

Supporting information for

Relative stability of benziporphyrin and naphthiporphyrin tautomers and the emergence of macrocyclic diatropicity.

Deyaa I. AbuSalim and Timothy D. Lash*

Department of Chemistry, Illinois State University, Normal, Illinois 61790-4160

E-mail: tdlash@ilstu.edu

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Molecule	<i>a</i>	<i>b</i>	<i>c</i>	<i>d</i>
BzP-24-H	0.00	0.00	0.00	0.00
BzP-23-H	0.02	0.02	0.01	0.02
BzP-22-H	0.00	0.00	0.00	0.00
BzP-11-H	0.01	0.01	0.01	0.02
BzP-6-H	0.04	0.06	0.08	0.05
BzP-23,25-H ⁺	12.91	4.55	2.84	4.57
BzP-23,24-H ⁺	10.65	3.24	5.16	9.95
BzP-22,24-H ⁺	0.00	0.00	0.00	0.00
BzP-22,23-H ⁺	0.00	0.00	0.00	0.00
BzP-23,24,25-H ²⁺	17.54	14.83	15.18	2.12
BzP-22,23,25-H ²⁺	0.00	0.00	0.00	0.00
BzP-22,23,24-H ²⁺	0.00	0.00	0.00	0.00
24-O-BzP	0.00	0.00	0.00	0.00
24-S-BzP	0.00	0.00	0.01	0.00
24-O-BzPH ₂ ²⁺	16.50	9.28	4.63	9.28
24-S-BzPH ₂ ²⁺	13.83	10.68	17.03	10.68
DiOMe-BzP-24-H	0.01	0.01	0.01	0.01
DiOMe-BzP-23-H	0.01	0.01	0.01	0.01
DiOMe-BzPH ₂ ²⁺	10.24	16.09	17.06	16.09
NP-24-H	0.00	0.00	0.00	0.00
NP-23-H	0.00	0.00	0.00	0.00
NPH ₂ ²⁺	13.66	21.53	20.94	16.19
OBP-23,24-H	4.65	1.76	3.87	7.82
OBP-24,25-H	4.33	8.17	4.17	1.76
OBP-23,25-H	3.82	1.79	1.02	1.63
OBP-O,24-H-L	0.01	0.01	0.02	0.01
OBP-O,24-H-R	2.49	2.77	0.97	1.12
OBP-O,23-H-L	0.02	0.01	0.00	0.01
OBP-O,23-H-R	1.57	1.79	0.66	0.94
OBP-23,24,25-H ⁺	10.66	13.45	14.26	13.14
OBP-O,23,25-H ⁺ -L	10.82	5.52	3.21	4.63
OBP-O,23,25-H ⁺ -R	13.95	9.39	4.69	6.64
OBP-O,23,24-H ⁺ -L	7.97	3.59	5.38	9.64
OBP-O,23,24-H ⁺ -R	11.21	7.10	6.73	11.18
OBP-O,24,25-H ⁺ -L	8.59	10.82	5.70	3.37
OBP-O,24,25-H ⁺ -R	11.62	13.96	7.04	5.21
OBPH ₂ ²⁺ -L	14.44	15.93	15.62	14.41
OBPH ₂ ²⁺ -R	15.62	18.54	16.50	15.74

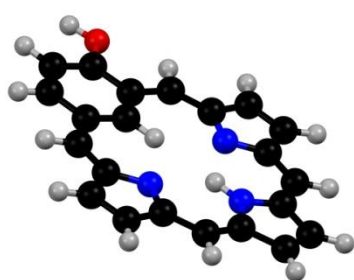
ONP-23,25-H	4.38	3.34	2.72	4.16
ONP-23,24-H	6.50	4.85	6.64	11.78
ONP-24,25-H	3.26	8.05	5.64	3.95
ONP-O,24-H-L	0.87	1.24	0.90	1.42
ONP-O,24-H-R	4.78	5.91	3.11	4.66
ONP-O,23-H-L	0.95	1.23	0.99	1.45
ONP-O,23-H-R	3.98	4.61	2.76	4.14
ONP-23,24,25-H⁺	11.05	15.04	18.98	19.62
ONP-O,23,25-H⁺-L	10.35	9.45	7.65	11.57
ONP-O,23,25-H⁺-R	12.29	12.54	8.68	13.23
ONP-O,23,24-H⁺-L	9.13	8.57	10.08	16.39
ONP-O,23,24-H⁺-R	11.14	11.33	11.14	17.72
ONP-O,24,25-H⁺-L	8.17	12.33	9.52	9.20
ONP-O,24,25-H⁺-R	10.09	15.45	10.52	10.70
ONPH₂²⁺-L	13.01	17.62	20.55	22.17
ONPH₂²⁺-R	12.57	20.27	21.07	27.98
HDBP-23,25-H	8.15	4.29	3.52	4.28
HDBP-23,24-H	8.46	4.84	6.74	9.54
HDBPH₂²⁺	12.44	14.55	16.97	14.76
5-BPhlH⁺	46.95	18.06	21.93	12.36
10-BPhlH⁺	17.87	11.14	46.25	12.06
5-BPhl-23,25-H	40.18	22.44	13.81	5.54
5-BPhl-24,25-H	39.54	19.84	15.48	6.60
5-BPhl-23,24-H	34.16	28.08	10.65	5.15
10-BPhl-24,25-H	9.09	9.89	22.28	8.85

Table S1. Angles (deg.) between the plane of each of the individual rings (pyrrole and benzene) and the overall plane of the macrocycle.

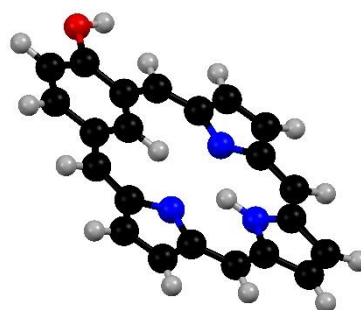
Molecule	Dihedral <i>ab</i>	Dihedral <i>bc</i>	Dihedral <i>cd</i>	Dihedral <i>da</i>
BzP-24-H	0.00	-0.01	0.00	0.00
BzP-23-H	-0.02	0.02	0.01	-0.01
BzP-22-H	-0.01	0.00	0.00	0.00
BzP-11-H	0.00	0.00	0.02	-0.02
BzP-6-H	-0.08	0.10	-0.08	0.06
BzP-23,25-H+	-12.57	2.09	-2.09	12.58
BzP-23,24-H+	-9.89	2.45	-8.05	14.20
BzP-22,24-H+	0.00	0.00	0.00	0.00
BzP-22,23-H+	0.00	0.00	0.00	0.00
BzP-23,24,25-H2+	-21.32	15.71	-15.71	21.32
BzP-22,23,25-H2+	0.00	0.00	0.00	0.00
BzP-22,23,24-H2+	0.00	0.00	0.00	0.00
24-O-BzP	0.01	0.00	0.00	-0.01
24-S-BzP	-0.01	0.02	-0.02	0.01
24-O-BzPH2 2+	-18.09	5.83	-5.83	18.09
24-S-BzPH2 2+	17.50	-18.14	18.13	-17.50
DiOMe-BzP-24-H	0.02	-0.01	0.01	-0.01
DiOMe-BzP-23-H	0.00	0.00	0.01	-0.01
DiOMe-BzPH2 2+	-19.13	15.66	-15.66	19.14
NP-24-H	0.01	-0.01	0.00	0.00
NP-23-H	0.00	0.00	0.00	0.00
NPH2 2+	27.07	-17.84	15.39	-20.59
OBP-23,24-H	4.56	-1.75	6.57	-8.90
OBP-24,25-H	9.02	-6.82	2.07	-3.96
OBP-23,25-H	4.40	-0.84	0.75	-4.07
OBP-O,24-H-L	0.01	0.00	-0.02	0.00
OBP-O,24-H-R	-4.41	1.34	-0.43	2.03
OBP-O,23-H-L	-0.02	0.01	0.00	0.01
OBP-O,23-H-R	2.74	-1.06	0.29	-1.39

Molecule	Dihedral <i>ab</i>	Dihedral <i>bc</i>	Dihedral <i>cd</i>	Dihedral <i>da</i>
OBP-23,24,25-H+	-16.61	13.95	-14.29	16.21
OBP-O,23,25-H+-L	12.32	-2.66	2.10	-11.08
OBP-O,23,25-H+-R	18.53	-4.69	2.72	-13.77
OBP-O,23,24-H+-L	-8.68	2.72	-8.12	12.30
OBP-O,23,24-H+-R	-14.59	4.25	-8.66	15.13
OBP-O,24,25-H+-L	13.91	-8.66	2.75	-8.32
OBP-O,24,25-H+-R	19.38	-10.09	3.42	-11.14
OBPH2 2+-L	-20.87	15.88	-15.54	19.49
OBPH2 2+-R	-24.79	17.15	-16.06	20.80
ONP-23,25-H	-3.93	0.63	-1.90	6.91
ONP-23,24-H	5.41	-2.45	8.13	-13.66
ONP-24,25-H	-8.49	6.62	-2.66	6.03
ONP-O,24-H-L	1.33	-0.45	0.54	-1.59
ONP-O,24-H-R	8.95	-2.55	1.52	-5.97
ONP-O,23-H-L	-1.31	0.55	-0.43	1.75
ONP-O,23-H-R	-7.03	2.42	-1.17	5.70
ONP-23,24,25-H+	-17.10	14.53	-16.32	22.72
ONP-O,23,25-H+-L	-13.85	2.83	-4.92	18.44
ONP-O,23,25-H+-R	-19.77	4.88	-5.35	20.32
ONP-O,23,24-H+-L	-12.34	3.97	-10.66	20.36
ONP-O,23,24-H+-R	-17.63	5.34	-11.09	22.21
ONP-O,24,25-H+-L	15.25	-8.86	4.60	-14.27
ONP-O,24,25-H+-R	20.24	-10.36	5.17	-16.03
ONPH2 2+-L	21.44	-16.10	17.92	-26.40
ONPH2 2+-R	25.29	-17.31	18.33	-27.32
HDBP-23,25-H	-5.68	1.13	-1.26	5.55
HDBP-23,24-H	-5.41	2.53	-7.30	10.04
HDBPH2 2+	-16.33	14.43	-14.56	16.21
5-BPhlH+	35.32	-9.91	15.96	-40.84
10-BPhlH+	8.30	-25.84	33.70	-15.55
5-BPhl-23,25-H	17.98	7.29	5.12	-31.79
5-BPhl-24,25-H	-18.22	-4.12	-8.67	21.53
5-BPhl-23,24-H	-7.56	-15.44	0.29	26.32
10-BPhl-24,25-H	-0.90	-7.98	17.38	-9.54

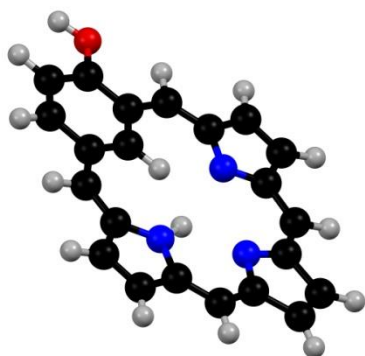
Table S2. Dihedral angles (deg.) between the four individual rings in each macrocycle.



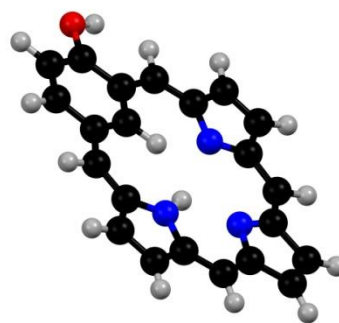
OBP-O,24-H-L



OBP-O,24-H-R



OBP-O,23-H-L



OBP-O,23-H-R

Figure S1. Mercury 3.1 renderings of the minimized conformations for 2-hydroxybenzoporphyrins.

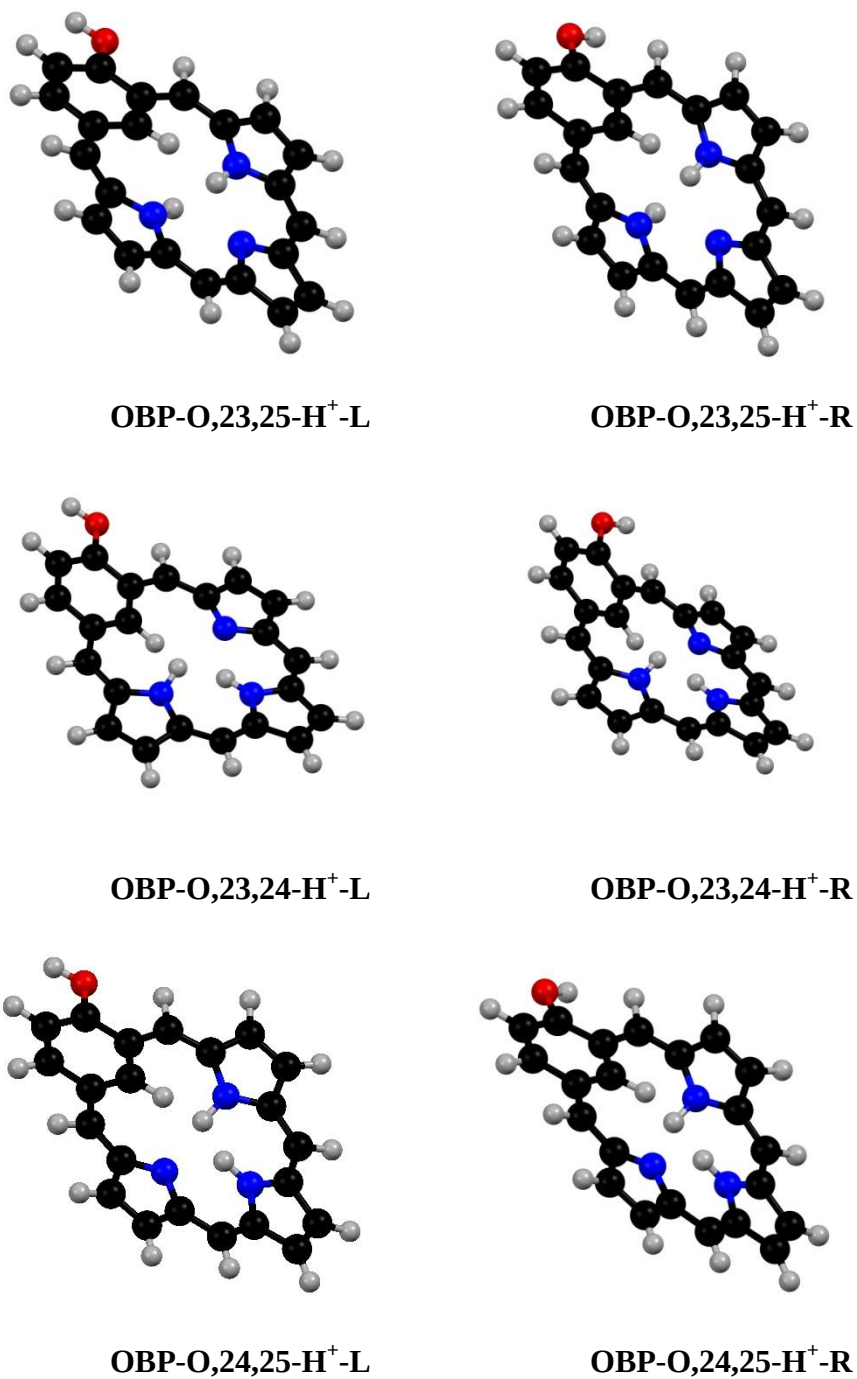


Figure S2. Mercury 3.1 renderings of the minimized conformations for monoprotonated 2-hydroxybenziporphyrins.

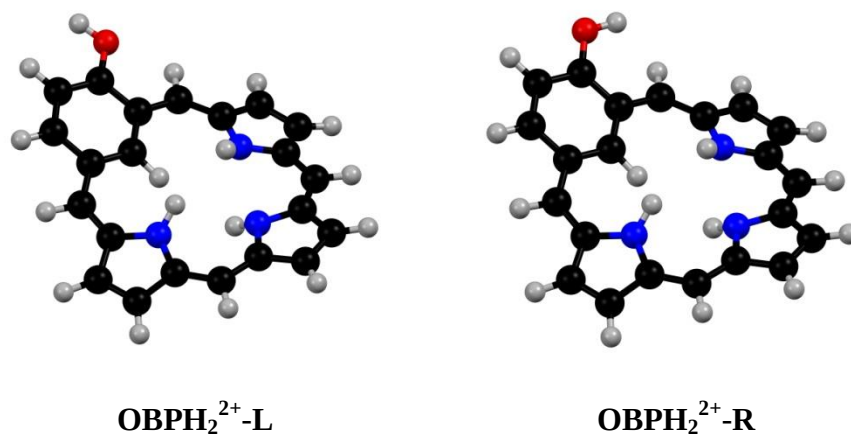
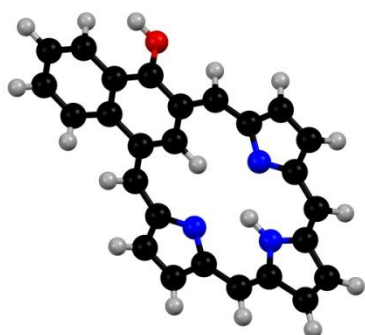
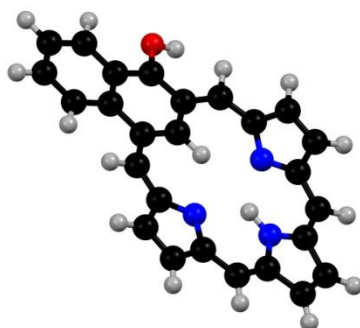


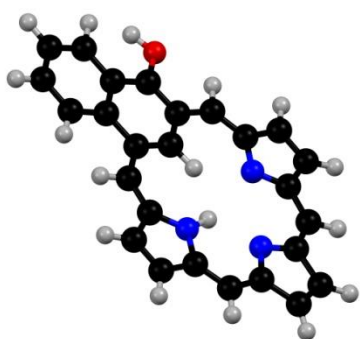
Figure S3. Mercury 3.1 renderings of the minimized conformations for diprotonated oxybenzporphyrin.



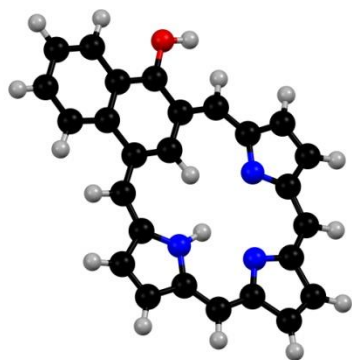
ONP-O,24-H-L



ONP-O,24-H-R



ONP-O,23-H-L



ONP-O,23-H-R

Figure S4. Mercury 3.1 renderings of the minimized conformations for hydroxy-naphthiporphyrins.

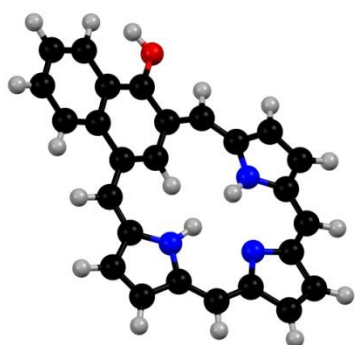
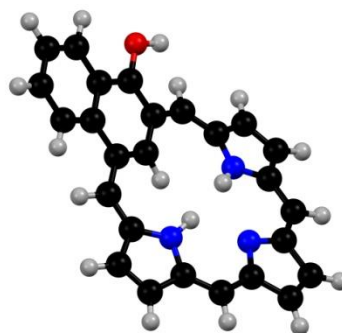
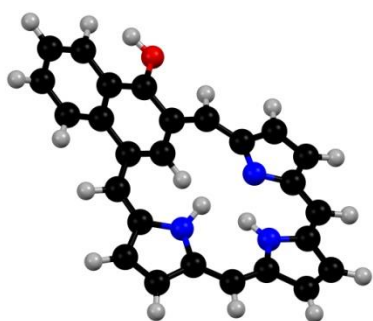
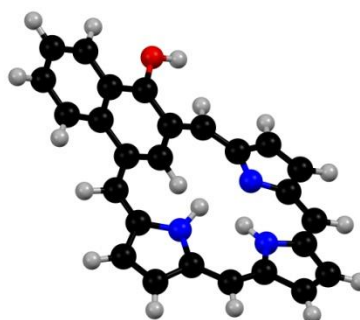
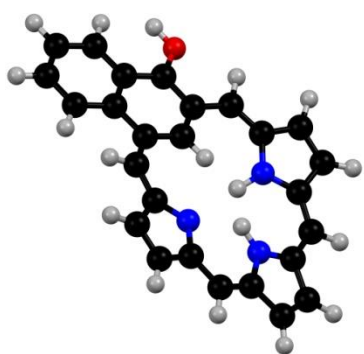
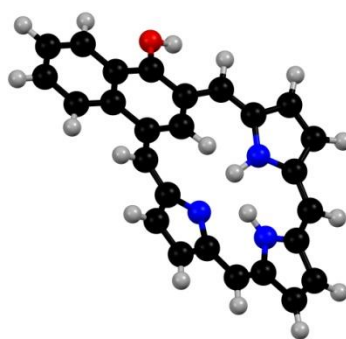
ONP-O,23,25-H⁺-LONP-O,23,25-H⁺-RONP-O,23,24-H⁺-LONP-O,23,24-H⁺-RONP-O,24,25-H⁺-LONP-O,24,25-H⁺-R

Figure S5. Mercury 3.1 renderings of the minimized conformations for monoprotinated hydroxynaphthoporphyrins.

