.673770
H	5.216165	0.171231	-0.965933
C	-0.048814	-2.579808	-1.580254
H	-0.847559	-2.057974	-2.116401
H	0.079346	-3.558811	-2.048446
H	-0.379902	-2.753354	-0.564901

(12c^{ery}→9c+10^z)[‡]

$E = -1788.073300729$ au

ZPE = 0.48521560 au

$G_{\text{corr}} = 0.43146682$ au

$\nu = -236.63$ cm⁻¹

O	0.068688	-0.784381	-0.058163	H	3.599087	-0.053185	3.658504
P	0.103412	-0.055043	1.498619	C	0.611791	1.779766	-1.293668
C	1.863901	-0.296406	1.603638	H	-0.012845	1.715772	-0.405702
P	1.546399	-0.714391	-0.752290	H	0.974097	2.807484	-1.348641
C	-0.959836	-1.246289	2.487035	H	-0.013162	1.600603	-2.175810
C	-0.609279	-0.976156	3.951808	C	3.435711	-2.719549	-1.167196
H	-0.660690	0.088251	4.195506	H	4.106891	-2.716129	-2.032259
H	-1.315423	-1.492112	4.607302	H	3.943681	-3.236657	-0.349659
H	0.393466	-1.327994	4.198176	H	2.550389	-3.288707	-1.430078
C	-2.398198	-0.782955	2.215771	C	1.665473	-1.521171	-3.361845
H	-3.097373	-1.351285	2.835225	H	1.678808	-2.486091	-3.876096
H	-2.536497	0.275546	2.441636	H	1.164656	-0.803405	-4.022728
H	-2.681679	-0.940162	1.172957	H	2.698412	-1.203199	-3.255147
C	-0.870092	-2.737705	2.184790	N	1.760226	0.891971	-1.229844
H	-0.955023	-2.948941	1.117977	N	3.100244	-1.368477	-0.761725
H	0.054375	-3.177165	2.548235	N	0.994627	-1.641212	-2.083396
H	-1.691984	-3.258425	2.684436	C	2.778463	1.282387	-2.187807
H	2.328387	0.664344	1.829087	H	3.168292	2.267987	-1.922735
C	2.542769	-1.379673	2.319820	H	3.615841	0.592652	-2.202369
C	2.391879	-2.725663	1.962019	H	2.382818	1.345480	-3.207321
C	3.101874	-3.699830	2.629466	C	4.211439	-0.695035	-0.126968
C	3.993551	-3.425346	3.649120	H	3.927424	0.286818	0.239313
C	4.138299	-2.090600	3.981279	H	4.606073	-1.272545	0.711020
C	3.446949	-1.079863	3.350772	H	5.019617	-0.561255	-0.852648
H	1.734441	-3.017284	1.155475	C	-0.366333	-2.116003	-2.244219
F	2.936178	-4.980338	2.261882	H	-1.063800	-1.338594	-2.576174
H	4.544518	-4.205984	4.154971	H	-0.366037	-2.899816	-3.005373
F	4.992416	-1.773503	4.966104	H	-0.759166	-2.556043	-1.333432

13c

$E = -1213.718335310$ au

ZPE = 0.35202531 au

$G_{\text{corr}} = 0.30469207$ au

C	0.133268	-0.381071	0.139375	H	0.407750	-2.788672	1.043899
P	0.088187	-0.217648	1.824803	C	1.979378	0.153506	3.713465
H	1.063194	-0.100467	-0.334283	H	3.047877	-0.056809	3.792189
C	-0.896558	-0.866495	-0.724655	H	1.776464	1.072622	4.275145
C	-0.723762	-0.751172	-2.123279	H	1.456440	-0.664743	4.201510
C	-1.681016	-1.227161	-2.985686	N	-0.987554	0.892103	2.536809
C	-2.854534	-1.836205	-2.572180	N	-0.363502	-1.619174	2.601805
C	-3.003583	-1.950315	-1.202312	N	1.614502	0.260994	2.317159
C	-2.078885	-1.502502	-0.286990	C	-0.601168	2.287271	2.402090
H	0.163477	-0.276501	-2.522497	H	-1.295509	2.899245	2.978575
F	-1.476677	-1.091111	-4.306874	H	0.392387	2.464949	2.808405
H	-3.596286	-2.199246	-3.268874	H	-0.621913	2.643590	1.365296
F	-4.115786	-2.547033	-0.738347	C	-0.913145	-1.703310	3.941093
H	-2.270333	-1.669108	0.763225	H	-1.109695	-0.715482	4.346832
C	-2.410954	0.709318	2.290816	H	-1.850430	-2.266015	3.932401
H	-2.715584	-0.318313	2.475409	H	-0.224167	-2.220324	4.616063
H	-2.973910	1.342533	2.978499	C	2.452020	1.184839	1.577264
H	-2.703345	0.972636	1.269044	H	2.543016	2.144152	2.097178
C	0.047234	-2.901384	2.063413	H	3.456800	0.773273	1.456627
H	0.842464	-3.348940	2.666897	H	2.049030	1.389088	0.590007
H	-0.799531	-3.590982	2.050618				