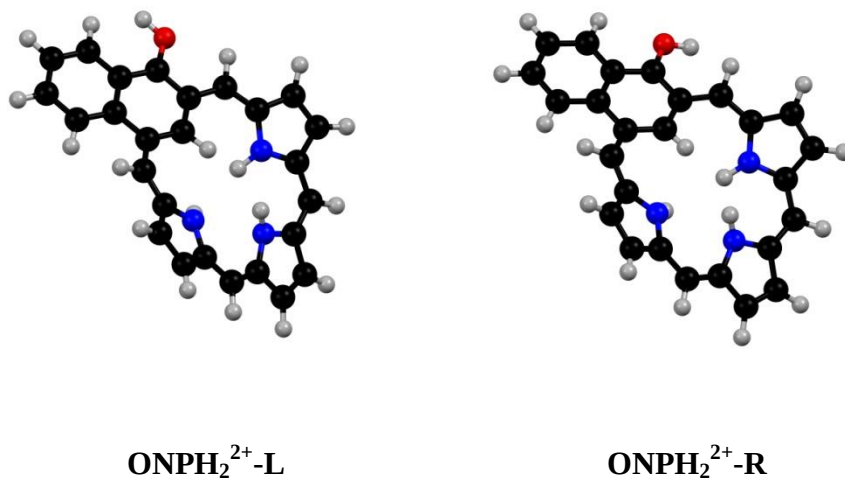


Figure S6. Mercury 3.1 renderings of the minimized conformations for diprotonated oxynaphthiporphyrin.

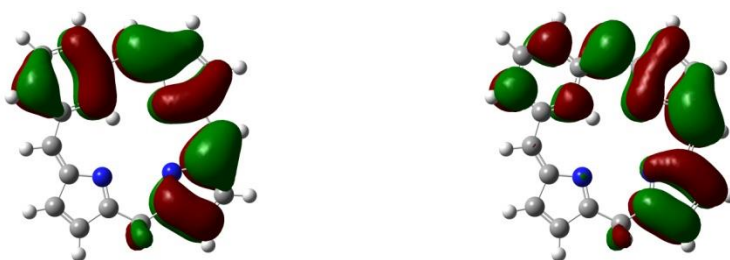
BzP-24-H**BzP-23-H****BzP-22-H****BzP-11-H**

Figure S7. HOMO and LUMO surfaces for benziporphyrin tautomers.

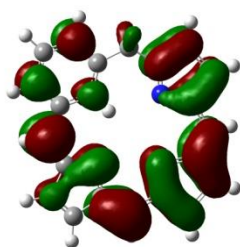
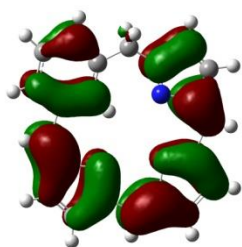
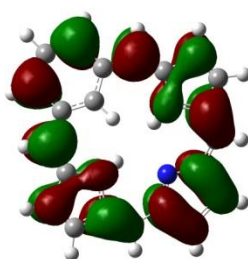
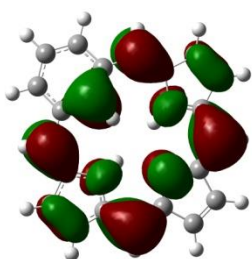
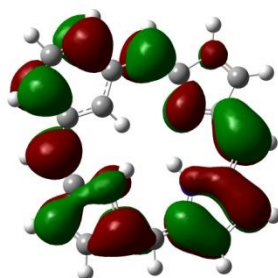
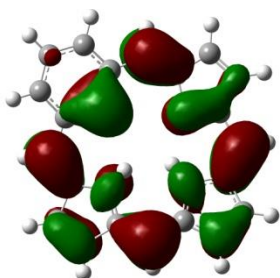
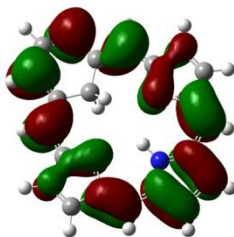
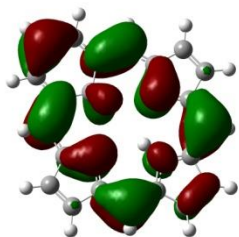
BzP-6-H**BzP-23,25-H⁺****BzP-23,24-H⁺****BzP-22,24-H⁺**

Figure S8. HOMO and LUMO surfaces for benziporphyrin tautomer **BzP-6-H** and benziporphyrin cations.

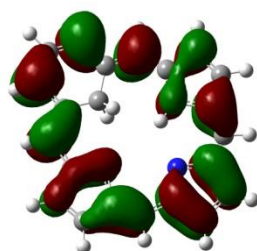
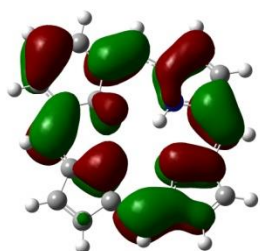
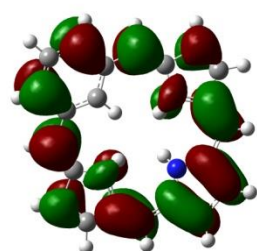
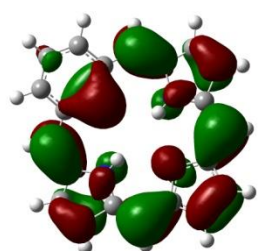
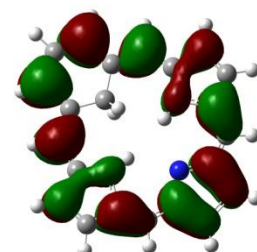
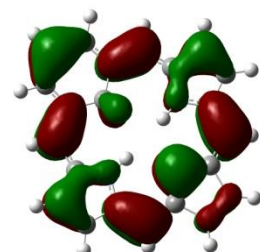
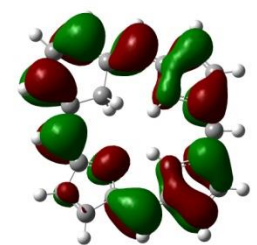
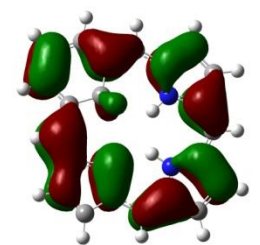
BzP-22,23-H⁺**BzP-23,24,25-H²⁺****BzP-22,23,25-H²⁺****BzP-22,23,24-H²⁺**

Figure S9. HOMO and LUMO surfaces for benziporphyrin mono- and dications.

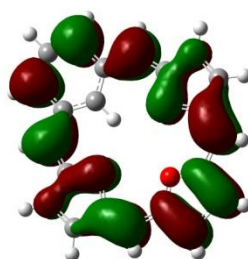
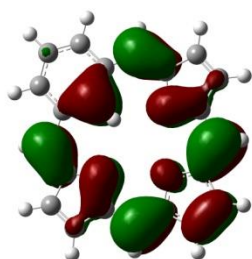
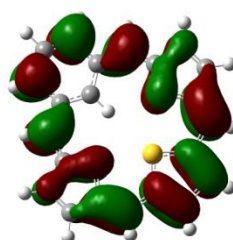
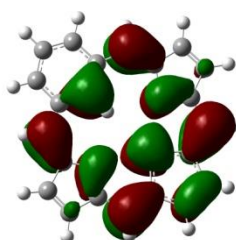
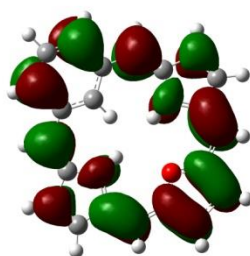
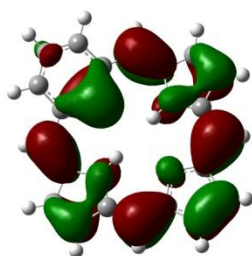
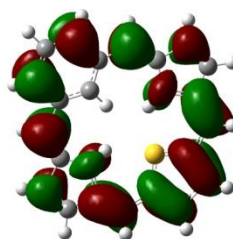
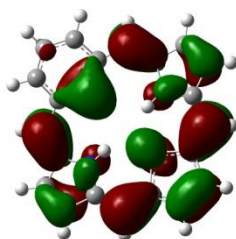
24-O-BzP**24-S-BzP****24-O-BzP-H²⁺****24-S-BzP-H²⁺**

Figure S10. HOMO and LUMO surfaces for heterobenziporphyrins and the related dications.

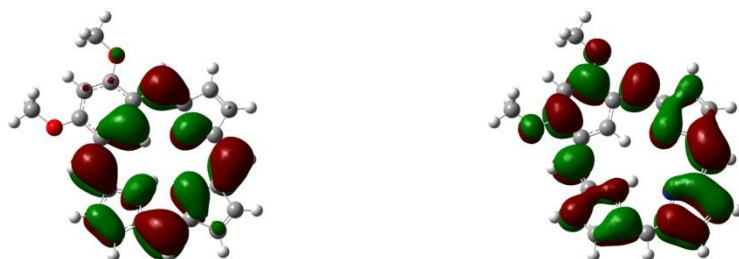
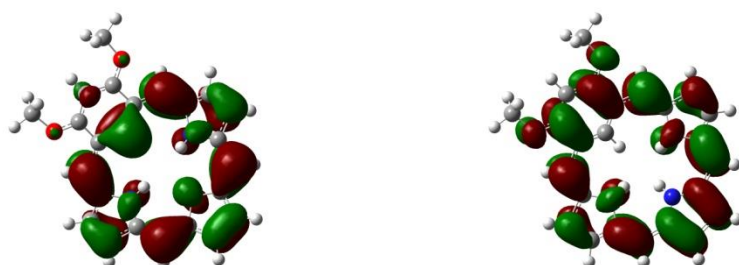
DiOMe-BzP-24-H**DiOMe-BzP-23-H****DiOMe-BzPH₂²⁺**

Figure S11. HOMO and LUMO surfaces for dimethoxybenziporphyrins and a related dication.

NP-24-H



NP-23-H

 NPH_2^{2+} 

Figure S12. HOMO and LUMO surfaces for naphthiporphyrins and a related dication.

OBP-23,24-H



OBP-24,25-H



OBP-23,25-H



Figure S13. HOMO and LUMO surfaces for oxybenziporphyrins.

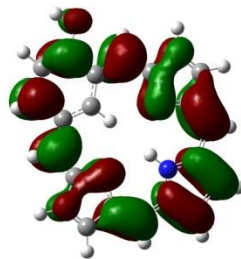
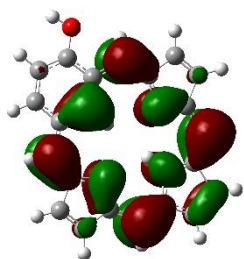
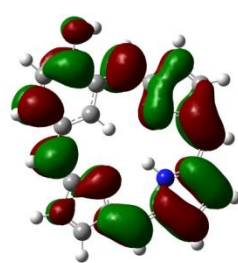
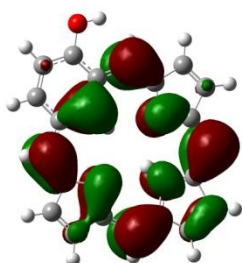
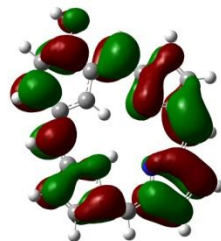
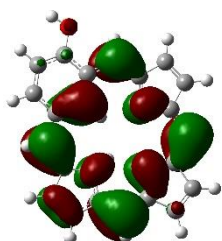
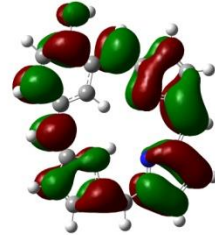
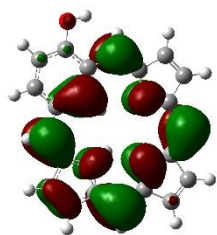
OBP-O,24-H-L**OBP-O,24-H-R****OBP-O,23-H-L****OBP-O,23-H-R**

Figure S14. HOMO and LUMO surfaces for hydroxybenziporphyrins.

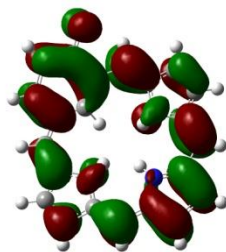
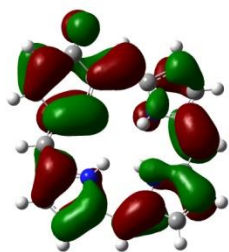
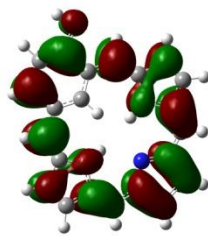
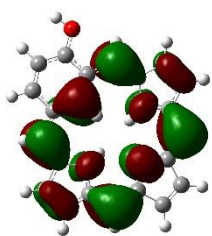
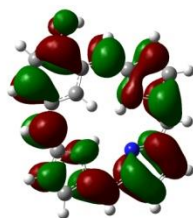
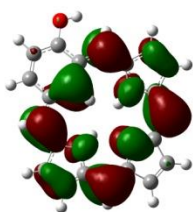
OBP-23,24,25-H⁺**OBP-O,23,25-H⁺-L****OBP-O,23,25-H⁺-R**

Figure S15. HOMO and LUMO surfaces for oxybenziporphyrin cations.

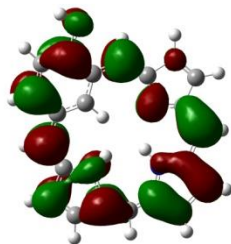
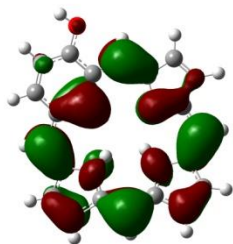
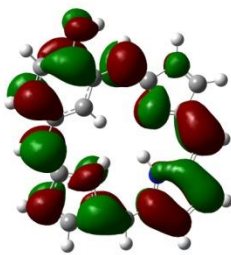
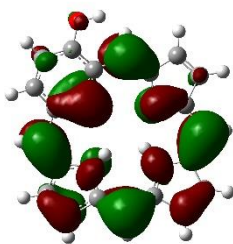
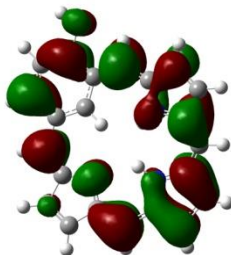
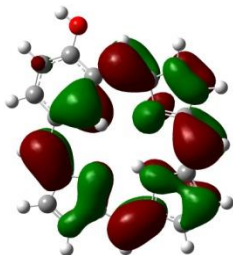
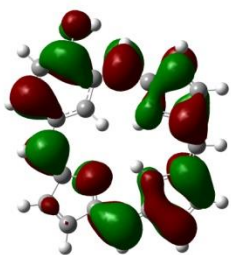
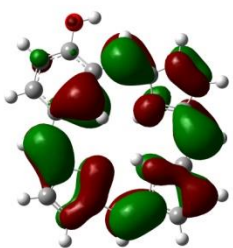
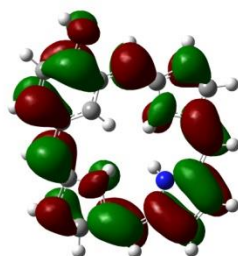
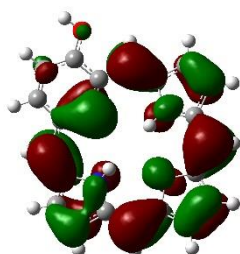
OBP-O,23,24-H⁺-LOBP-O,23,24-H⁺-ROBP-O,24,25-H⁺-LOBP-O,24,25-H⁺-R

Figure S16. HOMO and LUMO surfaces for oxybenziporphyrin cations.

OBPH₂²⁺-L



OBPH₂²⁺-R

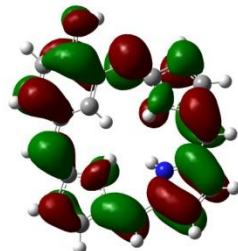
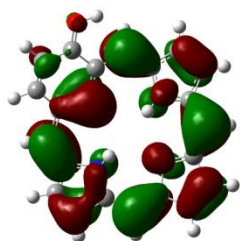


Figure S17. HOMO and LUMO surfaces for oxybenziporphyrin dications.

ONP-23,25-H



ONP-23,24-H



ONP-24,25-H

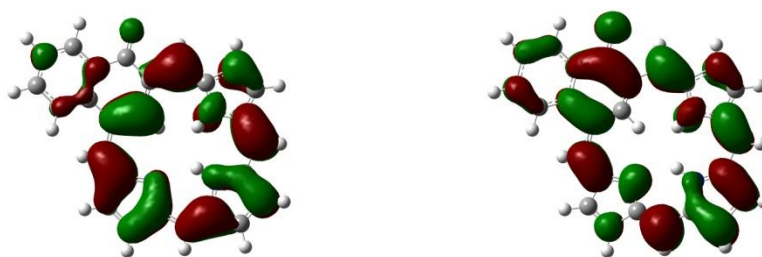


Figure S18. HOMO and LUMO surfaces for oxynaphthiporphyrins.

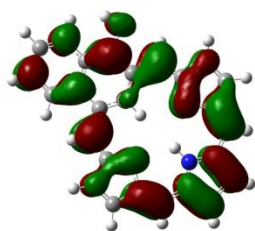
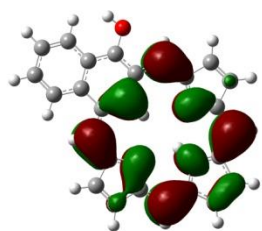
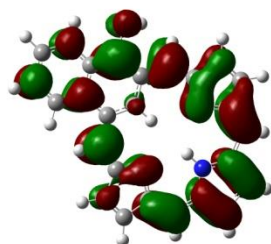
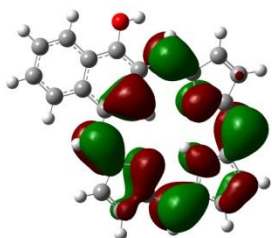
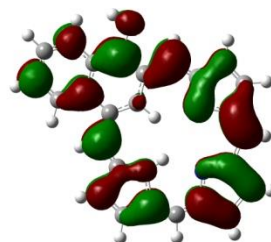
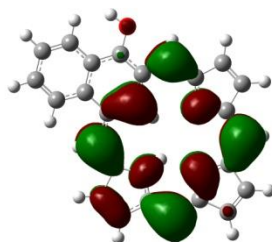
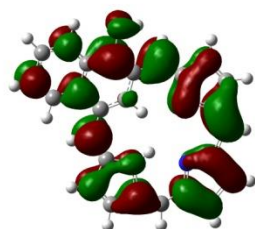
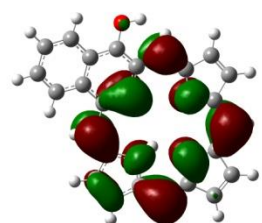
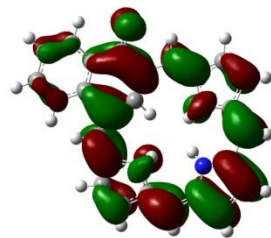
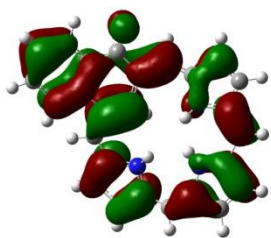
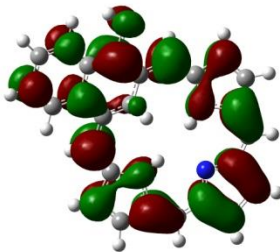
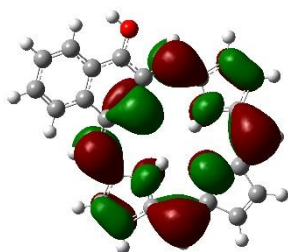
ONP-O,24-H-L**ONP-O,24-H-R****ONP-O,23-H-L****ONP-O,23-H-R**

Figure S19. HOMO and LUMO surfaces for hydroxynaphthiporphyrins.

ONP-23,24,25-H⁺



ONP-O,23,25-H⁺-L



ONP-O,23,25-H⁺-R

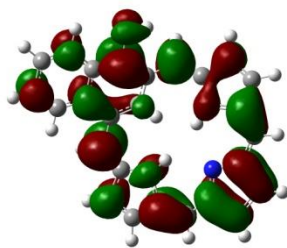
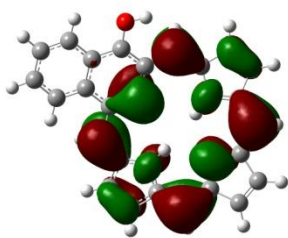
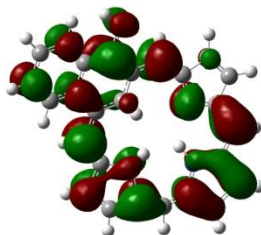
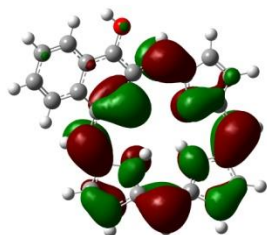
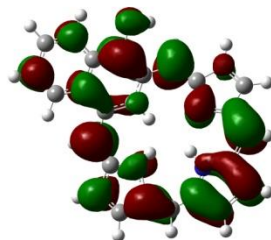
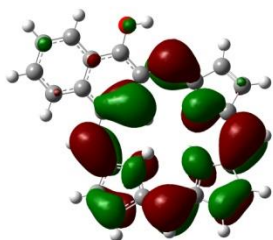


Figure S20. HOMO and LUMO surfaces for oxynaphthiporphyrin cations.

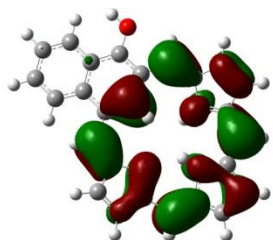
ONP-O,23,24-H⁺-L



ONP-O,23,24-H⁺-R



ONP-O,24,25-H⁺-L



ONP-O,24,25-H⁺-R

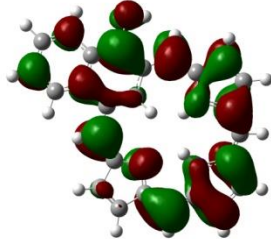
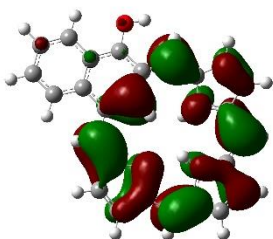
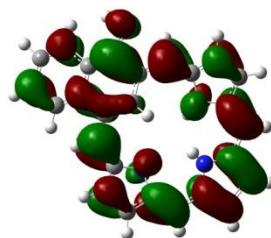
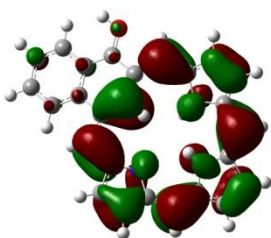


Figure S21. HOMO and LUMO surfaces for oxynaphthiporphyrin cations.

ONPH₂²⁺-L



ONPH₂²⁺-R

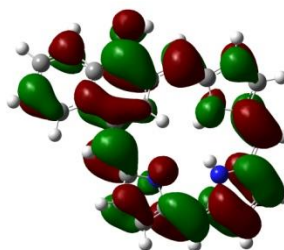
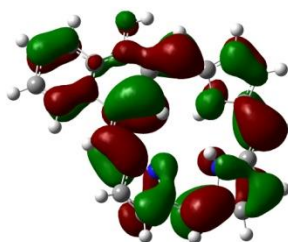


Figure S22. HOMO and LUMO surfaces for oxynaphthiporphyrin dications.

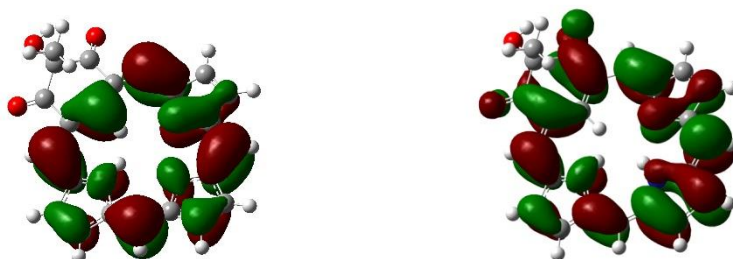
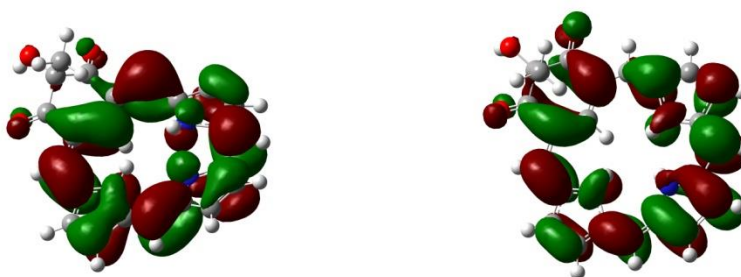
HDBP-23,25-H**HDBP-23,24-H****HDBPH⁺**

Figure S23. HOMO and LUMO surfaces for 3-hydroxy-3-methyl-2,4-dioxotetrahydrobenzporphyrin and a related cation.

5-BPhlH⁺**10-BPhlH⁺**

Figure S24. HOMO and LUMO surfaces for benziphlorin cations.

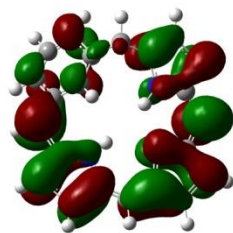
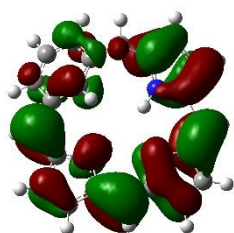
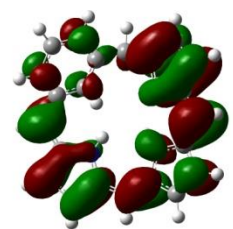
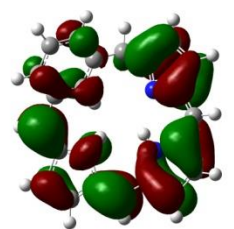
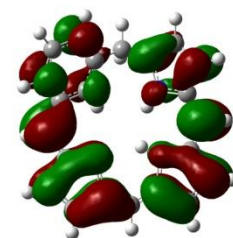
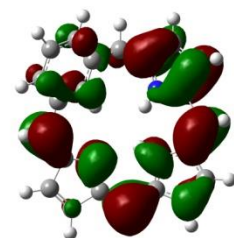
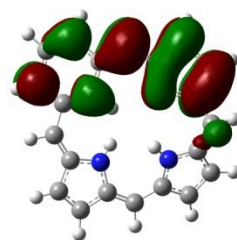
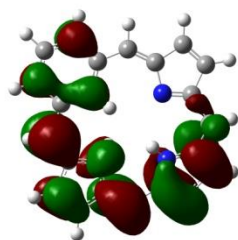
5-BPhl-23,25-H**5-BPhl-24,25-H****5-BPhl-23,24-H****10-BPhl-24,25-H**

Figure S25. HOMO and LUMO surfaces for benziphlorins.

Cartesian Coordinates

The following pages contain Cartesian coordinates for all of the benziporphyrin tautomers, heterobenziporphyrins, naphthiporphyrins, oxybenziporphyrins and related systems examined in this study.

BzP-24-H $\Delta G(\text{B3LYP})$: -1011.564961 $E(\text{B3LYP})$: -1011.830884 $E(\text{M06-2X})$: -1011.397259 $E(\text{B3LYP-D})$: -1011.870395

	X	Y	Z
C	0.42448	-4.29682	-0.00002
C	-0.92538	-4.28477	-0.00002
C	-1.31774	-2.87008	0.00001
N	-0.25566	-2.06109	-0.00002
C	0.85297	-2.89374	0.00000
C	2.79818	-1.22089	0.00001
C	2.79818	1.22088	0.00000
C	2.17211	-2.52703	0.00000
C	-0.92538	4.28477	0.00001
C	0.42449	4.29682	0.00001
C	0.85297	2.89374	0.00000
N	-0.25566	2.06109	0.00007
C	-1.31774	2.87008	-0.00006
C	2.17211	2.52703	-0.00001
C	-4.48622	-0.67824	0.00003
C	-4.48622	0.67824	0.00002
C	-3.10860	1.13236	-0.00002
N	-2.32699	0.00000	-0.00003
C	-3.10860	-1.13236	0.00001
C	-2.67091	-2.43552	0.00002
C	-2.67091	2.43552	-0.00004
C	2.10292	0.00000	0.00000
C	4.21149	1.19850	0.00000
C	4.91193	0.00000	0.00001
C	4.21149	-1.19850	0.00001
H	1.08765	-5.15036	-0.00002
H	-1.60454	-5.12561	-0.00003
H	2.87117	-3.35894	0.00000
H	-1.60453	5.12561	0.00001
H	1.08766	5.15036	0.00001
H	2.87118	3.35894	-0.00003
H	-5.33906	-1.34033	0.00006

H	-5.33906	1.34033	0.00003
H	-1.31078	0.00000	-0.00007
H	-3.43689	-3.20192	0.00005
H	-3.43689	3.20192	-0.00003
H	1.02538	0.00000	-0.00001
H	4.75366	2.13837	0.00000
H	5.99574	0.00000	0.00001
H	4.75366	-2.13838	0.00001

BzP-23-H $\Delta G(\text{B3LYP})$: -1011.553889 $E(\text{B3LYP})$: -1011.819398 $E(\text{M06-2X})$: -1011.397259 $E(\text{B3LYP-D})$: -1011.858503

	X	Y	Z
C	0.36679	-4.23149	0.00013
C	1.70861	-4.04108	-0.00027
C	1.95569	-2.61575	-0.00054
N	0.72962	-1.99649	-0.00066
C	-0.29327	-2.93551	0.00002
C	-2.51935	-1.62530	0.00017
C	-3.02997	0.76774	-0.00023
C	-1.65329	-2.78587	0.00027
C	0.15900	4.34538	-0.00027
C	-1.18300	4.19480	-0.00046
C	-1.42786	2.74824	-0.00018
N	-0.22638	2.06051	0.00013
C	0.72694	2.98491	0.00023
C	-2.66940	2.17207	-0.00039
C	4.60367	0.15889	0.00022
C	4.28845	1.47101	0.00035
C	2.81784	1.54993	0.00050
N	2.28302	0.28532	0.00000
C	3.32199	-0.56226	0.00000
C	3.17760	-1.96609	-0.00040
C	2.13391	2.74506	0.00062
C	-2.09728	-0.28666	-0.00028
C	-4.40658	0.45992	0.00003

C	-4.84208	-0.85987	0.00042
C	-3.91114	-1.88763	0.00049
H	-0.16640	-5.17059	0.00029
H	2.48444	-4.79164	-0.00030
H	0.69629	-0.97454	0.00030
H	-2.18184	-3.73375	0.00073
H	0.72820	5.26457	-0.00037
H	-1.94421	4.96215	-0.00078
H	-3.50847	2.86219	-0.00061
H	5.58400	-0.29617	0.00022
H	4.95750	2.32000	0.00045
H	4.06912	-2.58051	-0.00041
H	2.75137	3.63817	0.00076
H	-1.05363	-0.01269	-0.00062
H	-5.13043	1.26800	0.00004
H	-5.90221	-1.08536	0.00056
H	-4.25132	-2.91791	0.00078

BzP-22-H $\Delta G(\text{B3LYP})$: -1011.501311 $E(\text{B3LYP})$: -1011.762764 $E(\text{M06-2X})$: -1011.333353 $E(\text{B3LYP-D})$: -1011.801933

	X	Y	Z
C	0.38095	-4.35523	0.00003
C	-0.96953	-4.29819	-0.00005
C	-1.31894	-2.86796	-0.00003
N	-0.20511	-2.10042	-0.00007
C	0.83744	-2.95707	0.00003
C	2.74217	-1.28367	0.00008
C	2.74477	1.27871	0.00003
C	2.18288	-2.57018	0.00004
C	-0.96043	4.29978	0.00005
C	0.39012	4.35454	-0.00006
C	0.84407	2.95559	-0.00002
N	-0.19980	2.10069	-0.00009
C	-1.31250	2.87015	0.00000
C	2.18881	2.56631	0.00002
C	-4.50778	-0.67152	-0.00002

C	-4.50630	0.68044	0.00004
C	-3.08675	1.07973	0.00001
N	-2.27953	0.00209	0.00003
C	-3.08890	-1.07373	-0.00002
C	-2.63994	-2.40077	-0.00003
C	-2.63453	2.40572	0.00001
C	1.93444	-0.00170	0.00012
C	4.14520	1.20629	-0.00007
C	4.83014	-0.00477	-0.00006
C	4.14242	-1.21457	0.00002
H	1.01574	-5.23018	0.00007
H	-1.67389	-5.11832	-0.00008
H	2.89843	-3.38815	-0.00003
H	-1.66328	5.12125	0.00011
H	1.02619	5.22855	-0.00008
H	2.90587	3.38292	0.00004
H	-5.35744	-1.34005	-0.00004
H	-5.35456	1.35070	0.00007
H	-3.41080	-3.16624	-0.00004
H	-3.40360	3.17299	0.00004
H	1.22445	-0.00094	0.83738
H	1.22438	-0.00097	-0.83707
H	4.71133	2.13206	-0.00014
H	5.91422	-0.00625	-0.00011
H	4.70707	-2.14122	0.00002

BzP-11-H $\Delta G(\text{B3LYP})$: -1011.509964 $E(\text{B3LYP})$: -1011.772804 $E(\text{M06-2X})$: -1011.356942 $E(\text{B3LYP-D})$: -1011.810757

	X	Y	Z
C	0.29979	-4.34279	-0.00053
C	-1.04909	-4.26643	-0.00038
C	-1.37519	-2.82627	0.00015
N	-0.30983	-2.07693	0.00028
C	0.78084	-2.95766	-0.00017
C	2.74963	-1.30071	-0.00004
C	2.84386	1.13789	0.00013

C	2.09153	-2.60246	-0.00027
C	-0.75864	4.33150	-0.00021
C	0.59331	4.33181	-0.00008
C	0.99368	2.92095	-0.00005
N	-0.12561	2.10482	-0.00013
C	-1.16607	2.91501	-0.00022
C	2.28620	2.47979	0.00009
C	-4.55867	-0.43881	0.00023
C	-4.49562	0.91011	-0.00003
C	-3.06491	1.24628	-0.00013
N	-2.30203	0.07218	0.00007
C	-3.15206	-0.90836	0.00027
C	-2.80394	-2.36512	0.00058
C	-2.55170	2.50594	-0.00027
C	2.09135	-0.05598	0.00001
C	4.25480	1.06216	0.00027
C	4.90901	-0.16012	0.00026
C	4.16141	-1.32921	0.00008
H	0.92183	-5.22669	-0.00091
H	-1.76254	-5.07944	-0.00057
H	2.78435	-3.44072	-0.00057
H	-1.42616	5.18212	-0.00028
H	1.26404	5.17928	-0.00003
H	3.03480	3.26859	0.00017
H	-5.44127	-1.06429	0.00038
H	-5.31099	1.61954	-0.00015
H	-3.30335	-2.82970	0.86491
H	-3.30407	-2.83026	-0.86302
H	-3.27137	3.32012	-0.00039
H	1.00823	-0.01391	-0.00007
H	4.83174	1.98092	0.00038
H	5.99190	-0.20256	0.00036
H	4.66810	-2.28861	0.00004

BzP-6-H $\Delta G(\text{B3LYP}): -1011.507884$ $E(\text{B3LYP}): -1011.770864$ $E(\text{M06-2X}): -1011.352655$ $E(\text{B3LYP-D}): -1011.808967$

	X	Y	Z
C	-0.29764	-4.35176	-0.00208
C	1.05354	-4.28098	-0.00142
C	1.38493	-2.84748	-0.00033
N	0.29675	-2.09173	0.00012
C	-0.77023	-2.96373	-0.00092
C	-2.74086	-1.30257	0.00007
C	-2.83043	1.13211	0.00072
C	-2.09122	-2.59576	-0.00082
C	0.92930	4.30934	-0.00188
C	-0.41990	4.33396	-0.00211
C	-0.84691	2.91650	-0.00051
N	0.15987	2.09233	0.00035
C	1.31296	2.89193	-0.00058
C	-2.29845	2.55775	0.00021
C	4.56511	-0.61362	0.00232
C	4.52557	0.73773	0.00227
C	3.09236	1.09842	0.00027
N	2.31713	0.03515	-0.00092
C	3.16293	-1.05572	0.00050
C	2.73579	-2.35782	0.00053
C	2.60387	2.45290	-0.00044
C	-2.07950	-0.04427	0.00001
C	-4.23565	1.04843	0.00173
C	-4.89563	-0.17320	0.00186
C	-4.15125	-1.34171	0.00093
H	-0.92258	-5.23361	-0.00311
H	1.76460	-5.09545	-0.00184
H	-2.78601	-3.43246	-0.00150
H	1.61591	5.14398	-0.00274
H	-1.07301	5.19594	-0.00310
H	-2.74192	3.07429	0.86430
H	-2.74269	3.07391	-0.86370
H	5.43268	-1.25818	0.00365
H	5.35670	1.42945	0.00347

H	3.50800	-3.12220	0.00133
H	3.36819	3.22525	-0.00079
H	-0.99677	-0.00558	-0.00053
H	-4.81824	1.96509	0.00235
H	-5.97889	-0.21055	0.00261
H	-4.65430	-2.30275	0.00090

BzP-23,25-H⁺ $\Delta G(\text{B3LYP}): -1011.959691$ $E(\text{B3LYP}): -1012.238897$ $E(\text{M06-2X}): -1011.809356$ $E(\text{B3LYP-D}): -1012.280638$

	X	Y	Z
C	0.40795	-4.28182	-0.22170
C	-0.95003	-4.27953	-0.15392
C	-1.38282	-2.90943	-0.04104
N	-0.26569	-2.13094	-0.05283
C	0.87930	-2.91413	-0.15126
C	2.80179	-1.22395	-0.04533
C	2.80090	1.22542	-0.04642
C	2.19247	-2.53050	-0.14512
C	-0.95266	4.27912	-0.15280
C	0.40523	4.28185	-0.22200
C	0.87713	2.91422	-0.15250
N	-0.26749	2.13074	-0.05283
C	-1.38485	2.90878	-0.04023
C	2.19053	2.53145	-0.14698
C	-4.48040	-0.67371	0.20370
C	-4.48089	0.67099	0.20439
C	-3.07239	1.08505	0.12576
N	-2.24414	-0.00051	0.09219
C	-3.07163	-1.08669	0.12499
C	-2.68861	-2.42478	0.06202
C	-2.69030	2.42344	0.06333
C	2.13527	0.00043	-0.21852
C	4.18303	1.20037	0.25778
C	4.86495	0.00172	0.41063
C	4.18388	-1.19757	0.25893
H	1.06009	-5.13736	-0.31306

H	-1.61446	-5.12942	-0.17686
H	-0.34757	-1.13085	0.06656
H	2.89021	-3.36029	-0.18032
H	-1.61741	5.12878	-0.17451
H	1.05709	5.13761	-0.31337
H	-0.34938	1.13025	0.06338
H	2.88765	3.36172	-0.18303
H	-5.32353	-1.34751	0.24440
H	-5.32451	1.34414	0.24570
H	-3.47610	-3.16763	0.07848
H	-3.47824	3.16580	0.08039
H	1.11861	-0.00008	-0.58075
H	4.71359	2.13853	0.37552
H	5.92291	0.00220	0.64193
H	4.71513	-2.13522	0.37759

BzP-23,24-H⁺ $\Delta G(\text{B3LYP}): -1011.954557$ $E(\text{B3LYP}): -1012.233965$ $E(\text{M06-2X}): -1011.805370$ $E(\text{B3LYP-D}): -1012.275739$

	X	Y	Z
C	-0.78188	-4.21661	-0.32948
C	0.57634	-4.28653	-0.27213
C	1.08740	-2.96478	-0.01693
N	0.00299	-2.12618	0.05343
C	-1.18359	-2.84838	-0.11677
C	-2.93315	-0.99731	0.00382
C	-2.67978	1.43406	-0.00974
C	-2.45886	-2.35862	-0.11016
C	1.29018	4.18277	-0.18425
C	-0.05557	4.28057	-0.23202
C	-0.57782	2.91440	-0.17288
N	0.47260	2.00638	-0.10633
C	1.58554	2.75568	-0.09891
C	-1.92645	2.66198	-0.12536
C	4.39628	-1.03324	0.26699
C	4.55950	0.31623	0.23953
C	3.25598	0.91903	0.10284

N	2.34264	-0.12193	0.06523
C	2.98381	-1.32777	0.14602
C	2.43007	-2.60439	0.09284
C	2.91249	2.24211	0.01141
C	-2.13384	0.14895	-0.13882
C	-4.06552	1.55788	0.24560
C	-4.87411	0.43677	0.38194
C	-4.31689	-0.82680	0.25596
H	-1.47080	-5.02283	-0.53236
H	1.19693	-5.15782	-0.41458
H	0.01754	-1.23142	0.51776
H	-3.22969	-3.11718	-0.19591
H	2.02224	4.97675	-0.19545
H	-0.65955	5.17416	-0.29178
H	-2.54129	3.55702	-0.14440
H	5.16163	-1.78808	0.36310
H	5.48378	0.86943	0.30876
H	1.36806	0.10355	-0.11441
H	3.13779	-3.42332	0.09730
H	3.72091	2.96293	0.03326
H	-1.09461	0.08094	-0.41686
H	-4.50033	2.54725	0.33440
H	-5.93375	0.54855	0.57544
H	-4.94724	-1.70381	0.35243

BzP-22,24-H⁺

$\Delta G(\text{B3LYP}): -1011.929439$

$E(\text{B3LYP}): -1012.206743$

$E(\text{M06-2X}): -1011.771712$

$E(\text{B3LYP-D}): -1012.248620$

	X	Y	Z
C	0.40476	-4.32515	-0.00001
C	-0.94333	-4.30636	-0.00001
C	-1.32344	-2.89008	0.00000
N	-0.23311	-2.07996	0.00000
C	0.83398	-2.91950	0.00000
C	2.76391	-1.27632	-0.00001
C	2.76382	1.27646	-0.00001
C	2.18307	-2.55073	-0.00001

C	-0.94357	4.30631	0.00001
C	0.40453	4.32515	0.00000
C	0.83379	2.91952	0.00000
N	-0.23322	2.07994	0.00000
C	-1.32362	2.89001	0.00001
C	2.18293	2.55082	0.00000
C	-4.45768	-0.68247	0.00001
C	-4.45774	0.68224	0.00002
C	-3.08874	1.12130	0.00001
N	-2.30272	-0.00004	0.00001
C	-3.08864	-1.12143	0.00001
C	-2.64600	-2.44209	0.00000
C	-2.64614	2.44199	0.00001
C	1.96540	0.00004	-0.00001
C	4.16401	1.21279	-0.00001
C	4.84868	0.00014	-0.00002
C	4.16406	-1.21258	-0.00001
H	1.06371	-5.18109	-0.00001
H	-1.62807	-5.14162	-0.00001
H	2.88093	-3.38244	-0.00001
H	-1.62833	5.14154	0.00002
H	1.06343	5.18113	0.00000
H	2.88074	3.38258	0.00000
H	-5.30984	-1.34474	0.00001
H	-5.30994	1.34443	0.00002
H	-3.42311	-3.19767	0.00000
H	-3.42327	3.19754	0.00002
H	1.27297	0.00002	0.85084
H	1.27297	0.00002	-0.85084
H	4.72965	2.13804	-0.00001
H	5.93225	0.00015	-0.00002
H	4.72978	-2.13778	-0.00001
H	-1.28483	0.00002	0.00001

BzP-22,23-H⁺ $\Delta G(\text{B3LYP}): -1011.917976$ $E(\text{B3LYP}): -1012.195103$ $E(\text{M06-2X}): -1011.759433$ $E(\text{B3LYP-D}): -1012.236612$