12c^{thr}

$E = -1788.097907107$ au

ZPE = 0.48611778 au

$G_{\text{corr}} = 0.43302053$ au

O	0.177687	-0.179777	0.134226	H	-1.033323	-1.125100	4.219304
P	0.087268	-0.117933	1.789364	H	-0.461549	-2.790997	4.302709
C	1.921435	0.066492	1.693166	H	0.695067	-1.463392	4.308808
P	1.855925	0.311269	-0.207820	C	-1.549216	-2.309673	1.800220
C	-0.185598	-1.888144	2.352387	H	-1.840054	-3.279736	2.211650
C	-0.250295	-1.805545	3.879918	H	-2.332199	-1.594301	2.061481

H	-1.535334	-2.403209	0.713283
C	0.876235	-2.903399	1.943175
H	1.081720	-2.893319	0.873086
H	1.820669	-2.744865	2.466232
H	0.543358	-3.912677	2.199740
H	2.416475	-0.899134	1.830761
C	2.608550	1.084488	2.533196
C	3.697189	0.713602	3.319925
C	4.332349	1.664179	4.094814
C	3.931347	2.983971	4.132462
C	2.837987	3.318849	3.354743
C	2.169303	2.407346	2.566827
H	4.050856	-0.309261	3.329075
F	5.379164	1.293523	4.841892
H	4.439357	3.716751	4.744503
F	2.415866	4.588834	3.372526
H	1.319298	2.731808	1.983528
C	0.080551	2.425394	-0.489991
H	-0.247970	2.271511	0.535145
H	0.153909	3.505566	-0.637329
H	-0.705866	2.050710	-1.152659
C	4.504771	-0.415792	0.015425

H	5.361594	-0.421130	-0.669122
H	4.912266	-0.324500	1.030921
H	4.031821	-1.394087	-0.061948
C	2.917648	-0.914841	-2.479354
H	3.427927	-1.880511	-2.544887
H	2.399132	-0.753269	-3.430293
H	3.666355	-0.141428	-2.369935
N	1.383019	1.848154	-0.759462
N	3.588206	0.653767	-0.303472
N	1.957845	-0.918384	-1.384522
C	1.873850	2.286740	-2.055002
H	1.956181	3.376193	-2.071884
H	2.855695	1.882158	-2.277098
H	1.196786	1.990876	-2.865062
C	4.199600	1.939176	-0.054497
H	3.475320	2.746362	-0.089778
H	4.685475	1.983330	0.928052
H	4.974822	2.149597	-0.803082
C	0.914789	-1.878623	-1.709622
H	0.304607	-1.540232	-2.553990
H	1.386523	-2.819472	-2.005699
H	0.250899	-2.083768	-0.883371

$(12c^{thr} \rightarrow 11c^{thr-sc})^\ddagger$

$E = -1788.090788675$ au

ZPE = 0.48557710 au

$G_{corr} = 0.43252960$ au

$\nu = -178.04$ cm⁻¹

O	-0.037604	-0.480655	-0.147040
P	-0.073177	-0.172662	1.411786
C	1.805351	-0.070981	1.423234
P	2.105527	0.365871	-0.352386
C	-0.410460	-1.745705	2.394254
C	0.073584	-1.473890	3.818416
H	-0.306187	-0.523360	4.201298
H	-0.268219	-2.260786	4.496571
H	1.163555	-1.440410	3.881763
C	-1.934319	-1.897406	2.392453
H	-2.236653	-2.759794	2.993382
H	-2.426523	-1.015323	2.806863
H	-2.319313	-2.047859	1.381596
C	0.213454	-3.024473	1.856932
H	-0.152267	-3.254205	0.856092
H	1.304445	-2.977785	1.821003
H	-0.042244	-3.871843	2.500325
H	2.224900	-1.083226	1.491669
C	2.498205	0.820478	2.399192
C	3.601638	0.362606	3.114195
C	4.222179	1.207233	4.013630
C	3.792727	2.499553	4.240892