	X	Y	Z
C	-1.18547	4.20954	0.00000
C	0.15326	4.36260	-0.00001
C	0.72013	3.00205	0.00001
N	-0.25597	2.06436	0.00000
C	-1.42060	2.75718	0.00000
C	-3.01087	0.80679	0.00000
C	-2.48385	-1.69794	-0.00001
C	-2.68941	2.17084	0.00000
C	1.74469	-4.02663	0.00001
C	0.39742	-4.24214	-0.00001
C	-0.26601	-2.96438	-0.00001
N	0.72012	-2.00643	-0.00002
C	1.95539	-2.60908	0.00000
C	-1.65595	-2.82503	-0.00001
C	4.27011	1.48838	0.00000
C	4.59773	0.17933	0.00002
C	3.32363	-0.54458	0.00001
N	2.26599	0.30517	0.00002
C	2.79869	1.54797	0.00001
C	2.09777	2.76038	0.00001
C	3.17482	-1.93303	0.00001
C	-1.96442	-0.28281	0.00000
C	-3.86877	-1.92054	-0.00001
C	-4.78518	-0.87411	-0.00001
C	-4.36485	0.45559	0.00000
H	-1.94956	4.97304	0.00001
H	0.72365	5.28005	-0.00002
H	-3.52907	2.85893	0.00000
H	2.53265	-4.76396	0.00003
H	-0.11839	-5.19023	-0.00002
H	-2.17271	-3.77920	-0.00001
H	4.93022	2.34348	0.00000
H	5.58028	-0.26886	0.00004
H	2.72104	3.64924	0.00000

H	4.06867	-2.54562	0.00002
H	-1.29982	-0.12145	0.85865
H	-1.29981	-0.12144	-0.85865
H	-4.23448	-2.94147	-0.00001
H	-5.84567	-1.09640	-0.00001
H	-5.10911	1.24424	0.00000
H	0.66155	-0.98438	-0.00004

BzP-23,24,25-H²⁺ $\Delta G(\text{B3LYP}): -1012.216461$ $E(\text{B3LYP}): -1012.508652$ $E(\text{M06-2X}): -1012.073439$ $E(\text{B3LYP-D}): -1012.553370$

	X	Y	Z
C	-0.41542	-4.22328	-0.61033
C	0.95150	-4.20600	-0.55341
C	1.36183	-2.89127	-0.16877
N	0.22900	-2.12266	-0.04903
C	-0.90533	-2.91523	-0.27125
C	-2.79561	-1.22430	0.06682
C	-2.79561	1.22430	0.06682
C	-2.21690	-2.52650	-0.17189
C	0.95150	4.20600	-0.55341
C	-0.41542	4.22328	-0.61033
C	-0.90533	2.91523	-0.27124
N	0.22900	2.12266	-0.04903
C	1.36183	2.89127	-0.16877
C	-2.21690	2.52650	-0.17189
C	4.40645	-0.68076	0.62109
C	4.40645	0.68076	0.62109
C	3.09496	1.13924	0.23999
N	2.30303	0.00000	0.06372
C	3.09496	-1.13924	0.23999
C	2.67812	-2.44309	0.06925
C	2.67812	2.44309	0.06925
C	-2.13497	0.00000	-0.13820
C	-4.15157	1.19894	0.48676
C	-4.81310	0.00000	0.71287
C	-4.15157	-1.19894	0.48675

H	-1.04536	-5.05546	-0.88912
H	1.62679	-5.02013	-0.76938
H	0.19938	-1.31316	0.55342
H	-2.92861	-3.33939	-0.27649
H	1.62679	5.02013	-0.76938
H	-1.04536	5.05546	-0.88912
H	0.19938	1.31316	0.55342
H	-2.92861	3.33939	-0.27649
H	5.22530	-1.33421	0.88410
H	5.22530	1.33421	0.88410
H	1.58268	0.00000	-0.64839
H	3.44248	-3.20898	0.11778
H	3.44248	3.20898	0.11777
H	-1.15248	0.00000	-0.58955
H	-4.67904	2.13579	0.62815
H	-5.84710	0.00000	1.03445
H	-4.67904	-2.13579	0.62815

BzP-22,23,25-H²⁺

$\Delta G(\text{B3LYP}): -1012.195062$

$E(\text{B3LYP}): -1012.485161$

$E(\text{M06-2X}): -1012.042155$

$E(\text{B3LYP-D}): -1012.529105$

	X	Y	Z
C	0.39686	-4.30472	0.00000
C	-0.96795	-4.29439	-0.00003
C	-1.39125	-2.92200	-0.00001
N	-0.26140	-2.14510	-0.00001
C	0.86062	-2.93990	0.00000
C	2.79390	-1.28631	0.00001
C	2.79391	1.28629	0.00000
C	2.20325	-2.55678	0.00001
C	-0.96792	4.29440	0.00003
C	0.39689	4.30471	-0.00003
C	0.86064	2.93989	0.00000
N	-0.26138	2.14510	-0.00001
C	-1.39123	2.92201	0.00001
C	2.20327	2.55676	-0.00001
C	-4.49606	-0.67382	0.00000

C	-4.49606	0.67385	0.00003
C	-3.08808	1.08054	0.00001
N	-2.25408	0.00001	0.00004
C	-3.08810	-1.08052	0.00001
C	-2.69203	-2.42410	-0.00001
C	-2.69200	2.42412	0.00001
C	1.99787	-0.00001	0.00001
C	4.19307	1.21682	-0.00001
C	4.87446	-0.00002	-0.00001
C	4.19305	-1.21685	0.00000
H	1.04732	-5.16660	0.00001
H	-1.63419	-5.14393	-0.00004
H	2.89201	-3.39501	0.00001
H	-1.63415	5.14395	0.00004
H	1.04736	5.16659	-0.00005
H	2.89203	3.39499	-0.00002
H	-5.34101	-1.34663	-0.00002
H	-5.34100	1.34667	0.00005
H	-3.48291	-3.16554	-0.00002
H	-3.48289	3.16556	0.00002
H	1.34399	0.00000	0.88409
H	1.34398	-0.00001	-0.88408
H	4.76463	2.13842	-0.00002
H	5.95820	-0.00002	-0.00001
H	4.76461	-2.13845	0.00000
H	-0.34124	1.13783	-0.00004
H	-0.34125	-1.13783	-0.00002

BzP-22,23,24-H²⁺

$\Delta G(\text{B3LYP}): -1012.188076$

$E(\text{B3LYP}): -1012.478517$

$E(\text{M06-2X}): -1012.03493$

$E(\text{B3LYP-D}): -1012.522258$

	X	Y	Z
C	0.14216	4.30457	0.00013
C	1.48047	4.15433	0.00011
C	1.72198	2.71065	0.00006
N	0.55091	2.00195	0.00008
C	-0.42808	2.94915	0.00010

C	-2.59450	1.59143	-0.00001
C	-2.97656	-0.94875	-0.00012
C	-1.81930	2.75818	0.00007
C	0.40961	-4.34177	0.00021
C	-0.95310	-4.23472	0.00018
C	-1.29347	-2.83970	-0.00003
N	-0.10226	-2.14680	-0.00011
C	0.96325	-3.01658	0.00004
C	-2.57794	-2.29339	-0.00008
C	4.58424	0.13697	-0.00014
C	4.35808	-1.21018	-0.00013
C	2.93312	-1.43117	-0.00001
N	2.34446	-0.18961	0.00005
C	3.30471	0.78759	-0.00003
C	3.00521	2.14917	0.00000
C	2.31701	-2.68269	0.00003
C	-2.00157	0.20705	-0.00009
C	-4.35127	-0.67452	-0.00014
C	-4.84419	0.63032	-0.00011
C	-3.98914	1.73285	-0.00004
H	-0.42937	5.22117	0.00015
H	2.24427	4.91792	0.00011
H	-2.38807	3.68281	0.00010
H	0.99669	-5.24794	0.00036
H	-1.67364	-5.03884	0.00030
H	-3.37370	-3.03062	-0.00006
H	5.53662	0.64540	-0.00023
H	5.09467	-1.99979	-0.00021
H	3.84685	2.83213	-0.00003
H	2.99679	-3.52695	0.00006
H	-1.34544	0.13473	0.87804
H	-1.34550	0.13482	-0.87825
H	-5.05365	-1.50094	-0.00017
H	-5.91604	0.79094	-0.00012
H	-4.41675	2.72943	0.00001
H	-0.04208	-1.14593	-0.00044
H	1.37237	0.11028	0.00023

24-O-BzP $\Delta G(\text{B3LYP}): -1031.415552$ $E(\text{B3LYP}): -1031.667899$ $E(\text{M06-2X}): -1031.242675$ $E(\text{B3LYP-D}): -1031.704833$

	X	Y	Z
C	0.42052	-4.30480	-0.00009
C	-0.92915	-4.26188	-0.00008
C	-1.28955	-2.83313	-0.00001
N	-0.21749	-2.05375	-0.00002
C	0.87202	-2.90817	-0.00006
C	2.80112	-1.21983	0.00000
C	2.80112	1.21983	0.00000
C	2.18742	-2.53453	-0.00006
C	-0.92916	4.26188	-0.00011
C	0.42052	4.30480	-0.00005
C	0.87201	2.90817	-0.00006
N	-0.21749	2.05375	0.00000
C	-1.28955	2.83312	-0.00001
C	2.18741	2.53453	-0.00006
C	-4.50358	-0.67861	0.00006
C	-4.50358	0.67861	0.00006
C	-3.13185	1.11081	0.00005
O	-2.33208	0.00000	0.00006
C	-3.13185	-1.11082	0.00006
C	-2.64713	-2.38669	0.00003
C	-2.64714	2.38669	0.00002
C	2.09837	0.00000	-0.00004
C	4.21466	1.19683	0.00008
C	4.91666	0.00000	0.00013
C	4.21466	-1.19682	0.00008
H	1.06385	-5.17340	-0.00013
H	-1.62521	-5.08929	-0.00009
H	2.89561	-3.35922	-0.00009
H	-1.62521	5.08928	-0.00014
H	1.06384	5.17340	-0.00007
H	2.89560	3.35923	-0.00009
H	-5.35230	-1.34556	0.00008
H	-5.35230	1.34555	0.00006
H	-3.40771	-3.15976	0.00003

H	-3.40772	3.15975	0.00001
H	1.01642	0.00000	-0.00006
H	4.75632	2.13707	0.00010
H	6.00040	0.00001	0.00022
H	4.75632	-2.13706	0.00010

24-S-BzP $\Delta G(\text{B3LYP}): -1354.399894$ $E(\text{B3LYP}): -1354.688150$ $E(\text{M06-2X}): -1354.221200$ $E(\text{B3LYP-D}): -1354.648636$

	X	Y	Z
C	0.52567	-4.43966	0.00011
C	-0.82749	-4.47249	0.00005
C	-1.26655	-3.07090	0.00009
N	-0.22920	-2.24071	-0.00007
C	0.90725	-3.02008	0.00002
C	2.77182	-1.22638	-0.00006
C	2.77192	1.22616	-0.00006
C	2.19830	-2.56520	0.00000
C	-0.82712	4.47256	0.00008
C	0.52604	4.43962	0.00009
C	0.90750	3.02002	0.00002
N	-0.22901	2.24073	-0.00006
C	-1.26629	3.07100	0.00008
C	2.19851	2.56503	0.00000
C	-4.26098	-0.67992	-0.00017
C	-4.26092	0.68026	-0.00017
C	-2.94107	1.26157	-0.00004
S	-1.70820	0.00006	0.00021
C	-2.94117	-1.26134	-0.00003
C	-2.61588	-2.59557	-0.00002
C	-2.61566	2.59577	-0.00003
C	2.06999	-0.00008	-0.00007
C	4.18646	1.19537	-0.00006
C	4.88801	-0.00020	-0.00007
C	4.18636	-1.19571	-0.00006
H	1.21223	-5.27462	0.00016
H	-1.47274	-5.33971	0.00004

H	2.94597	-3.35389	0.00007
H	-1.47231	5.33983	0.00009
H	1.21266	5.27453	0.00013
H	2.94625	3.35366	0.00006
H	-5.15450	-1.29240	-0.00030
H	-5.15439	1.29283	-0.00030
H	-3.41834	-3.32641	-0.00013
H	-3.41806	3.32668	-0.00014
H	0.99059	-0.00003	-0.00002
H	4.73082	2.13368	-0.00005
H	5.97173	-0.00025	-0.00006
H	4.73063	-2.13406	-0.00005

24-O-BzPH₂²⁺ $\Delta G(\text{B3LYP}): -1032.096660$ $E(\text{B3LYP}): -1032.374944$ $E(\text{M06-2X}): -1031.934411$ $E(\text{B3LYP-D}): -1032.417066$

	X	Y	Z
C	-0.41704	-4.24416	-0.40104
C	0.94623	-4.21675	-0.32249
C	1.34465	-2.86165	-0.07996
N	0.21597	-2.10258	-0.04257
C	-0.91288	-2.90484	-0.21447
C	-2.83148	-1.22309	-0.01943
C	-2.83149	1.22308	-0.01943
C	-2.23085	-2.52471	-0.18081
C	0.94621	4.21675	-0.32250
C	-0.41707	4.24415	-0.40105
C	-0.91290	2.90484	-0.21446
N	0.21595	2.10258	-0.04256
C	1.34463	2.86166	-0.07996
C	-2.23086	2.52471	-0.18081
C	4.49079	-0.67992	0.32322
C	4.49079	0.67995	0.32322
C	3.13597	1.11568	0.19869
O	2.31619	0.00001	0.14999
C	3.13598	-1.11566	0.19869
C	2.66814	-2.39909	0.08760

C	2.66813	2.39910	0.08760
C	-2.17323	0.00000	-0.23057
C	-4.19670	1.19865	0.37067
C	-4.86628	-0.00002	0.57258
C	-4.19669	-1.19868	0.37066
H	-1.04464	-5.10378	-0.58471
H	1.62804	-5.04734	-0.42414
H	0.20576	-1.14567	0.26352
H	-2.92821	-3.35359	-0.24990
H	1.62801	5.04734	-0.42417
H	-1.04467	5.10378	-0.58473
H	0.20575	1.14568	0.26357
H	-2.92824	3.35358	-0.24989
H	5.34113	-1.34226	0.38916
H	5.34112	1.34229	0.38917
H	3.43254	-3.16661	0.10297
H	3.43252	3.16662	0.10297
H	-1.19270	0.00000	-0.68749
H	-4.72284	2.13612	0.51273
H	-5.90791	-0.00002	0.86846
H	-4.72282	-2.13615	0.51272

24-S-BzPH₂²⁺

$\Delta G(\text{B3LYP}): -1355.058267$

$E(\text{B3LYP}): -1355.333144$

$E(\text{M06-2X}): -1354.890163$

$E(\text{B3LYP-D}): -1355.377269$

	X	Y	Z
C	0.52959	4.38803	0.38111
C	-0.83737	4.41100	0.28946
C	-1.28583	3.07700	0.02010
N	-0.17307	2.28672	-0.03734
C	0.97832	3.03554	0.16427
C	2.81890	1.23026	-0.01285
C	2.81965	-1.22873	-0.01283
C	2.26870	2.56278	0.14771
C	-0.83484	-4.41146	0.28949
C	0.53211	-4.38777	0.38109
C	0.98012	-3.03505	0.16427

N	-0.17166	-2.28685	-0.03739
C	-1.28401	-3.07769	0.02009
C	2.27023	-2.56157	0.14772
C	-4.26622	0.68214	-0.44976
C	-4.26580	-0.68453	-0.44977
C	-2.99497	-1.27832	-0.13148
S	-1.87322	-0.00047	0.32025
C	-2.99576	1.27670	-0.13147
C	-2.61740	2.60212	-0.14510
C	-2.61584	-2.60352	-0.14512
C	2.14360	0.00056	0.15432
C	4.20296	-1.19510	-0.33969
C	4.87950	0.00138	-0.51852
C	4.20224	1.19745	-0.33971
H	1.18046	5.22116	0.60257
H	-1.48695	5.26319	0.42057
H	-0.16331	1.36978	-0.45632
H	3.01524	3.34482	0.24435
H	-1.48398	-5.26398	0.42063
H	1.18341	-5.22056	0.60256
H	-0.16237	-1.36992	-0.45642
H	3.01722	-3.34319	0.24439
H	-5.12852	1.28691	-0.70103
H	-5.12773	-1.28983	-0.70104
H	-3.38609	3.35231	-0.29625
H	-3.38411	-3.35415	-0.29627
H	1.13073	0.00025	0.53480
H	4.74075	-2.13037	-0.44752
H	5.93309	0.00170	-0.76833
H	4.73946	2.13305	-0.44755

DiOMe-BzP-24-H $\Delta G(\text{B3LYP}): -1240.947339$ $E(\text{B3LYP}): -1240.439681$ $E(\text{M06-2X}): -1240.996857$ $E(\text{B3LYP-D}): -1240.623199$

	X	Y	Z
C	0.49860	4.27747	0.00038
C	1.85027	4.27123	0.00025
C	2.24657	2.86155	0.00007
N	1.18190	2.04705	0.00008
C	0.07594	2.87463	0.00027
C	-1.89279	1.23432	0.00013
C	-1.89276	-1.23433	0.00020
C	-1.25271	2.52106	0.00028
C	1.85034	-4.27121	0.00023
C	0.49868	-4.27743	0.00042
C	0.07603	-2.87457	0.00033
N	1.18199	-2.04701	0.00008
C	2.24664	-2.86152	0.00002
C	-1.25263	-2.52104	0.00040
C	5.41892	0.67955	-0.00038
C	5.41895	-0.67948	-0.00040
C	4.04395	-1.13176	-0.00026
N	3.26254	0.00001	-0.00014
C	4.04392	1.13180	-0.00022
C	3.59865	2.43458	-0.00011
C	3.59872	-2.43454	-0.00018
C	-1.22485	0.00002	0.00026
C	-3.32225	-1.20568	-0.00003
C	-4.02116	-0.00005	-0.00019
C	-3.32232	1.20563	-0.00012
H	-0.16826	5.12829	0.00053
H	2.52623	5.11476	0.00027
H	-1.93434	3.36226	0.00040
H	2.52631	-5.11473	0.00021
H	-0.16818	-5.12824	0.00059
H	-1.93425	-3.36225	0.00060
H	6.27234	1.34097	-0.00047
H	6.27238	-1.34088	-0.00050
H	2.24581	-0.00001	-0.00003

H	4.36077	3.20503	-0.00015
H	4.36085	-3.20498	-0.00025
H	-0.14563	0.00003	0.00043
H	-5.09883	-0.00007	-0.00037
O	-3.95391	2.40147	-0.00031
C	-5.37700	2.45880	-0.00021
H	-5.62640	3.51812	-0.00018
H	-5.79280	1.98785	0.89586
H	-5.79292	1.98788	-0.89624
O	-3.95377	-2.40157	-0.00014
C	-5.37688	-2.45894	-0.00042
H	-5.79255	-1.98823	-0.89669
H	-5.62624	-3.51826	-0.00022
H	-5.79292	-1.98778	0.89542

DiOMe-BzP-23-H $\Delta G(\text{B3LYP}): -1240.612013$ $E(\text{B3LYP}): -1240.935713$ $E(\text{M06-2X}): -1240.426869$ $E(\text{B3LYP-D}): -1240.984808$

	X	Y	Z
C	0.72244	-4.18006	0.00017
C	2.08002	-4.17739	-0.00010
C	2.51945	-2.80313	-0.00035
N	1.38944	-2.01914	-0.00040
C	0.24846	-2.80864	0.00005
C	-1.80440	-1.24229	0.00001
C	-1.99869	1.22346	-0.00012
C	-1.08634	-2.48863	0.00023
C	1.66118	4.31185	0.00036
C	0.30933	4.33831	0.00028
C	-0.12231	2.93833	0.00008
N	0.97137	2.09928	0.00016
C	2.04445	2.89236	0.00023
C	-1.44073	2.54816	-0.00005
C	5.51919	-0.41324	-0.00014
C	5.37754	0.93063	0.00004
C	3.93164	1.20012	0.00012
N	3.23713	0.01999	-0.00005

C	4.15649	-0.95965	-0.00018
C	3.82130	-2.32766	-0.00034
C	3.40457	2.47540	0.00027
C	-1.23866	0.03982	-0.00007
C	-3.41854	1.09164	-0.00021
C	-4.02180	-0.16576	-0.00013
C	-3.23526	-1.31502	-0.00003
H	0.06405	-5.03610	0.00029
H	2.74494	-5.02783	-0.00020
H	1.50030	-1.00165	0.00014
H	-1.72083	-3.36462	0.00055
H	2.34681	5.14789	0.00053
H	-0.34578	5.19822	0.00026
H	-2.16373	3.35418	-0.00014
H	6.43215	-0.99198	-0.00029
H	6.15230	1.68459	0.00013
H	4.61896	-3.06012	-0.00040
H	4.13167	3.28199	0.00040
H	-0.16661	0.17244	-0.00004
O	-4.13752	2.23734	-0.00013
H	-5.09642	-0.24886	-0.00032
O	-3.77769	-2.55456	0.00004
C	-5.56079	2.18713	-0.00077
C	-5.19267	-2.71627	0.00088
H	-5.36377	-3.79100	0.00142
H	-5.64232	-2.27746	-0.89516
H	-5.64134	-2.27664	0.89699
H	-5.93944	1.68648	-0.89727
H	-5.88952	3.22454	-0.00063
H	-5.94033	1.68594	0.89503

DiOMe-BzPH₂²⁺

$\Delta G(\text{B3LYP}): -1241.306474$

$E(\text{B3LYP}): -1241.657614$

$E(\text{M06-2X}): -1241.134159$

$E(\text{B3LYP-D}): -1241.712287$

	X	Y	Z
C	0.52165	4.18911	-0.69908
C	1.88729	4.18452	-0.57403

C	2.28899	2.88213	-0.15651
N	1.14719	2.10470	-0.08138
C	0.02640	2.88834	-0.36572
C	-1.90612	1.23615	-0.12751
C	-1.90606	-1.23621	-0.12739
C	-1.30190	2.50927	-0.32502
C	1.88746	-4.18440	-0.57442
C	0.52181	-4.18901	-0.69943
C	0.02653	-2.88832	-0.36586
N	1.14730	-2.10467	-0.08151
C	2.28912	-2.88206	-0.15675
C	-1.30179	-2.50930	-0.32500
C	5.29690	0.68310	0.77017
C	5.29694	-0.68298	0.77009
C	4.00644	-1.13835	0.33988
N	3.22326	0.00004	0.13663
C	4.00638	1.13844	0.33999
C	3.58996	2.44261	0.13866
C	3.59007	-2.44252	0.13844
C	-1.25423	-0.00001	-0.23648
C	-3.34100	-1.20798	0.12420
C	-4.02454	-0.00006	0.24557
C	-3.34113	1.20789	0.12390
H	-0.09943	5.01267	-1.01892
H	2.56507	5.00154	-0.76992
H	1.09510	1.31814	0.54904
H	-1.99270	3.33305	-0.45731
H	2.56525	-5.00138	-0.77045
H	-0.09925	-5.01256	-1.01936
H	1.09524	-1.31813	0.54894
H	-1.99258	-3.33309	-0.45724
H	6.10664	1.33542	1.06171
H	6.10672	-1.33529	1.06155
H	2.51736	0.00006	-0.58931
H	4.35112	3.21043	0.20452
H	4.35128	-3.21030	0.20423
H	-0.22134	0.00001	-0.55317
O	-3.92183	-2.38619	0.23161
C	-5.08554	-0.00011	0.43819
O	-3.92209	2.38608	0.23078
C	-5.34893	2.51343	0.45443

H	-5.53429	3.58316	0.47999
H	-5.61820	2.06465	1.41176
H	-5.90041	2.05659	-0.36868
C	-5.34867	-2.51366	0.45516
H	-5.61800	-2.06495	1.41253
H	-5.90018	-2.05681	-0.36793
H	-5.53397	-3.58341	0.48070

NP-24-H $\Delta G(\text{B3LYP})$: -1165.196106 $E(\text{B3LYP})$: -1165.504717 $E(\text{M06-2X})$: -1165.023017 $E(\text{B3LYP-D})$: -1165.551090

	X	Y	Z
C	1.23481	4.32191	-0.00007
C	2.56171	4.07496	-0.00003
C	2.70164	2.61394	0.00001
N	1.51384	2.00145	-0.00002
C	0.56869	3.01459	-0.00006
C	-1.66308	1.73594	-0.00007
C	-2.14003	-0.67634	-0.00004
C	-0.79498	2.89339	-0.00009
C	1.03281	-4.32608	-0.00005
C	-0.29635	-4.08988	-0.00018
C	-0.46241	-2.63141	-0.00008
N	0.77659	-2.01685	-0.00003
C	1.67536	-3.00810	-0.00006
C	-1.70950	-2.05519	-0.00008
C	5.43526	-0.09938	0.00012
C	5.19083	-1.43426	0.00011
C	3.75433	-1.63178	0.00006
N	3.18946	-0.37814	0.00005
C	4.16187	0.59430	0.00008
C	3.95929	1.95390	0.00007
C	3.08387	-2.83221	0.00001
C	-1.23589	0.38153	-0.00007
C	-3.56849	-0.39527	0.00002
C	-3.99588	0.97115	0.00000
C	-3.03133	1.99618	-0.00005

C	-4.58219	-1.38565	0.00012
C	-5.92006	-1.05151	0.00016
C	-6.33101	0.29752	0.00012
C	-5.38131	1.28785	0.00004
H	0.72989	5.27760	-0.00010
H	3.37726	4.78430	-0.00003
H	-1.32618	3.84123	-0.00012
H	1.54736	-5.27653	-0.00001
H	-1.10444	-4.80791	-0.00026
H	-2.50033	-2.79301	-0.00015
H	6.39341	0.39822	0.00016
H	5.91052	-2.23910	0.00013
H	2.18916	-0.19475	0.00000
H	4.84627	2.57625	0.00009
H	3.69451	-3.72733	0.00002
H	-0.17875	0.16627	-0.00010
H	-3.37700	3.02559	-0.00007
H	-4.32393	-2.43493	0.00018
H	-6.66550	-1.83889	0.00024
H	-7.38627	0.54429	0.00015
H	-5.67291	2.33287	0.00001

NP-23-H $\Delta G(\text{B3LYP})$: -1165.185676 $E(\text{B3LYP})$: -1165.493327 $E(\text{M06-2X})$: -1165.010660 $E(\text{B3LYP-D})$: -1165.539366

	X	Y	Z
C	-1.11212	4.39874	0.00009
C	-2.43130	4.11206	0.00005
C	-2.53449	2.64202	-0.00003
N	-1.33468	2.06888	0.00004
C	-0.41840	3.10638	0.00013
C	1.75643	1.77182	0.00009
C	2.08152	-0.67053	0.00007
C	0.94306	2.96925	0.00015
C	-1.19611	-4.28909	0.00009
C	0.13390	-4.02852	0.00009
C	0.33505	-2.58805	0.00008

N	-0.93701	-2.03556	0.00010
C	-1.89420	-3.02440	0.00009
C	1.58786	-2.02761	0.00012
C	-5.43077	0.07484	-0.00019
C	-5.30505	-1.26937	-0.00009
C	-3.85945	-1.53716	-0.00007
N	-3.15078	-0.39950	-0.00008
C	-4.06459	0.62344	-0.00015
C	-3.79457	1.97322	-0.00013
C	-3.26179	-2.81485	0.00001
C	1.24903	0.44319	0.00010
C	3.52681	-0.46773	-0.00001
C	4.03453	0.87116	-0.00004
C	3.13441	1.95492	0.00003
C	4.48226	-1.51408	-0.00007
C	5.83791	-1.25924	-0.00014
C	6.32702	0.06245	-0.00018
C	5.43565	1.10592	-0.00013
H	-0.63531	5.36872	0.00014
H	-3.26517	4.80025	0.00005
H	1.50552	3.89867	0.00020
H	-1.68371	-5.25210	0.00013
H	0.94487	-4.74172	0.00005
H	-1.24277	-1.05932	0.00000
H	2.34689	-2.79595	0.00015
H	-6.33831	0.66203	-0.00026
H	-6.08601	-2.01658	-0.00005
H	-4.66149	2.62688	-0.00019
H	-3.90024	-3.68942	0.00002
H	0.17466	0.34361	0.00013
H	3.53928	2.96225	0.00004
H	4.16636	-2.54737	-0.00008
H	6.53530	-2.08949	-0.00017
H	7.39475	0.24789	-0.00024
H	5.78717	2.13226	-0.00017

NPH₂²⁺

$\Delta G(\text{B3LYP}): -1165.862272$

$E(\text{B3LYP}): -1166.197731$

$E(\text{M06-2X}): -1165.700610$

$E(\text{B3LYP-D}): -1166.249512$

	X	Y	Z
C	1.27279	4.24214	-0.69381
C	2.60144	3.98259	-0.48311
C	2.72752	2.61978	-0.07791
N	1.46600	2.06534	-0.10023
C	0.52586	3.04724	-0.42981
C	-1.67620	1.75477	-0.28039
C	-2.13635	-0.66492	-0.24519
C	-0.84396	2.90987	-0.45877
C	1.09737	-4.21959	-0.76419
C	-0.23259	-3.96991	-0.96837
C	-0.51686	-2.62308	-0.55811
N	0.70494	-2.07719	-0.15124
C	1.69257	-3.03691	-0.22728
C	-1.75251	-2.01920	-0.54344
C	5.22534	-0.10052	0.98750
C	4.98177	-1.44203	0.95162
C	3.65860	-1.65146	0.43064
N	3.10605	-0.38829	0.21059
C	4.06577	0.58830	0.48891
C	3.90693	1.94605	0.29479
C	3.03194	-2.85403	0.16070
C	-1.25661	0.40551	-0.40344
C	-3.52223	-0.39885	0.12529
C	-3.95824	0.96887	0.20860
C	-3.03987	1.99843	-0.01662
C	-4.45994	-1.40099	0.41739
C	-5.77301	-1.07775	0.73163
C	-6.20750	0.26022	0.78337
C	-5.31158	1.27059	0.53016
H	0.83606	5.17247	-1.02603
H	3.42954	4.66357	-0.60900
H	1.22436	1.27607	0.48065
H	-1.37301	3.84379	-0.61907
H	1.63432	-5.13016	-0.98302

H	-0.96411	-4.64473	-1.38813
H	0.75206	-1.32267	0.51800
H	-2.55726	-2.69406	-0.80944
H	6.11769	0.39149	1.34533
H	5.64100	-2.23429	1.27416
H	2.45784	-0.25337	-0.55548
H	4.78592	2.56336	0.43427
H	3.63796	-3.74856	0.23619
H	-0.26529	0.20727	-0.78796
H	-3.39040	3.02446	0.03251
H	-4.17501	-2.44459	0.42267
H	-6.47633	-1.87390	0.94676
H	-7.23739	0.48553	1.03042
H	-5.61949	2.30863	0.58231

OBP-23,24-H

$\Delta G(\text{B3LYP}): -1086.823269$

$E(\text{B3LYP}): -1087.092372$

$E(\text{M06-2X}): -1086.641956$

$E(\text{B3LYP-D}): -1087.135253$

	X	Y	Z
C	0.48379	-4.32750	0.22512
C	1.83431	-4.06837	0.19630
C	2.01840	-2.66888	0.00010
N	0.75274	-2.11806	-0.07060
C	-0.21926	-3.10034	0.05060
C	-2.38806	-1.75811	-0.00985
C	-2.74791	0.67769	0.01890
C	-1.60112	-2.92488	0.03398
C	0.43170	4.30678	0.12823
C	-0.89804	4.05062	0.15295
C	-1.04798	2.59883	0.12044
N	0.18309	1.99485	0.08591
C	1.08941	3.01001	0.07998
C	-2.31549	2.01734	0.08695
C	4.74716	0.03027	-0.18326
C	4.56864	1.38714	-0.16216
C	3.16392	1.64577	-0.06097
N	2.53759	0.41764	-0.03316

C	3.46048	-0.60425	-0.09524
C	3.22975	-1.97555	-0.06387
C	2.48582	2.85181	0.00702
C	-1.90935	-0.43609	0.06627
C	-4.23112	0.47884	-0.10460
C	-4.69243	-0.91052	-0.16509
C	-3.82861	-1.94413	-0.11789
O	-5.02140	1.41872	-0.14896
H	0.00529	-5.28218	0.38335
H	2.64005	-4.77472	0.32535
H	0.55550	-1.21265	-0.46336
H	-2.15030	-3.86100	0.06402
H	0.93204	5.26450	0.13352
H	-1.71648	4.75543	0.18295
H	-3.13523	2.72942	0.08373
H	5.67999	-0.50797	-0.25753
H	5.32983	2.15064	-0.21399
H	1.53137	0.40418	0.11525
H	4.11842	-2.59491	-0.06249
H	3.08851	3.75218	-0.00675
H	-0.86197	-0.22937	0.21982
H	-5.76267	-1.05992	-0.24643
H	-4.20113	-2.96342	-0.16444

OBP-24,25-H

$\Delta G(\text{B3LYP}): -1086.824575$

$E(\text{B3LYP}): -1087.136712$

$E(\text{M06-2X}): -1086.643427$

$E(\text{B3LYP-D}): -1087.093831$

	X	Y	Z
C	0.82356	4.25389	-0.13533
C	2.14807	3.96189	-0.10410
C	2.23790	2.51366	-0.06027
N	0.99812	1.94182	-0.07426
C	0.11358	2.98138	-0.11065
C	-2.21550	1.89056	-0.02442
C	-2.83052	-0.49226	0.01566
C	-1.28914	2.94559	-0.08528
C	0.11840	-4.28627	-0.23092

C	-1.21969	-3.98934	-0.25251
C	-1.38069	-2.58036	-0.06531
N	-0.09470	-2.06471	0.05390
C	0.84688	-3.07274	-0.02533
C	-2.57408	-1.87920	-0.04125
C	4.78651	-0.35546	0.17919
C	4.41636	-1.67549	0.18679
C	2.98711	-1.75034	0.08558
N	2.54090	-0.44934	0.02949
C	3.59993	0.43397	0.07372
C	3.45216	1.81187	0.01551
C	2.22985	-2.92154	0.03951
C	-1.87770	0.52696	-0.05989
C	-4.28455	-0.12456	0.12833
C	-4.59462	1.30562	0.14775
C	-3.62410	2.23928	0.07717
O	-5.16893	-0.97556	0.19941
H	0.35507	5.22738	-0.16555
H	2.98610	4.64400	-0.10342
H	-1.73637	3.93626	-0.08932
H	0.57854	-5.25275	-0.36958
H	-2.04066	-4.67170	-0.41261
H	0.08258	-1.16776	0.47486
H	-3.46736	-2.49463	-0.07193
H	5.78619	0.04646	0.24405
H	5.06135	-2.53786	0.26091
H	1.61150	-0.07038	-0.13210
H	4.36315	2.39849	0.03961
H	2.80034	-3.84220	0.02875
H	-0.83156	0.30863	-0.20415
H	-5.64306	1.56931	0.22194
H	-3.88287	3.29402	0.09579

OBP-23,25-H $\Delta G(\text{B3LYP})$: -1086.831695 $E(\text{B3LYP})$: -1087.100405 $E(\text{M06-2X})$: -1086.649791 $E(\text{B3LYP-D})$: -1087.143187

	X	Y	Z
C	-0.74859	4.29734	0.07416
C	-2.09073	4.00994	0.04802
C	-2.23152	2.59031	0.00846
N	-0.96229	2.06674	0.01619
C	-0.01366	3.06804	0.05262
C	2.25295	1.86682	0.03118
C	2.78990	-0.54189	0.02606
C	1.37775	2.96907	0.05197
C	-0.20353	-4.34104	0.07047
C	1.12847	-4.02660	0.09052
C	1.26829	-2.59646	0.05876
N	-0.02108	-2.09907	0.02296
C	-0.94261	-3.11538	0.02367
C	2.47733	-1.91644	0.05308
C	-4.75316	-0.28480	-0.07992
C	-4.45388	-1.60479	-0.07517
C	-2.99894	-1.69835	-0.04614
N	-2.43338	-0.45503	-0.03884
C	-3.48130	0.42693	-0.05373
C	-3.39464	1.81977	-0.03157
C	-2.32063	-2.92255	-0.01603
C	1.87644	0.51327	0.08548
C	4.25664	-0.22726	-0.07148
C	4.61339	1.19193	-0.10478
C	3.67557	2.15962	-0.05763
O	5.11366	-1.10674	-0.11924
H	-0.28827	5.27330	0.10694
H	-2.91356	4.70818	0.05482
H	-0.84093	1.06507	-0.03370
H	1.86240	3.94056	0.04934
H	-0.64896	-5.32395	0.08572
H	1.96520	-4.70769	0.12605
H	-0.33984	-1.14314	-0.04133
H	3.35064	-2.56060	0.04818

H	-5.72793	0.18127	-0.09590
H	-5.13216	-2.44590	-0.08658
H	-4.32900	2.36864	-0.04012
H	-2.92880	-3.81934	-0.01821
H	0.83419	0.28022	0.22704
H	5.67066	1.42031	-0.16965
H	3.97307	3.20370	-0.08856

OBP-O,24-H-L $\Delta G(\text{B3LYP}): -1086.811853$ $E(\text{B3LYP}): -1087.080498$ $E(\text{M06-2X}): -1086.636837$ $E(\text{B3LYP-D}): -1087.121823$

	X	Y	Z
C	-0.90950	4.30930	-0.00020
C	-2.21590	3.96367	0.00023
C	-2.24634	2.49826	0.00035
N	-1.01463	1.97722	0.00018
C	-0.14899	3.05702	-0.00012
C	2.15415	1.92607	-0.00017
C	2.77851	-0.45006	0.00026
C	1.22220	3.02789	-0.00034
C	-0.07964	-4.32662	0.00011
C	1.23077	-4.00209	0.00024
C	1.29712	-2.53636	0.00031
N	0.01868	-2.00568	-0.00013
C	-0.81124	-3.05485	-0.00035
C	2.49286	-1.86422	0.00055
C	-4.76716	-0.41377	0.00018
C	-4.42701	-1.72816	-0.00021
C	-2.98098	-1.82209	-0.00046
N	-2.50796	-0.53097	-0.00025
C	-3.54848	0.36989	0.00021
C	-3.44808	1.74133	0.00053
C	-2.22776	-2.97395	-0.00064
C	1.80676	0.56543	0.00014
C	4.14703	-0.05792	0.00011
C	4.50951	1.28985	-0.00024
C	3.52827	2.26193	-0.00037

H	-0.47929	5.30096	-0.00046
H	-3.08127	4.61135	0.00044
H	1.69063	4.00854	-0.00067
H	-0.52799	-5.31011	0.00010
H	2.08602	-4.66301	0.00043
H	3.36744	-2.50312	0.00084
H	-5.75904	0.01267	0.00042
H	-5.08722	-2.58245	-0.00035
H	-1.52407	-0.27615	-0.00005
H	-4.38064	2.29323	0.00087
H	-2.77618	-3.90851	-0.00082
H	0.76634	0.28209	0.00028
H	5.55961	1.56699	-0.00029
H	3.81872	3.30716	-0.00058
O	5.09323	-1.03355	0.00009
H	5.97193	-0.63853	-0.00023

OBP-O,24-H-R $E(\text{B3LYP}): -1087.078708$

	X	Y	Z
C	-0.90176	4.30481	-0.06544
C	-2.20984	3.96388	-0.03627
C	-2.24402	2.50040	-0.00654
N	-1.01337	1.97467	-0.01780
C	-0.14617	3.05077	-0.05178
C	2.15921	1.92041	-0.03175
C	2.79437	-0.45266	-0.00750
C	1.22672	3.01798	-0.05916
C	-0.08710	-4.32160	-0.08711
C	1.22222	-3.99767	-0.12245
C	1.28967	-2.53153	-0.06609
N	0.01664	-2.00097	-0.00796
C	-0.81707	-3.05013	-0.01904
C	2.48833	-1.85986	-0.06369
C	-4.76789	-0.40724	0.07679
C	-4.42818	-1.72235	0.07424
C	-2.98305	-1.81596	0.04688
N	-2.50911	-0.52735	0.03800
C	-3.54980	0.37481	0.05013

C	-3.44645	1.74556	0.03050
C	-2.22953	-2.97022	0.02091
C	1.81734	0.56095	-0.04115
C	4.16228	-0.05053	0.07154
C	4.51820	1.30041	0.06087
C	3.53527	2.26306	0.00633
C	-0.46839	5.29469	-0.09166
C	-3.07293	4.61449	-0.03369
C	1.69479	3.99862	-0.08008
C	-0.53617	-5.30446	-0.10677
C	2.07421	-4.66111	-0.17614
C	3.33196	-2.54164	-0.14233
C	-5.75953	0.01947	0.09230
C	-5.08851	-2.57637	0.08757
C	-1.52541	-0.27150	0.01880
C	-4.37794	2.29931	0.04079
C	-2.77851	-3.90432	0.02154
C	0.77912	0.27261	-0.08375
C	5.56839	1.55939	0.10997
C	3.81850	3.31033	0.00418
O	5.19803	-0.91909	0.16195
C	4.88049	-1.82085	0.27666

OBP-O,23-H-L

$\Delta G(\text{B3LYP}): -1086.800451$

$E(\text{B3LYP}): -1087.068692$

$E(\text{M06-2X}): -1086.623637$

$E(\text{B3LYP-D}): -1087.109593$

	X	Y	Z
C	-1.21030	-4.16363	0.00026
C	-2.51457	-3.78957	0.00013
C	-2.56208	-2.34589	0.00001
N	-1.26249	-1.90118	0.00010
C	-0.37976	-2.97273	0.00022
C	2.00985	-1.98891	0.00011
C	2.86623	0.31852	0.00014
C	0.98961	-3.01144	0.00027
C	0.19294	4.28825	0.00015
C	1.50097	3.95221	0.00031

C	1.54233	2.48561	0.00027
N	0.26009	1.97130	0.00011
C	-0.55837	3.02082	0.00008
C	2.70160	1.75268	0.00029
C	-4.79587	0.77187	-0.00026
C	-4.29648	2.02621	-0.00029
C	-2.83008	1.89468	-0.00017
N	-2.48051	0.56964	-0.00014
C	-3.63069	-0.12390	-0.00018
C	-3.68352	-1.53162	-0.00012
C	-1.98203	2.98216	-0.00008
C	1.79960	-0.60232	0.00031
C	4.18887	-0.19818	-0.00022
C	4.41865	-1.57604	-0.00046
C	3.35004	-2.44947	-0.00028
O	5.22341	0.68332	-0.00035
H	-0.81267	-5.16770	0.00037
H	-3.38642	-4.42608	0.00010
H	-1.08936	-0.89276	0.00003
H	1.37944	-4.02454	0.00038
H	-0.24316	5.27755	0.00011
H	2.36263	4.60474	0.00043
H	3.62068	2.32575	0.00039
H	-5.83111	0.46112	-0.00030
H	-4.83778	2.96188	-0.00036
H	-4.65154	-2.01682	-0.00016
H	-2.46732	3.95348	-0.00012
H	0.80845	-0.17388	0.00061
H	5.43674	-1.95406	-0.00078
H	3.54159	-3.51714	-0.00045
H	6.06127	0.20779	-0.00082