C	2.686609	2.919650	3.525908
C	2.029003	2.113781	2.620591
H	3.975090	-0.643522	2.973345
F	5.284154	0.759497	4.693463
H	4.289752	3.147074	4.950470
F	2.238311	4.163748	3.728506
H	1.154829	2.485737	2.103752
C	0.052097	2.247043	-0.654575
H	-0.255133	2.073301	0.372293
H	0.047647	3.327427	-0.812848
H	-0.690207	1.795268	-1.313640
C	4.820394	-0.004913	-0.131922
H	5.624472	0.200679	-0.845896
H	5.246759	0.079951	0.873329
H	4.507644	-1.035551	-0.276366
C	3.066168	-0.724845	-2.643644
H	3.713626	-1.582870	-2.837242
H	2.370111	-0.633635	-3.483000
H	3.697154	0.157144	-2.623152
N	1.402053	1.779349	-0.920772
N	3.723340	0.922281	-0.317998
N	2.362338	-0.926568	-1.386226

C	1.886259	2.310998	-2.188828	H	4.561960	2.319645	1.024669
H	1.795128	3.398467	-2.176976	H	4.860163	2.644832	-0.685149
H	2.932146	2.078982	-2.360793	C	1.652365	-2.190125	-1.373333
H	1.304095	1.933688	-3.035416	H	0.752949	-2.179156	-1.990778
C	4.114418	2.273841	0.026140	H	2.331230	-2.950786	-1.766633
H	3.268891	2.953712	0.012778	H	1.370881	-2.485354	-0.373510

11c^{thr-sc}

$E = -1788.102799634$ au

ZPE = 0.48525392 au

$G_{\text{corr}} = 0.43174636$ au

O	-0.662503	-0.850821	-0.073090	H	0.926695	2.409744	1.943970
P	-0.273526	-0.269891	1.297851	C	0.182917	2.121881	-0.829782
C	1.703212	-0.099932	1.162780	H	-0.180495	1.866147	0.161623
P	2.327187	0.449486	-0.440243	H	0.039931	3.194024	-0.966704
C	-0.359150	-1.702678	2.544118	H	-0.424129	1.586944	-1.560620
C	0.238647	-1.292805	3.885744	C	4.977569	-0.094256	-0.274361
H	-0.110636	-0.305146	4.197356	H	5.839370	0.225799	-0.863621
H	-0.044882	-2.003676	4.668191	H	5.311798	-0.243313	0.756669
H	1.328503	-1.260290	3.862067	H	4.642044	-1.050618	-0.666378
C	-1.867420	-1.917634	2.714575	C	2.823028	-0.606595	-2.849474
H	-2.062017	-2.723293	3.428754	H	3.421272	-1.464853	-3.161454
H	-2.360981	-1.018116	3.090647	H	1.995443	-0.494713	-3.554424
H	-2.341536	-2.185607	1.769089	H	3.461036	0.270643	-2.920322
C	0.265012	-2.997172	2.043182	N	1.607868	1.847059	-0.977254
H	-0.139522	-3.273511	1.068408	N	3.931945	0.909155	-0.354880
H	1.352971	-2.928795	1.954950	N	2.344800	-0.822537	-1.494022
H	0.060955	-3.822115	2.733096	C	2.166571	2.557795	-2.122726
H	2.137906	-1.101866	1.251778	H	2.034820	3.630221	-1.971671
C	2.297886	0.766328	2.230220	H	3.229488	2.370252	-2.242798
C	3.374595	0.303071	2.986399	H	1.660248	2.281769	-3.051640
C	3.910964	1.110908	3.967107	C	4.354064	2.196770	0.172899
C	3.432136	2.379674	4.234036	H	3.533194	2.906542	0.197608
C	2.362265	2.807685	3.473066	H	4.744013	2.099854	1.189439
C	1.782276	2.034524	2.486706	H	5.145936	2.609707	-0.456858
H	3.785692	-0.684076	2.817271	C	1.718074	-2.120221	-1.318294
F	4.942591	0.655342	4.687997	H	0.831509	-2.219500	-1.943345
H	3.865756	3.000541	5.006182	H	2.439528	-2.892713	-1.595866
F	1.866892	4.028202	3.707542	H	1.403485	-2.289172	-0.298827