OBP-O,23-H-R

E(B3LYP): -1087.067147

	X	Y	Z
C	-1.19481	-4.16145	-0.04184
C	-2.50161	-3.79242	-0.02370
C	-2.55336	-2.35070	-0.00337
N	-1.25705	-1.90028	-0.00971
C	-0.37074	-2.96839	-0.03197
C	2.01892	-1.98111	-0.02013
C	2.88193	0.32406	-0.00558
C	1.00025	-3.00132	-0.03714
C	0.17801	4.28413	-0.05432
C	1.48566	3.95040	-0.07694
C	1.52875	2.48287	-0.04060
N	0.25202	1.96656	-0.00238
C	-0.57123	3.01564	-0.01019
C	2.69274	1.75278	-0.04086
C	-4.80067	0.75786	0.04867
C	-4.30461	2.01325	0.04789
C	-2.83729	1.88502	0.02957
N	-2.48346	0.56467	0.02141
C	-3.63305	-0.13467	0.03040
C	-3.68000	-1.53911	0.01812
C	-1.99093	2.97693	0.01476
C	1.81161	-0.59654	-0.02682
C	4.20535	-0.20106	0.04457
C	4.42981	-1.58141	0.03800
C	3.36119	-2.44706	0.00419
O	5.32121	0.56465	0.10091
H	-0.79336	-5.16380	-0.05929
H	-3.37094	-4.43227	-0.02388
H	-1.08746	-0.89101	0.00169
H	1.39143	-4.01386	-0.05145
H	-0.25970	5.27254	-0.06725
H	2.34431	4.60645	-0.11170
H	3.58176	2.37707	-0.09202
H	-5.83492	0.44414	0.05902
H	-4.84820	2.94753	0.05778
H	-4.64561	-2.02909	0.02313
H	-2.47799	3.94718	0.01616

H	0.82145	-0.16678	-0.05465
H	5.45122	-1.93949	0.06888
H	3.54707	-3.51580	0.00332
H	5.09516	1.49713	0.18144

OBP-23,24,25-H⁺ $\Delta G(B3LYP)$: -1087.201996

E(B3LYP): -1087.484530

E(M06-2X): -1087.029225

E(B3LYP-D): -1087.530275

	X	Y	Z
C	0.68358	4.25580	0.52337
C	2.02701	3.96497	0.46610
C	2.17082	2.59165	0.12763
N	0.88753	2.06837	0.02741
C	-0.05134	3.07286	0.22390
C	-2.27957	1.84648	-0.03485
C	-2.76900	-0.56708	-0.03102
C	-1.43995	2.96289	0.12718
C	0.26202	-4.27000	0.52878
C	-1.07854	-3.98311	0.58020
C	-1.26338	-2.60055	0.26900
N	0.01063	-2.07203	0.07346
C	0.96120	-3.07690	0.17923
C	-2.47332	-1.93267	0.16218
C	4.68403	-0.21556	-0.58045
C	4.39757	-1.55760	-0.57002
C	3.02787	-1.72632	-0.21084
N	2.49236	-0.44609	-0.05754
C	3.50380	0.50390	-0.22982
C	3.35485	1.87563	-0.07499
C	2.33239	-2.91721	-0.03006
C	-1.87668	0.49971	0.09067
C	-4.22408	-0.27612	-0.32383
C	-4.60031	1.13638	-0.43341
C	-3.69081	2.11759	-0.29316
O	-5.03779	-1.17700	-0.45391
H	0.23323	5.20425	0.77417
H	2.84925	4.63621	0.66167

H	0.69040	1.27023	-0.55650
H	-1.94467	3.92257	0.17521
H	0.73656	-5.21802	0.73127
H	-1.88246	-4.65828	0.83178
H	0.15796	-1.27540	-0.52747
H	-3.35078	-2.57069	0.20769
H	5.62625	0.24688	-0.83312
H	5.06789	-2.36851	-0.81166
H	1.75801	-0.28496	0.62011
H	4.26494	2.46199	-0.10991
H	2.92227	-3.82517	-0.05161
H	-0.86782	0.29583	0.42325
H	-5.64597	1.34317	-0.62610
H	-3.99540	3.15578	-0.37546

OBP-O,23,25-H⁺-L

$\Delta G(\text{B3LYP}): -1087.210399$

$E(\text{B3LYP}): -1087.492664$

$E(\text{M06-2X}): -1087.040321$

$E(\text{B3LYP-D}): -1087.536202$

	X	Y	Z
C	0.94417	4.28431	-0.21438
C	2.25932	3.93960	-0.13258
C	2.33122	2.50745	-0.02377
N	1.05274	2.03554	-0.05192
C	0.14519	3.08158	-0.15731
C	-2.15057	1.94528	-0.08405
C	-2.78416	-0.43529	-0.07435
C	-1.22636	3.04316	-0.16588
C	0.08013	-4.32881	-0.20564
C	-1.23328	-3.98200	-0.27783
C	-1.34076	-2.54172	-0.18133
N	-0.03638	-2.07896	-0.06433
C	0.84734	-3.11839	-0.06491
C	-2.52118	-1.84490	-0.17595
C	4.75193	-0.44572	0.23851
C	4.40777	-1.74661	0.22549
C	2.94258	-1.78573	0.13292
N	2.41988	-0.52543	0.10454

C	3.49853	0.31413	0.15244
C	3.46940	1.70477	0.09226
C	2.23037	-2.98275	0.05108
C	-1.83149	0.58598	-0.22166
C	-4.13341	-0.04072	0.18950
C	-4.47824	1.31075	0.29946
C	-3.50837	2.27892	0.16356
O	-5.04660	-1.01466	0.32836
H	0.53031	5.27719	-0.30629
H	3.11594	4.59558	-0.14327
H	0.88292	1.04520	0.05746
H	-1.68553	4.02533	-0.20344
H	0.50517	-5.31982	-0.24467
H	-2.08237	-4.63944	-0.38859
H	0.30005	-1.13756	0.08185
H	-3.40007	-2.47490	-0.22389
H	5.73942	-0.01147	0.29142
H	5.05102	-2.61330	0.26597
H	4.41988	2.22270	0.12137
H	2.80334	-3.90147	0.06078
H	-0.83821	0.31183	-0.54018
H	-5.50852	1.58994	0.49344
H	-3.78698	3.32253	0.25568
H	-5.92817	-0.65280	0.48376

OBP-O,23,25-H⁺-R

$E(\text{B3LYP}): -1087.487586$

	X	Y	Z
C	0.94408	4.27421	-0.30218
C	2.25749	3.93001	-0.17626
C	2.32285	2.50293	-0.02926
N	1.04588	2.03099	-0.07985
C	0.14430	3.07518	-0.23281
C	-2.15061	1.94444	-0.13078
C	-2.78786	-0.43308	-0.07916
C	-1.22918	3.03681	-0.25072
C	0.08203	-4.31580	-0.32722
C	-1.22748	-3.96988	-0.44031

C	-1.34618	-2.53646	-0.26477
N	-0.05301	-2.07612	-0.07047
C	0.83927	-3.11166	-0.09421
C	-2.52590	-1.83723	-0.25563
C	4.73499	-0.44674	0.34638
C	4.38860	-1.74718	0.32192
C	2.92646	-1.78250	0.18894
N	2.40613	-0.52559	0.15130
C	3.48640	0.31486	0.22369
C	3.45867	1.70143	0.13967
C	2.21401	-2.98025	0.06665
C	-1.83864	0.58467	-0.27651
C	-4.11189	-0.03180	0.29357
C	-4.45714	1.32331	0.37733
C	-3.50049	2.28529	0.16591
O	-5.09321	-0.89534	0.58479
H	0.53419	5.26492	-0.42861
H	3.11500	4.58488	-0.17938
H	0.86915	1.04311	0.04280
H	-1.68734	4.01830	-0.31439
H	0.51296	-5.30235	-0.40115
H	-2.06564	-4.62483	-0.62536
H	0.26552	-1.13904	0.13218
H	-3.38536	-2.47899	-0.42507
H	5.72172	-0.01471	0.42508
H	5.02909	-2.61506	0.37771
H	4.40756	2.22117	0.18654
H	2.78746	-3.89875	0.06718
H	-0.86868	0.30772	-0.66266
H	-5.47689	1.58052	0.63366
H	-3.77272	3.33126	0.25008
H	-4.77603	-1.80381	0.65064

OBP-O,23,24-H⁺-L $\Delta G(\text{B3LYP})$: -1087.205309 $E(\text{B3LYP})$: -1087.487747 $E(\text{M06-2X})$: -1087.036042 $E(\text{B3LYP-D})$: -1087.531335

	X	Y	Z
C	-0.71202	4.31524	-0.30667
C	-2.03664	3.99513	-0.25188
C	-2.15011	2.58471	-0.00511
N	-0.86984	2.08868	0.06284
C	0.05970	3.11929	-0.10112
C	2.27596	1.85799	-0.01401
C	2.75133	-0.55446	-0.03424
C	1.42610	3.01444	-0.10119
C	-0.27533	-4.30829	-0.20740
C	1.04140	-4.01444	-0.25788
C	1.14908	-2.55615	-0.18876
N	-0.11420	-1.98848	-0.11425
C	-0.96841	-3.02767	-0.11126
C	2.37790	-1.93816	-0.14600
C	-4.75797	-0.22206	0.27669
C	-4.51997	-1.56122	0.24533
C	-3.09908	-1.75649	0.10138
N	-2.52940	-0.49636	0.06407
C	-3.49492	0.47186	0.15126
C	-3.33341	1.85257	0.10274
C	-2.38328	-2.92310	0.00338
C	1.85835	0.52248	-0.12315
C	4.13471	-0.25451	0.16585
C	4.57342	1.07242	0.26246
C	3.66478	2.10145	0.16803
O	4.98936	-1.28458	0.25426
H	-0.28161	5.28544	-0.50454
H	-2.87869	4.65529	-0.39204
H	-0.63242	1.22632	0.52767
H	1.94116	3.96613	-0.17985
H	-0.74873	-5.27888	-0.22393
H	1.87758	-4.69498	-0.32476
H	3.21503	-2.62500	-0.17597
H	-5.71000	0.27583	0.37950

H	-5.24209	-2.36024	0.31673
H	-1.53436	-0.42615	-0.12827
H	-4.24661	2.43367	0.11271
H	-2.94639	-3.84831	0.02348
H	0.83402	0.26803	-0.34230
H	5.62796	1.28262	0.40681
H	4.01650	3.12462	0.23902
H	5.89823	-0.98089	0.37242

OBP-O,23,24-H⁺-R

E(B3LYP): -1087.483317

	X	Y	Z
C	-0.68979	4.30735	-0.39171
C	-2.01466	3.99354	-0.29210
C	-2.12481	2.59156	-0.00789
N	-0.84560	2.09216	0.03690
C	0.08142	3.11521	-0.17511
C	2.29004	1.84925	-0.06111
C	2.74896	-0.56624	-0.04201
C	1.44919	3.00527	-0.18526
C	-0.30036	-4.29760	-0.32336
C	1.01368	-4.00666	-0.41891
C	1.13195	-2.55264	-0.27840
N	-0.12255	-1.98477	-0.13146
C	-0.98314	-3.01907	-0.14170
C	2.36267	-1.93807	-0.22869
C	-4.74058	-0.19755	0.37876
C	-4.51147	-1.53766	0.34163
C	-3.09522	-1.74109	0.16060
N	-2.51867	-0.48605	0.11300
C	-3.47676	0.48935	0.21958
C	-3.30926	1.86622	0.15040
C	-2.39103	-2.91226	0.02516
C	1.86793	0.51762	-0.18318
C	4.11623	-0.27016	0.26792
C	4.56434	1.05712	0.34565
C	3.67501	2.08781	0.17700
O	5.04804	-1.20148	0.50252

H	-0.26159	5.27087	-0.62391
H	-2.85810	4.65360	-0.42400
H	-0.59531	1.23671	0.50854
H	1.96802	3.95274	-0.28803
H	-0.77886	-5.26497	-0.36392
H	1.84034	-4.68897	-0.55457
H	3.17573	-2.64734	-0.36196
H	-5.68709	0.30597	0.50319
H	-5.23635	-2.33255	0.42925
H	-1.52735	-0.42146	-0.09963
H	-4.21842	2.45311	0.17910
H	-2.95887	-3.83437	0.04584
H	0.85756	0.27582	-0.47330
H	5.61132	1.23570	0.55456
H	4.02928	3.11031	0.24488
H	4.67712	-2.09049	0.55120

OBP-O,24,25-H⁺-L

$\Delta G(B3LYP)$: -1087.205572

E(B3LYP): -1087.488110

E(M06-2X): -1087.036455

E(B3LYP-D): -1087.531713

	X	Y	Z
C	-0.98095	4.25410	0.22392
C	-2.28670	3.91115	0.16265
C	-2.31499	2.45596	0.08067
N	-1.07877	1.92416	0.10254
C	-0.21868	3.00759	0.17606
C	2.12434	1.94938	0.04692
C	2.82191	-0.40720	0.01834
C	1.15865	3.00854	0.14579
C	-0.03378	-4.27112	0.31958
C	1.28770	-3.94672	0.37932
C	1.42823	-2.53240	0.14409
C	0.12984	-2.04608	-0.03871
N	-0.78108	-3.07399	0.04246
C	2.59903	-1.82420	0.13363
C	-4.78799	-0.48448	-0.27598
C	-4.38302	-1.78415	-0.28962

C	-2.94494	-1.81732	-0.14774
N	-2.53341	-0.51420	-0.06869
C	-3.61860	0.34322	-0.12703
C	-3.52067	1.70941	-0.04088
C	-2.16518	-2.97016	-0.07628
C	1.83311	0.58225	0.13865
C	4.16837	0.02882	-0.19360
C	4.47959	1.38968	-0.27320
C	3.47763	2.32828	-0.15117
O	5.11127	-0.92028	-0.31268
H	-0.55216	5.24367	0.28586
H	-3.15161	4.55800	0.16348
H	1.59406	4.00329	0.17016
H	-0.48078	-5.24080	0.47611
H	2.11479	-4.60553	0.59736
H	-0.05038	-1.18604	-0.53310
H	3.48976	-2.43242	0.22790
H	-5.79593	-0.10814	-0.36256
H	-4.99846	-2.66498	-0.39019
H	-1.61892	-0.11862	0.13031
H	-4.44683	2.27037	-0.07712
H	-2.70954	-3.90579	-0.07439
H	0.81587	0.31481	0.37314
H	5.50747	1.69964	-0.42951
H	3.72903	3.38121	-0.21212
H	5.98808	-0.53321	-0.42933

OBP-O,24,25-H⁺-R

E(B3LYP): -1087.760203

	X	Y	Z
C	-0.99243	4.24222	0.30462
C	-2.29689	3.89960	0.20900
C	-2.32058	2.44805	0.08848
N	-1.08231	1.91732	0.12188
C	-0.22837	2.99829	0.23867
C	2.11756	1.95057	0.08580
C	2.83088	-0.39979	0.03216
C	1.15166	3.00180	0.21626
C	-0.02810	-4.25551	0.41486

C	1.28764	-3.92589	0.52438
C	1.43831	-2.52166	0.23288
N	0.15111	-2.04490	-0.02195
C	-0.76543	-3.06996	0.06453
C	2.60820	-1.81041	0.22081
C	-4.76923	-0.49571	-0.37125
C	-4.35849	-1.79507	-0.37930
C	-2.92604	-1.82157	-0.20292
N	-2.52036	-0.51840	-0.11395
C	-3.60805	0.33431	-0.19059
C	-3.51796	1.70064	-0.07963
C	-2.14254	-2.97267	-0.09684
C	1.83944	0.58298	0.19419
C	4.15567	0.04639	-0.28539
C	4.45996	1.41160	-0.34722
C	3.46414	2.34004	-0.16036
O	5.17444	-0.78641	-0.54051
H	-0.56647	5.23038	0.39956
H	-3.16236	4.54565	0.20869
H	1.58426	3.99709	0.26282
H	-0.48058	-5.21991	0.58774
H	2.10293	-4.57557	0.80554
H	-0.01067	-1.19468	-0.54008
H	3.47725	-2.42767	0.42867
H	-5.77669	-0.12351	-0.47871
H	-4.96844	-2.67782	-0.49488
H	-1.61141	-0.11982	0.10631
H	-4.44579	2.25809	-0.12810
H	-2.68498	-3.90945	-0.09014
H	0.84124	0.30383	0.49178
H	5.47930	1.70396	-0.56436
H	3.70520	3.39540	-0.22099
H	4.88654	-1.70234	-0.63051

OBPH₂²⁺-L $\Delta G(\text{B3LYP}): -1087.473023$ $E(\text{B3LYP}): -1087.768659$ $E(\text{M06-2X}): -1087.310258$ $E(\text{B3LYP-D}): -1087.815174$

	X	Y	Z
C	-0.88842	4.23805	-0.58801
C	-2.21142	3.88691	-0.51248
C	-2.28307	2.51229	-0.13747
N	-0.99065	2.04285	-0.04134
C	-0.09193	3.08993	-0.27006
C	2.17084	1.92945	0.00672
C	2.77544	-0.45697	0.00315
C	1.28287	3.03666	-0.19294
C	-0.13965	-4.25057	-0.61156
C	1.18700	-3.92401	-0.68851
C	1.34193	-2.54194	-0.32944
N	0.05178	-2.05934	-0.07854
C	-0.85931	-3.08678	-0.19870
C	2.52589	-1.85037	-0.23955
C	-4.67802	-0.38454	0.66514
C	-4.34143	-1.70584	0.65115
C	-2.96494	-1.82228	0.25241
N	-2.48150	-0.52317	0.08064
C	-3.52698	0.38480	0.27614
C	-3.44360	1.75299	0.11179
C	-2.23854	-2.98233	0.05699
C	1.83748	0.57503	-0.16046
C	4.11766	-0.08413	0.36722
C	4.46854	1.26533	0.53238
C	3.52341	2.24313	0.34273
O	4.98886	-1.07067	0.53208
H	-0.48592	5.20090	-0.86675
H	-3.06725	4.51400	-0.71176
H	-0.75717	1.26833	0.56237
H	1.76278	4.00556	-0.28863
H	-0.59369	-5.20428	-0.83453
H	2.00000	-4.56773	-0.99093
H	-0.11073	-1.28712	0.55111
H	3.40892	-2.46651	-0.36315

H	-5.62999	0.04379	0.94233
H	-4.97113	-2.54290	0.91435
H	-1.78568	-0.33905	-0.63179
H	-4.37229	2.30706	0.17455
H	-2.79004	-3.91371	0.09668
H	0.86464	0.32027	-0.55611
H	5.48696	1.52936	0.79617
H	3.81065	3.28246	0.45659
H	5.87921	-0.75641	0.74766

OBPH₂²⁺-R $E(\text{B3LYP}): -1087.760203$

	X	Y	Z
C	-0.86828	4.22467	-0.64571
C	-2.19296	3.88320	-0.53714
C	-2.26471	2.51882	-0.13121
N	-0.97289	2.04423	-0.04679
C	-0.07456	3.08038	-0.31481
C	2.18336	1.91712	-0.02543
C	2.77548	-0.47357	0.00999
C	1.30305	3.02160	-0.24862
C	-0.17040	-4.22925	-0.69358
C	1.15342	-3.90604	-0.79859
C	1.32751	-2.53922	-0.38628
N	0.04906	-2.05951	-0.08473
C	-0.87429	-3.07599	-0.22131
C	2.51568	-1.85537	-0.28852
C	-4.66023	-0.36206	0.73005
C	-4.33044	-1.68576	0.70730
C	-2.96234	-1.80660	0.28523
N	-2.47476	-0.51191	0.11177
C	-3.51224	0.40197	0.32350
C	-3.42468	1.76828	0.14997
C	-2.24520	-2.97030	0.05922
C	1.84490	0.56296	-0.18107
C	4.10200	-0.10016	0.43707
C	4.46582	1.25362	0.55409
C	3.53786	2.23165	0.31780
O	5.05257	-0.97017	0.74082

H	-0.46547	5.17855	-0.95334
H	-3.04860	4.51103	-0.73504
H	-0.73046	1.28125	0.56811
H	1.78684	3.98616	-0.36716
H	-0.63583	-5.17185	-0.93948
H	1.95179	-4.54275	-1.15101
H	-0.09358	-1.30276	0.56844
H	3.37781	-2.47866	-0.50925
H	-5.60586	0.07002	1.02288
H	-4.96050	-2.52049	0.97680
H	-1.78119	-0.32840	-0.60280
H	-4.34926	2.32789	0.22478
H	-2.80301	-3.89838	0.08613
H	0.88339	0.31022	-0.60589
H	5.48279	1.48850	0.84243
H	3.82949	3.27179	0.41037
H	4.75870	-1.89031	0.76413

ONP-23,25-H

$\Delta G(\text{B3LYP}): -1240.472827$

$E(\text{B3LYP}): -1240.784722$

$E(\text{M06-2X}): -1240.276419$

$E(\text{B3LYP-D}): -1240.834550$

	X	Y	Z
C	-0.10059	-4.16112	0.20650
C	-1.45858	-4.34591	0.16172
C	-2.06926	-3.06025	0.05746
N	-1.04956	-2.13712	0.04569
C	0.18031	-2.75641	0.13039
C	1.98485	-0.91513	0.07523
C	1.63955	1.54705	0.11543
C	1.47102	-2.22556	0.12866
C	-2.46732	4.11669	0.01775
C	-1.10715	4.25678	0.09645
C	-0.50661	2.95248	0.10011
N	-1.55703	2.05896	0.02711
C	-2.76087	2.71784	-0.02790
C	0.86213	2.71914	0.14072
C	-5.41150	-1.21361	-0.15890

C	-5.57203	0.13098	-0.18775
C	-4.23485	0.70705	-0.13112
N	-3.28614	-0.27534	-0.07882
C	-3.97665	-1.45584	-0.08767
C	-3.42233	-2.73635	-0.01959
C	-3.99858	2.08502	-0.10979
C	1.17363	0.22799	0.13799
C	3.11370	1.78184	0.07333
C	3.98533	0.58474	-0.01911
C	3.45099	-0.72322	-0.03473
O	3.59045	2.91121	0.10591
C	5.36862	0.79494	-0.10644
C	6.24327	-0.27226	-0.21862
C	5.72836	-1.57073	-0.25166
C	4.36099	-1.78986	-0.16472
H	0.66151	-4.92165	0.28671
H	-1.99827	-5.27977	0.19841
H	-1.27469	-1.15816	-0.06114
H	2.20408	-3.01900	0.17331
H	-3.21044	4.89894	-0.00842
H	-0.54123	5.17467	0.14559
H	-1.54506	1.04919	0.00001
H	1.45686	3.62592	0.16916
H	-6.17316	-1.97988	-0.17981
H	-6.49245	0.69506	-0.23636
H	-4.11309	-3.57133	-0.01818
H	-4.86563	2.73365	-0.15078
H	0.11395	0.07585	0.26761
H	5.72417	1.81757	-0.08691
H	7.31166	-0.10330	-0.28688
H	6.39721	-2.41870	-0.34993
H	4.01163	-2.81205	-0.20996

ONP-23,24-H $\Delta G(\text{B3LYP})$: -1240.464668 $E(\text{B3LYP})$: -1240.777324 $E(\text{M06-2X})$: -1240.269431 $E(\text{B3LYP-D})$: -1240.827345

	X	Y	Z
C	0.07160	-4.14040	0.45394
C	1.43458	-4.28883	0.37009
C	2.00620	-3.01734	0.07439
N	0.95047	-2.12380	-0.00045
C	-0.25764	-2.77351	0.20997
C	-2.01981	-0.91843	0.08365
C	-1.62511	1.52901	0.15356
C	-1.54411	-2.24044	0.19736
C	2.47426	4.08476	0.09399
C	1.13001	4.21161	0.20265
C	0.57713	2.86077	0.18660
N	1.58137	1.93629	0.08315
C	2.73717	2.65718	0.01550
C	-0.80675	2.66990	0.22026
C	5.38327	-1.23601	-0.34136
C	5.59814	0.11715	-0.36351
C	4.33302	0.76607	-0.20722
N	3.38622	-0.23081	-0.11107
C	3.97757	-1.47303	-0.17170
C	3.36106	-2.71662	-0.06569
C	4.02530	2.11579	-0.13329
C	-1.18038	0.20397	0.16604
C	-3.09163	1.79959	0.09622
C	-3.98648	0.62253	-0.04587
C	-3.47615	-0.69420	-0.07505
O	-3.54752	2.93628	0.15271
C	-5.36158	0.85933	-0.17458
C	-6.24970	-0.18964	-0.34609
C	-5.75619	-1.49545	-0.40226
C	-4.39605	-1.74093	-0.27456
H	-0.65517	-4.90348	0.68854
H	2.00735	-5.19043	0.52488
H	1.00902	-1.22876	-0.45840
H	-2.29186	-3.01396	0.31158

H	3.22319	4.86303	0.06197
H	0.54517	5.11703	0.27792
H	-1.37641	3.59253	0.26875
H	6.11959	-2.01967	-0.43661
H	6.54053	0.63095	-0.47745
H	2.42870	0.04381	0.09870
H	4.02945	-3.56902	-0.05949
H	4.85377	2.81130	-0.19670
H	-0.12128	0.07278	0.32573
H	-5.70068	1.88728	-0.14088
H	-7.31207	0.00024	-0.44655
H	-6.43513	-2.32745	-0.55373
H	-4.05692	-2.76528	-0.34948

ONP-24,25-H $\Delta G(\text{B3LYP})$: -1240.466042 $E(\text{B3LYP})$: -1240.778435 $E(\text{M06-2X})$: -1240.270369 $E(\text{B3LYP-D})$: -1240.828387

	X	Y	Z
C	-0.14177	4.12069	-0.25549
C	-1.48290	4.30819	-0.19503
C	-2.06752	2.98353	-0.09818
N	-1.10233	2.01490	-0.10764
C	0.08673	2.68100	-0.19160
C	1.96807	0.90859	-0.07968
C	1.68515	-1.55497	-0.06481
C	1.40420	2.19322	-0.17324
C	-2.41331	-4.09134	-0.18575
C	-1.05481	-4.26493	-0.25557
C	-0.42137	-2.99367	-0.09705
N	-1.45000	-2.07188	0.05171
C	-2.68045	-2.70295	0.01914
C	0.94297	-2.75122	-0.11319
C	-5.45148	1.19190	0.25580
C	-5.55828	-0.17502	0.28634
C	-4.24518	-0.73869	0.15992
N	-3.38042	0.32816	0.06846
C	-4.06840	1.52141	0.11148

C	-3.44847	2.75863	0.01537
C	-3.93042	-2.09589	0.11910
C	1.17912	-0.25120	-0.10800
C	3.16549	-1.74975	-0.00922
C	4.00746	-0.53022	0.05339
C	3.43860	0.76282	0.03258
O	3.66902	-2.86833	-0.00804
C	5.39558	-0.70179	0.14708
C	6.24116	0.39156	0.22874
C	5.69190	1.67646	0.22327
C	4.31918	1.85693	0.12962
H	0.63404	4.86985	-0.32701
H	-2.03326	5.23796	-0.20768
H	2.11534	3.00713	-0.22702
H	-3.17826	-4.84548	-0.29152
H	-0.51857	-5.18590	-0.42710
H	-1.29755	-1.15849	0.44628
H	1.55581	-3.64444	-0.17076
H	-6.24983	1.91463	0.32911
H	-6.45887	-0.76093	0.39078
H	-2.38115	0.36280	-0.11626
H	-4.09250	3.62993	0.03602
H	-4.77660	-2.77171	0.14054
H	0.11970	-0.07916	-0.22632
H	5.77856	-1.71463	0.15640
H	7.31367	0.25328	0.30198
H	6.33831	2.54420	0.29622
H	3.94083	2.86966	0.14277

ONP-O,24-H-L

E(B3LYP): -1240.751414

	X	Y	Z
C	0.16633	-4.20299	0.06987
C	1.50989	-4.34440	0.04733
C	2.05561	-2.98646	0.01419
N	1.08617	-2.06048	0.01557
C	-0.10240	-2.76177	0.04784
C	-1.93206	-0.94515	0.02777

C	-1.65108	1.50838	0.02720
C	-1.39124	-2.27922	0.05263
C	2.40079	4.13014	0.01892
C	1.05915	4.27450	0.04429
C	0.49398	2.91994	0.03359
N	1.51048	1.98303	0.00501
C	2.65102	2.68525	-0.00451
C	-0.86277	2.71445	0.04422
C	5.44295	-1.15763	-0.05764
C	5.58500	0.19341	-0.06258
C	4.26379	0.78649	-0.04188
N	3.36887	-0.25617	-0.02785
C	4.02765	-1.46319	-0.03385
C	3.44646	-2.70977	-0.01463
C	3.95402	2.12744	-0.03172
C	-1.12917	0.18979	0.02817
C	-3.04905	1.66005	0.01758
C	-3.93168	0.54016	-0.01637
C	-3.37810	-0.77857	0.00091
O	-3.54183	2.92144	0.03099
C	-5.34019	0.71089	-0.07325
C	-6.19336	-0.36566	-0.09071
C	-5.65802	-1.66557	-0.05944
C	-4.29443	-1.85972	-0.01949
H	-0.58771	-4.97727	0.09675
H	2.09017	-5.25622	0.05219
H	-2.11872	-3.07859	0.08057
H	3.15996	4.89954	0.01625
H	0.48202	5.18810	0.06625
H	-1.44447	3.62679	0.06564
H	6.22244	-1.90465	-0.06780
H	6.50257	0.76221	-0.07761
H	2.35733	-0.14989	-0.01214
H	4.12029	-3.55838	-0.01896
H	4.78881	2.81811	-0.04181
H	-0.05616	0.07016	0.04025
H	-5.78236	1.70161	-0.12157
H	-7.26520	-0.21447	-0.13594
H	-6.32127	-2.52286	-0.07387
H	-3.93192	-2.87695	-0.00928
H	-4.49841	2.91177	0.13346

ONP-O,24-H-R $\Delta G(\text{B3LYP}): -1240.441087$ $E(\text{B3LYP}): -1240.752706$ $E(\text{M06-2X}): -1240.248418$ $E(\text{B3LYP-D}): -1240.801498$

	X	Y	Z
C	0.15801	-4.19849	0.20688
C	1.49927	-4.34457	0.11854
C	2.04349	-2.99071	0.02169
N	1.07607	-2.06175	0.04839
C	-0.10888	-2.75890	0.15572
C	-1.93654	-0.94163	0.10971
C	-1.65406	1.51264	0.07457
C	-1.39767	-2.27139	0.18282
C	2.41268	4.11831	0.16926
C	1.07456	4.26284	0.26395
C	0.50315	2.91318	0.16549
N	1.50908	1.98017	0.03309
C	2.65528	2.67810	0.03081
C	-0.85602	2.70641	0.17890
C	5.42612	-1.16913	-0.22318
C	5.57134	0.18237	-0.22158
C	4.25416	0.77698	-0.14019
N	3.35785	-0.26169	-0.10676
C	4.01355	-1.47124	-0.14233
C	3.43071	-2.71583	-0.08504
C	3.95016	2.12072	-0.07766
C	-1.13411	0.19331	0.13172
C	-3.04886	1.65498	-0.07498
C	-3.92832	0.53585	-0.07955
C	-3.38329	-0.77825	0.02193
O	-3.65222	2.85458	-0.22889
C	-5.32866	0.73095	-0.19147
C	-6.18715	-0.34219	-0.19147
C	-5.66440	-1.64425	-0.08950
C	-4.30436	-1.85339	0.00894
H	-0.59491	-4.96960	0.29180
H	2.07737	-5.25775	0.11645

H	-2.12723	-3.06605	0.26194
H	3.17442	4.88471	0.19204
H	0.50645	5.17550	0.37913
H	-1.39913	3.63675	0.32951
H	6.20298	-1.91755	-0.26859
H	6.48906	0.74929	-0.26581
H	2.34776	-0.15430	-0.04943
H	4.10257	-3.56570	-0.11324
H	4.78741	2.80814	-0.09485
H	-0.06393	0.07433	0.21035
H	-2.99354	3.54599	-0.35785
H	-5.70782	1.74022	-0.27460
H	-7.25676	-0.18831	-0.27240
H	-6.33522	-2.49618	-0.09288
H	-3.95360	-2.87314	0.07252

ONP-O,23-H-L $E(\text{B3LYP}): -1240.739724$

	X	Y	Z
C	-0.34082	-4.12444	0.07152
C	-1.68763	-4.28679	0.04865
C	-2.28885	-2.97594	0.01517
N	-1.26153	-2.05991	0.01746
C	-0.03480	-2.70499	0.05027
C	1.86540	-0.93444	0.03074
C	1.74634	1.53660	0.03018
C	1.25878	-2.24134	0.05600
C	-2.26292	4.16529	0.01523
C	-0.92548	4.34702	0.04192
C	-0.33469	3.00416	0.03405
N	-1.32594	2.04289	0.00594
C	-2.48060	2.70907	-0.00612
C	1.01875	2.78046	0.04608
C	-5.55527	-0.96609	-0.05963
C	-5.57288	0.38451	-0.06643
C	-4.16783	0.82181	-0.04393
N	-3.33986	-0.26804	-0.02676
C	-4.13686	-1.34821	-0.03353
C	-3.63882	-2.66512	-0.01236

C	-3.78789	2.14701	-0.03455
C	1.14228	0.25059	0.03249
C	3.14725	1.60499	0.01934
C	3.95636	0.42988	-0.01570
C	3.32195	-0.85267	0.00098
O	3.71557	2.83455	0.03128
C	5.37217	0.51342	-0.07430
C	6.15883	-0.61291	-0.09443
C	5.54508	-1.87683	-0.06470
C	4.17176	-1.98632	-0.02295
H	0.41489	-4.89554	0.09850
H	-2.24483	-5.21128	0.05401
H	-1.49570	-1.06332	0.00038
H	1.94978	-3.07042	0.08650
H	-3.04077	4.91622	0.01036
H	-0.37254	5.27547	0.06303
H	1.63290	3.67154	0.06640
H	-6.39350	-1.64843	-0.06994
H	-6.43055	1.04227	-0.08342
H	-4.33992	-3.49036	-0.01420
H	-4.59830	2.86943	-0.04678
H	0.06245	0.24873	0.04781
H	5.87336	1.47554	-0.12224
H	7.23779	-0.52692	-0.14081
H	6.15375	-2.77361	-0.08183
H	3.75069	-2.98059	-0.01484
H	4.66951	2.76795	0.13642

ONP-O,23-H-R

$\Delta G(\text{B3LYP}): -1240.430268$

$E(\text{B3LYP}): -1240.741230$

$E(\text{M06-2X}): -1240.235901$

$E(\text{B3LYP-D}): -1240.789630$

	X	Y	Z
C	0.33259	-4.11914	-0.18254
C	1.67842	-4.28483	-0.10657
C	2.27735	-2.97735	-0.01820
N	1.25353	-2.05980	-0.03987
C	0.02859	-2.70191	-0.13615

C	-1.87012	-0.93069	-0.09789
C	-1.75234	1.54232	-0.07169
C	-1.26451	-2.23358	-0.16201
C	2.27414	4.15573	-0.12469
C	0.93933	4.33783	-0.20428
C	0.34492	2.99707	-0.13372
N	1.32741	2.03859	-0.02817
C	2.48698	2.70201	-0.01920
C	-1.01139	2.77363	-0.15002
C	5.54522	-0.97786	0.18994
C	5.56562	0.37256	0.19175
C	4.16240	0.81257	0.11999
N	3.33337	-0.27168	0.08388
C	4.12767	-1.35677	0.11708
C	3.62841	-2.66876	0.06682
C	3.78767	2.14146	0.07164
C	-1.14890	0.25502	-0.12190
C	-3.15288	1.59970	0.04946
C	-3.95636	0.42348	0.06071
C	-3.32755	-0.85476	-0.01530
O	-3.83756	2.75888	0.16929
C	-5.36691	0.53028	0.15710
C	-6.15656	-0.59468	0.17099
C	-5.55157	-1.86166	0.09819
C	-4.17982	-1.98467	0.01230
H	-0.42226	-4.88776	-0.25847
H	2.23455	-5.20992	-0.11006
H	1.48735	-1.06382	0.00569
H	-1.95767	-3.05839	-0.23913
H	3.05359	4.90478	-0.13659
H	0.39292	5.26641	-0.29429
H	-1.58231	3.69209	-0.26611
H	6.38091	-1.66219	0.22911
H	6.42374	1.02865	0.23293
H	4.32676	-3.49620	0.08367
H	4.59998	2.86138	0.09139
H	-0.07171	0.25266	-0.19841
H	-3.23025	3.49877	0.27730
H	-5.80971	1.51477	0.21940
H	-7.23436	-0.50702	0.24128
H	-6.16610	-2.75487	0.11418

H -3.76739 -2.98214 -0.02797

ONP-23,24,25-H⁺

$\Delta G(\text{B3LYP}): -1240.847629$

$E(\text{B3LYP}): -1241.173889$

$E(\text{M06-2X}): -1240.660990$

$E(\text{B3LYP-D}): -1241.226900$

	X	Y	Z
C	0.12753	-4.05684	-0.89207
C	1.47966	-4.23543	-0.72840
C	2.03287	-3.02105	-0.23488
N	0.98352	-2.11099	-0.14575
C	-0.21141	-2.72791	-0.49727
C	-1.98097	-0.90291	-0.17007
C	-1.63762	1.54956	-0.20861
C	-1.50068	-2.20248	-0.43646
C	2.48182	4.04328	-0.43702
C	1.13120	4.20271	-0.62379
C	0.48345	2.95698	-0.36569
N	1.49301	2.04626	-0.06894
C	2.72395	2.69117	-0.05837
C	-0.88610	2.72636	-0.37324
C	5.24773	-1.23539	0.84369
C	5.40996	0.12785	0.89195
C	4.20455	0.74350	0.44590
N	3.30159	-0.28791	0.18586
C	3.93462	-1.51835	0.36854
C	3.36246	-2.75674	0.09868
C	3.94566	2.09778	0.26346
C	-1.16021	0.23629	-0.27306
C	-3.11903	1.77633	-0.04816
C	-3.96515	0.58093	0.16379
C	-3.41786	-0.72049	0.13101
O	-3.58441	2.90337	-0.07951
C	-5.32635	0.77538	0.42392
C	-6.15803	-0.30689	0.67194
C	-5.62276	-1.59581	0.67329
C	-4.27291	-1.79887	0.41229
H	-0.58259	-4.77657	-1.27038

H	2.05391	-5.12146	-0.95229
H	1.00768	-1.35053	0.51659
H	-2.25283	-2.95679	-0.62879
H	3.25288	4.78707	-0.56840
H	0.61494	5.09963	-0.93081
H	1.31682	1.24494	0.51783
H	-1.49219	3.61936	-0.48946
H	5.96717	-1.98706	1.13131
H	6.28307	0.66818	1.22512
H	2.60285	-0.18088	-0.53831
H	4.02611	-3.61190	0.13515
H	4.79011	2.76750	0.36956
H	-0.13201	0.08651	-0.57637
H	-5.70523	1.78967	0.43306
H	-7.21052	-0.15172	0.87615
H	-6.25802	-2.44738	0.88718
H	-3.89215	-2.81080	0.45258

ONP-O,23,25-H⁺-L

$\Delta G(\text{B3LYP}): -1240.843133$

$E(\text{B3LYP}): -1241.168371$

$E(\text{M06-2X}): -1240.656427$

$E(\text{B3LYP-D}): -1241.219334$

	X	Y	Z
C	0.19157	-4.17146	-0.55305
C	1.53437	-4.32689	-0.38470
C	2.09416	-3.03202	-0.11150
N	1.06242	-2.13615	-0.12332
C	-0.14100	-2.77624	-0.37807
C	-1.93405	-0.94377	-0.24783
C	-1.65531	1.51374	-0.28827
C	-1.41988	-2.27243	-0.41602
C	2.41875	4.11958	-0.14867
C	1.07952	4.25252	-0.35410
C	0.46949	2.94263	-0.30756
N	1.51273	2.05325	-0.09058
C	2.69939	2.71964	0.02142
C	-0.88196	2.71651	-0.39312
C	5.37695	-1.15839	0.48654

C	5.51649	0.18048	0.52875
C	4.17311	0.74103	0.34525
N	3.24222	-0.25032	0.22099
C	3.94740	-1.41802	0.28194
C	3.42995	-2.70198	0.11979
C	3.93327	2.11082	0.25402
C	-1.15160	0.19562	-0.39164
C	-3.04867	1.66328	-0.08221
C	-3.90770	0.53920	0.10601
C	-3.35333	-0.77625	0.04387
O	-3.52040	2.91505	-0.04225
C	-5.28834	0.70674	0.38448
C	-6.10807	-0.37591	0.59689
C	-5.56398	-1.67064	0.55464
C	-4.22201	-1.86090	0.29487
H	-0.53463	-4.93851	-0.77624
H	2.10656	-5.23981	-0.44348
H	1.23728	-1.16638	0.10037
H	-2.15345	-3.04714	-0.59322
H	3.16298	4.90006	-0.11343
H	0.52636	5.16518	-0.51667
H	1.49179	1.04868	0.01981
H	-1.46020	3.62395	-0.50588
H	6.14072	-1.91728	0.57229
H	6.41979	0.75890	0.65556
H	4.13050	-3.52728	0.14614
H	4.78572	2.77241	0.34438
H	-0.12743	0.07842	-0.71390
H	-5.73304	1.69443	0.45483
H	-7.15980	-0.23164	0.81024
H	-6.20060	-2.52784	0.73880
H	-3.84063	-2.87174	0.30669
H	-4.48152	2.93635	0.03176

ONP-O,23-25-H⁺-R

E(B3LYP): -1241.166710

	X	Y	Z
C	0.17435	-4.16180	-0.61292
C	1.51136	-4.32634	-0.39975
C	2.06693	-3.03794	-0.09896
N	1.04220	-2.13615	-0.13927
C	-0.15467	-2.76803	-0.43706
C	-1.94126	-0.93342	-0.29498
C	-1.64859	1.52402	-0.28708
C	-1.43214	-2.25630	-0.49123
C	2.45151	4.09234	-0.28610
C	1.11897	4.23213	-0.52219
C	0.48580	2.93813	-0.38664
N	1.50840	2.04978	-0.09750
C	2.70904	2.70173	-0.01947
C	-0.86805	2.71619	-0.46196
C	5.34453	-1.18420	0.58859
C	5.49192	0.15472	0.60978
C	4.15602	0.71949	0.39020
N	3.22166	-0.26374	0.26779
C	3.91888	-1.43794	0.35684
C	3.39819	-2.71588	0.18095
C	3.92930	2.09171	0.25299
C	-1.15515	0.20649	-0.43605
C	-3.02573	1.66795	0.02772
C	-3.89257	0.54616	0.15466
C	-3.35924	-0.76877	0.01325
O	-3.59501	2.85794	0.24585
C	-5.26421	0.73847	0.45603
C	-6.10017	-0.34223	0.61206
C	-5.58068	-1.64262	0.49431
C	-4.24321	-1.84922	0.21393
H	-0.54844	-4.92342	-0.86391
H	2.07967	-5.24246	-0.44421
H	1.21494	-1.16614	0.08548
H	-2.16771	-3.02463	-0.68860
H	3.20793	4.86184	-0.29587
H	0.58688	5.14123	-0.75909
H	1.46167	1.05599	0.07991

H	-1.41172	3.62680	-0.69741
H	6.10192	-1.94603	0.70062
H	6.39656	0.72959	0.74296
H	4.09146	-3.54646	0.22930
H	4.78846	2.74674	0.32628
H	-0.14505	0.09183	-0.80396
H	-2.94144	3.56542	0.29959
H	-5.64125	1.74594	0.56461
H	-7.14903	-0.19371	0.83723
H	-6.23281	-2.49673	0.63482
H	-3.88465	-2.86760	0.16669