(12c^{thr}→9c+10Z)[‡]

$E = -1788.092134879$ au

ZPE = 0.48434410 au

$G_{\text{corr}} = 0.43077608$ au

$\nu = -193.75$ cm⁻¹

O	0.421058	-0.505419	0.342505	C	0.433332	-2.036830	2.618123
P	0.335186	-0.258487	2.041666	C	0.620575	-1.963299	4.135017
C	2.010857	0.342550	2.121068	H	-0.156424	-1.362045	4.612971
P	1.786735	0.071217	-0.301354	H	0.570650	-2.965250	4.568294

H	1.586102	-1.532685	4.405526
C	-0.914225	-2.689316	2.298942
H	-0.940362	-3.712197	2.684158
H	-1.744448	-2.143677	2.750907
H	-1.094319	-2.740154	1.223543
C	1.553204	-2.855229	1.985527
H	1.430682	-2.945975	0.905685
H	2.540824	-2.435853	2.181703
H	1.547733	-3.868418	2.396647
H	2.722767	-0.383070	2.509332
C	2.251204	1.676092	2.649710
C	3.455493	1.967418	3.315322
C	3.721382	3.252544	3.732612
C	2.847222	4.307250	3.544214
C	1.658731	3.994574	2.907549
C	1.342306	2.731640	2.462290
H	4.176322	1.182818	3.510388
F	4.883508	3.498473	4.359322
H	3.072211	5.308805	3.882865
F	0.773337	4.985492	2.710321
H	0.391072	2.563699	1.974224
C	0.726062	2.390692	-1.124815
H	-0.194019	1.816755	-1.041480
H	0.549170	3.359042	-0.652304

H	0.924571	2.559611	-2.188623
C	3.499341	-1.922938	-1.042787
H	4.332978	-1.816448	-1.741667
H	3.743803	-2.731865	-0.348796
H	2.624886	-2.231149	-1.604125
C	2.119793	0.131971	-2.988337
H	2.685875	-0.686154	-3.450685
H	1.496676	0.578507	-3.769114
H	2.839190	0.885726	-2.673466
N	1.822098	1.738128	-0.436938
N	3.286089	-0.686127	-0.304960
N	1.300372	-0.319873	-1.889210
C	3.014908	2.537652	-0.299341
H	2.734386	3.553299	-0.018244
H	3.661761	2.170577	0.489658
H	3.597384	2.590735	-1.226870
C	4.394981	-0.443824	0.592941
H	4.310356	0.496381	1.120546
H	4.495083	-1.239344	1.338176
H	5.317855	-0.416041	0.008705
C	0.307814	-1.284547	-2.299085
H	-0.345710	-0.849142	-3.061602
H	0.762684	-2.180970	-2.742542
H	-0.315809	-1.601170	-1.471447

14

$E = -1118.388170323$ au

ZPE = 0.23031712 au

$G_{\text{corr}} = 0.18906029$ au

C	1.234854	0.710422	0.163139
O	0.874431	1.951777	-0.539083
H	1.932060	0.093852	-0.402768
C	-0.802590	0.287113	-2.072248
C	-1.507748	1.407911	-2.846367
H	-1.808631	1.032585	-3.826540
H	-2.404055	1.753772	-2.332197
H	-0.853515	2.265450	-3.008753
C	0.460122	-0.152244	-2.807695
H	0.966280	-0.975516	-2.301690
H	0.186784	-0.508958	-3.802510
H	1.169605	0.665069	-2.935196
C	-1.752779	-0.897137	-1.878415
H	-2.656334	-0.608272	-1.343446
H	-2.048692	-1.287408	-2.854089

H	-1.281721	-1.713674	-1.328437
C	1.580713	0.841743	1.595807
C	2.310770	-0.184457	2.189392
C	1.172967	1.937969	2.347029
C	2.613525	-0.097396	3.532449
H	2.644763	-1.040533	1.617338
C	1.511210	1.978883	3.684834
H	0.607722	2.747809	1.908736
C	2.228435	0.976873	4.310047
H	2.479803	1.033584	5.360023
F	1.131473	3.030520	4.411519
F	3.312591	-1.081655	4.101899
P	-0.421488	0.967087	-0.417313
O	-1.589575	1.308302	0.415706