ONP-O,23,24-H⁺-L

$\Delta G(\text{B3LYP}): -1240.838447$

$E(\text{B3LYP}): -1241.164132$

$E(\text{M06-2X}): -1240.652877$

$E(\text{B3LYP-D}): -1241.215183$

	X	Y	Z
C	0.16973	-4.14450	-0.66464
C	1.51706	-4.27242	-0.49348
C	2.04142	-2.99998	-0.08890
N	0.97603	-2.12782	-0.03699
C	-0.20813	-2.79063	-0.36334
C	-1.97050	-0.94840	-0.19948
C	-1.63803	1.49729	-0.23997
C	-1.48390	-2.28408	-0.39485
C	2.42856	4.09316	-0.21160
C	1.09608	4.21871	-0.39226
C	0.53514	2.86871	-0.32798
N	1.54473	1.94114	-0.13666
C	2.67790	2.66565	-0.04932
C	-0.82869	2.67381	-0.36793
C	5.35853	-1.17854	0.56344
C	5.55025	0.16971	0.57629
C	4.27948	0.80048	0.32941
N	3.35210	-0.21649	0.19900
C	3.96060	-1.43916	0.30784
C	3.37998	-2.69415	0.15500
C	3.97178	2.13262	0.19822

C	-1.15596	0.17207	-0.31644
C	-3.03060	1.68041	-0.05888
C	-3.91804	0.57496	0.12074
C	-3.39163	-0.75142	0.06348
O	-3.47880	2.94049	-0.03899
C	-5.29797	0.77084	0.37978
C	-6.14429	-0.29536	0.57502
C	-5.62801	-1.60100	0.53451
C	-4.28589	-1.81861	0.29486
H	-0.52215	-4.90503	-0.99416
H	2.12039	-5.15235	-0.65538
H	0.98153	-1.27392	0.49994
H	-2.22463	-3.04047	-0.61868
H	3.17922	4.86908	-0.18082
H	0.52222	5.12203	-0.53905
H	-1.39267	3.59229	-0.47038
H	6.09758	-1.95054	0.71384
H	6.47546	0.70151	0.73806
H	2.40640	0.02890	-0.08233
H	4.06018	-3.53598	0.17690
H	4.78868	2.83826	0.28886
H	-0.11286	0.06623	-0.57140
H	-5.72183	1.76774	0.44936
H	-7.19561	-0.12915	0.77389
H	-6.28569	-2.44509	0.70490
H	-3.92417	-2.83701	0.30924
H	-4.44068	2.98085	0.01449

ONP-O,23,24-H⁺-R

$E(\text{B3LYP}): -1241.163328$

	X	Y	Z
C	0.15694	-4.13640	-0.71538
C	1.49945	-4.27076	-0.50476
C	2.01475	-3.00454	-0.07524
N	0.95190	-2.12931	-0.04794
C	-0.22363	-2.78536	-0.41307
C	-1.98010	-0.94256	-0.24262
C	-1.62980	1.50306	-0.24423
C	-1.49887	-2.27351	-0.46013

C	2.45622	4.06905	-0.32959
C	1.12961	4.19583	-0.54496
C	0.55431	2.85569	-0.40894
N	1.54987	1.93214	-0.15457
C	2.69013	2.64909	-0.08668
C	-0.81117	2.66370	-0.43787
C	5.32672	-1.19925	0.65178
C	5.52766	0.14743	0.65136
C	4.26573	0.78364	0.37238
N	3.33362	-0.22681	0.24096
C	3.93191	-1.45393	0.37211
C	3.34862	-2.70428	0.20981
C	3.97311	2.11643	0.20302
C	-1.16055	0.17543	-0.36241
C	-3.00951	1.68457	0.03997
C	-3.90475	0.58245	0.16404
C	-3.39970	-0.74431	0.03786
O	-3.55926	2.88728	0.22945
C	-5.27609	0.80621	0.44020
C	-6.13885	-0.25563	0.58711
C	-5.64694	-1.56726	0.48388
C	-4.30907	-1.80432	0.22682
H	-0.52776	-4.89198	-1.07019
H	2.10398	-5.15194	-0.65485
H	0.94394	-1.27477	0.48815
H	-2.24088	-3.02407	-0.69995
H	3.21302	4.83958	-0.32722
H	0.57076	5.09651	-0.75462
H	-1.34109	3.59092	-0.64373
H	6.05801	-1.97429	0.82328
H	6.45381	0.67494	0.82145
H	2.39337	0.02145	-0.05534
H	4.02295	-3.55010	0.25279
H	4.79467	2.81721	0.28737
H	-0.12952	0.06379	-0.66196
H	-2.89498	3.58606	0.26501
H	-5.63298	1.82225	0.53678
H	-7.18781	-0.08255	0.79349
H	-6.32015	-2.40605	0.61725
H	-3.96977	-2.83010	0.19079

ONP-O,24,25-H⁺-L $\Delta G(\text{B3LYP})$: -1240.838264 $E(\text{B3LYP})$: -1241.163623 $E(\text{M06-2X})$: -1240.652006 $E(\text{B3LYP-D})$: -1241.214614

	X	Y	Z
C	-0.22416	-4.13720	-0.51639
C	-1.55782	-4.29839	-0.36861
C	-2.09935	-2.96380	-0.15297
N	-1.13615	-2.01837	-0.17292
C	0.04454	-2.70620	-0.37575
C	1.91630	-0.93522	-0.19485
C	1.70490	1.52448	-0.19330
C	1.34523	-2.23724	-0.37292
C	-2.37428	4.08970	-0.27449
C	-1.03150	4.25205	-0.44114
C	-0.38448	2.98185	-0.24518
N	-1.40870	2.06808	0.01623
C	-2.62812	2.70833	0.02647
C	0.96437	2.74834	-0.30760
C	-5.43162	-1.13232	0.49056
C	-5.51457	0.22668	0.53928
C	-4.19521	0.77340	0.32199
N	-3.35365	-0.29587	0.17123
C	-4.05723	-1.48326	0.24522
C	-3.47955	-2.71842	0.07585
C	-3.87622	2.12611	0.23898
C	1.15737	0.22380	-0.28173
C	3.10812	1.63292	-0.02852
C	3.94188	0.48471	0.11607
C	3.35096	-0.81501	0.04270
O	3.61352	2.87200	0.00922
C	5.33473	0.61282	0.35313
C	6.13387	-0.49398	0.51062
C	5.55638	-1.77373	0.45104
C	4.20237	-1.92572	0.23142
H	0.52498	-4.89660	-0.68761
H	-2.13144	-5.21313	-0.39388
H	2.05988	-3.03655	-0.51936

H	-3.14506	4.83856	-0.37303
H	-0.50855	5.16001	-0.70118
H	-1.23634	1.19237	0.48539
H	1.55794	3.64160	-0.45170
H	-6.23299	-1.84527	0.61089
H	-6.39565	0.82700	0.70678
H	-2.37096	-0.33713	-0.08568
H	-4.13524	-3.57968	0.11854
H	-4.71109	2.81229	0.30169
H	0.11062	0.10022	-0.51249
H	4.57720	2.86663	0.04406
H	5.80470	1.58791	0.43525
H	7.19513	-0.38094	0.69338
H	6.17754	-2.65067	0.58955
H	3.79918	-2.92794	0.22465

ONP-O,24,25-H⁺-R

E(B3LYP): -1241.161626

	X	Y	Z
C	-0.21467	-4.13020	-0.56533
C	-1.54367	-4.29925	-0.38329
C	-2.08453	-2.96966	-0.14189
N	-1.12432	-2.01905	-0.17943
C	0.05050	-2.69975	-0.41762
C	1.92021	-0.92847	-0.23230
C	1.70288	1.53184	-0.19711
C	1.35198	-2.22493	-0.42999
C	-2.39485	4.06407	-0.38414
C	-1.05788	4.22686	-0.58674
C	-0.39600	2.97487	-0.32609
N	-1.40500	2.06854	-0.00221
C	-2.63334	2.69736	-0.00939
C	0.95544	2.74494	-0.37758
C	-5.40373	-1.14775	0.57790
C	-5.49277	0.21293	0.61118
C	-4.18235	0.76099	0.36088
N	-3.33749	-0.30467	0.21009
C	-4.03462	-1.49385	0.30846
C	-3.45617	-2.72877	0.12589

C	-3.87161	2.11553	0.23784
C	1.16075	0.23184	-0.32259
C	3.09458	1.63308	0.07058
C	3.93203	0.48642	0.15674
C	3.35564	-0.81143	0.01699
O	3.70368	2.80638	0.27345
C	5.31909	0.63744	0.40817
C	6.13035	-0.46755	0.51527
C	5.57075	-1.75089	0.39455
C	4.21842	-1.91732	0.16115
H	0.53326	-4.88441	-0.76262
H	-2.11337	-5.21660	-0.40084
H	2.06800	-3.01992	-0.59378
H	-3.17310	4.80128	-0.50884
H	-0.55001	5.12430	-0.90673
H	-1.21728	1.21355	0.49912
H	1.51514	3.63992	-0.63437
H	-6.19935	-1.86277	0.72174
H	-6.37384	0.81083	0.78709
H	-2.36015	-0.34314	-0.06877
H	-4.10879	-3.59156	0.18478
H	-4.71101	2.79738	0.28735
H	0.12257	0.11423	-0.59372
H	3.07204	3.53076	0.35584
H	5.72772	1.63263	0.51623
H	7.19070	-0.35141	0.70239
H	6.20411	-2.62469	0.49416
H	3.83307	-2.92523	0.10484

ONPH₂²⁺-L

ΔG (B3LYP): -1241.115510

E(B3LYP): -1241.454366

E(M06-2X): -1240.936175

E(B3LYP-D): -1241.508381

	X	Y	Z
C	-0.12753	-4.05684	-0.89207
C	-1.47966	-4.23543	-0.72840
C	-2.03287	-3.02105	-0.23488
N	-0.98352	-2.11099	-0.14575

C	0.21141	-2.72791	-0.49727
C	1.98097	-0.90291	-0.17007
C	1.63762	1.54956	-0.20861
C	1.50068	-2.20248	-0.43646
C	-2.48182	4.04328	-0.43702
C	-1.13120	4.20271	-0.62380
C	-0.48345	2.95698	-0.36569
N	-1.49301	2.04626	-0.06894
C	-2.72395	2.69117	-0.05837
C	0.88610	2.72636	-0.37323
C	-5.24773	-1.23539	0.84369
C	-5.40996	0.12785	0.89194
C	-4.20455	0.74350	0.44590
N	-3.30159	-0.28791	0.18586
C	-3.93462	-1.51835	0.36854
C	-3.36246	-2.75674	0.09868
C	-3.94566	2.09778	0.26346
C	1.16021	0.23629	-0.27306
C	3.11903	1.77633	-0.04816
C	3.96515	0.58093	0.16379
C	3.41786	-0.72049	0.13100
O	3.58441	2.90337	-0.07950
C	5.32635	0.77538	0.42392
C	6.15803	-0.30689	0.67193
C	5.62276	-1.59581	0.67328
C	4.27291	-1.79887	0.41229
H	0.58259	-4.77657	-1.27038
H	-2.05391	-5.12146	-0.95229
H	-1.00768	-1.35052	0.51659
H	2.25283	-2.95679	-0.62879
H	-3.25288	4.78706	-0.56840
H	-0.61494	5.09963	-0.93081
H	-1.31682	1.24494	0.51784
H	1.49219	3.61936	-0.48946
H	-5.96718	-1.98706	1.13130
H	-6.28307	0.66818	1.22511
H	-2.60285	-0.18087	-0.53831
H	-4.02611	-3.61190	0.13515
H	-4.79011	2.76750	0.36956
H	0.13201	0.08651	-0.57637
H	5.70523	1.78967	0.43306

H	7.21052	-0.15172	0.87614
H	6.25802	-2.44738	0.88718
H	3.89216	-2.81080	0.45257

ONPH₂²⁺-R

E(B3LYP): -1241.450057

	X	Y	Z
C	-0.22095	-4.05108	-1.01136
C	-1.56314	-4.21281	-0.78013
C	-2.06165	-3.00563	-0.21001
N	-1.00367	-2.11700	-0.13843
C	0.16364	-2.74074	-0.58103
C	1.94312	-0.93177	-0.24686
C	1.65512	1.52583	-0.23257
C	1.44912	-2.23208	-0.56765
C	-2.46981	4.00051	-0.61865
C	-1.12995	4.14799	-0.85582
C	-0.46309	2.93031	-0.49356
N	-1.46323	2.04254	-0.09327
C	-2.69048	2.68191	-0.11604
C	0.89852	2.70940	-0.49851
C	-5.21616	-1.18260	1.00613
C	-5.36445	0.17567	1.02856
C	-4.16294	0.77182	0.51931
N	-3.27649	-0.26976	0.25452
C	-3.91532	-1.48912	0.48369
C	-3.37673	-2.73216	0.20335
C	-3.90939	2.11322	0.27943
C	1.15195	0.21221	-0.36475
C	3.04928	1.66557	0.08895
C	3.90213	0.53763	0.23377
C	3.35978	-0.77548	0.09001
O	3.61783	2.84350	0.28857
C	5.27069	0.71876	0.55438
C	6.09295	-0.37294	0.72974
C	5.56012	-1.66532	0.61653
C	4.21878	-1.86125	0.31602
H	0.45176	-4.76689	-1.46031
H	-2.16623	-5.07946	-1.00508
H	-0.98049	-1.38257	0.55404

H	2.19194	-2.96913	-0.84749
H	-3.24938	4.72595	-0.79602
H	-0.63459	5.01721	-1.26287
H	-1.27481	1.28855	0.55140
H	1.45609	3.59891	-0.77871
H	-5.93043	-1.92233	1.33618
H	-6.22029	0.73293	1.37952
H	-2.60484	-0.18550	-0.49811
H	-4.04375	-3.58215	0.28093
H	-4.74615	2.79315	0.38299
H	0.14589	0.10223	-0.74624
H	5.66067	1.72146	0.66366
H	7.14003	-0.23489	0.96849
H	6.19954	-2.52566	0.77594
H	3.84715	-2.87614	0.27935
H	2.99208	3.57883	0.31655

HDBP-23,25-H

$\Delta G(\text{B3LYP}): -1276.619105$

$E(\text{B3LYP}): -1276.919975$

$E(\text{M06-2X}): -1276.407466$

$E(\text{B3LYP-D}): -1276.972300$

	X	Y	Z
C	-0.44052	-4.26519	0.21516
C	-1.80805	-4.27356	0.11967
C	-2.24819	-2.91691	0.03181
N	-1.12230	-2.13192	0.08028
C	0.01572	-2.90591	0.18900
C	1.97321	-1.25932	0.20240
C	1.97765	1.23863	0.19836
C	1.35137	-2.51654	0.24388
C	-1.77566	4.28404	0.10788
C	-0.40848	4.26628	0.20665
C	0.03796	2.90371	0.18681
N	-1.10554	2.13730	0.07918
C	-2.22566	2.93031	0.02480
C	1.37008	2.50364	0.24223
C	-5.32225	-0.65865	-0.23362
C	-5.31701	0.69504	-0.23581

C	-3.92111	1.10220	-0.13762
N	-3.09980	0.00983	-0.08449
C	-3.92957	-1.07635	-0.13421
C	-3.54467	-2.41900	-0.07922
C	-3.52576	2.44200	-0.08650
C	1.33803	-0.01083	0.22653
C	3.46182	1.24271	0.17510
C	4.17053	-0.01902	-0.32949
C	3.47462	-1.29572	0.17774
O	4.14004	2.19884	0.51055
O	4.10882	-2.28062	0.47609
O	5.51797	-0.00304	0.05612
C	4.07445	-0.03615	-1.88279
H	0.21840	-5.11610	0.29855
H	-2.46251	-5.13163	0.11051
H	-1.21791	-1.12891	0.00831
H	2.04693	-3.34685	0.30472
H	-2.42366	5.14692	0.09323
H	0.25592	5.11324	0.28722
H	-1.20822	1.13445	0.01427
H	2.07153	3.32868	0.30198
H	-6.17046	-1.32583	-0.28818
H	-6.16003	1.36859	-0.29253
H	-4.33706	-3.15718	-0.11708
H	-4.31227	3.18624	-0.12805
H	0.26848	-0.00741	0.36968
H	5.69955	0.90129	0.35713
H	3.04519	-0.09458	-2.24137
H	4.63320	-0.90147	-2.24331
H	4.54086	0.87010	-2.27456

HDBP-23,24-H

$\Delta G(\text{B3LYP}): -1276.612333$

$E(\text{B3LYP}): -1276.913525$

$E(\text{M06-2X}): -1276.401204$

$E(\text{B3LYP-D}): -1276.965994$

	X	Y	Z
C	0.38351	-4.25874	-0.37429
C	1.75350	-4.23907	-0.28395

C	2.16894	-2.89629	-0.03830
N	1.01582	-2.13269	-0.00543
C	-0.10583	-2.93088	-0.19101
C	-2.01829	-1.25216	-0.15980
C	-1.95968	1.23811	-0.20559
C	-1.43517	-2.52853	-0.22360
C	1.80823	4.24286	-0.17295
C	0.45769	4.22437	-0.28373
C	0.05458	2.82325	-0.25301
N	1.14937	2.01210	-0.13848
C	2.22261	2.85310	-0.07861
C	-1.30058	2.47292	-0.28992
C	5.30077	-0.70915	0.34764
C	5.35259	0.66005	0.34417
C	4.02095	1.15065	0.16852
N	3.20056	0.04597	0.08379
C	3.93529	-1.11585	0.17427
C	3.47538	-2.42850	0.09776
C	3.56048	2.45558	0.07623
C	-1.34547	-0.02329	-0.20364
C	-3.44134	1.28653	-0.17528
C	-4.17971	0.05561	0.36463
C	-3.52102	-1.24672	-0.12654
O	-4.09817	2.24910	-0.53427
O	-4.18288	-2.21848	-0.40901
O	-5.52986	0.10033	-0.00942
C	-4.07157	0.06677	1.91655
H	-0.24762	-5.11006	-0.57944
H	2.43040	-5.07137	-0.40235
H	0.96386	-1.22412	0.42501
H	-2.14894	-3.34067	-0.31337
H	2.46909	5.09741	-0.15058
H	-0.21938	5.06194	-0.37096
H	-1.97499	3.32036	-0.36123
H	6.12446	-1.39716	0.46350
H	6.22602	1.28448	0.45453
H	2.22013	0.19693	-0.13782
H	4.24323	-3.19206	0.12128
H	4.30686	3.23918	0.13254
H	-0.27403	-0.00018	-0.33926
H	-5.68507	1.00008	-0.33833

H	-3.04135	-0.01062	2.26855
H	-4.64994	-0.77574	2.29972
H	-4.51068	0.99284	2.29320

HDBPH₂²⁺

$\Delta G(\text{B3LYP}): -1276.984581$

$E(\text{B3LYP}): -1277.298603$

$E(\text{M06-2X}): -1276.781477$

$E(\text{B3LYP-D}): -1277.353864$

	X	Y	Z
C	-0.44780	4.20676	-0.67914
C	-1.81564	4.20114	-0.54653
C	-2.22082	2.89198	-0.16140
N	-1.07037	2.11501	-0.11227
C	0.04459	2.90177	-0.38291
C	1.97817	1.25200	-0.19557
C	1.98231	-1.23530	-0.18868
C	1.38041	2.50958	-0.36225
C	-1.78788	-4.21161	-0.54165
C	-0.41984	-4.20937	-0.67203
C	0.06403	-2.90038	-0.37963
N	-1.05624	-2.11949	-0.11412
C	-2.20181	-2.90366	-0.16170
C	1.39712	-2.49941	-0.35527
C	-5.20957	0.67060	0.74467
C	-5.20516	-0.70173	0.74366
C	-3.92118	-1.15124	0.31640
N	-3.14330	-0.00849	0.11245
C	-3.92860	1.12899	0.31793
C	-3.51261	2.44024	0.12094
C	-3.49663	-2.45971	0.11906
C	1.33426	0.00841	-0.25938
C	3.47585	-1.23642	-0.05538
C	4.14372	0.01570	0.51572
C	3.48784	1.28153	-0.06587
O	4.15622	-2.18867	-0.37330
O	4.12680	2.25678	-0.36357
H	0.17587	5.03529	-0.97911
C	-2.49227	5.02393	-0.72021

H	-1.01294	1.30857	0.49048
H	2.09002	3.32276	-0.48188
H	-2.45908	-5.03929	-0.71309
H	0.20896	-5.03555	-0.96772
H	-1.00502	-1.30929	0.48412
H	2.11102	-3.30893	-0.47031
H	-6.02194	1.31876	1.03686
H	-6.01332	-1.35552	1.03497
H	-4.28061	3.20118	0.18655
H	-4.25971	-3.22556	0.18471
H	0.28663	0.00468	-0.53344
H	-2.43269	-0.00540	-0.60838
C	3.91687	0.03924	2.05686
H	4.34673	-0.86625	2.48890
H	4.45079	0.90222	2.45724
H	2.86351	0.10502	2.33727
O	5.51167	0.01383	0.24450
H	5.75003	-0.87586	-0.05748

5-BPhIH⁺

$\Delta G(\text{B3LYP}): -1013.160519$

$E(\text{B3LYP}): -1013.462688$

$E(\text{M06-2X}): -1013.037678$

$E(\text{B3LYP-D}): -1013.509015$

	X	Y	Z
C	2.10366	3.77008	-0.67936
C	3.18979	2.95423	-0.68647
C	2.76291	1.61533	-0.34868
N	1.38647	1.65911	-0.23687
C	0.93252	2.98639	-0.35292
C	-1.49564	2.57914	0.18960
C	-2.88533	0.60326	-0.21143
C	-0.33627	3.41393	-0.12010
C	-1.70406	-3.98195	-0.32444
C	-2.80361	-3.21606	-0.72175
C	-2.43307	-1.87080	-0.65514
N	-1.13096	-1.81854	-0.25494
C	-0.64362	-3.10712	-0.02486
C	-3.20496	-0.63905	-1.02732

C	3.90342	-1.85367	0.75840
C	3.08603	-2.95147	0.88640
C	1.78379	-2.61266	0.42205
N	1.84104	-1.25459	0.05187
C	3.13688	-0.78641	0.21027
C	3.56700	0.51313	-0.10799
C	0.67153	-3.42807	0.35053
C	-1.75895	1.37876	-0.50117
C	-3.74674	1.01972	0.80870
C	-3.51403	2.21682	1.48523
C	-2.41280	3.00153	1.16807
H	2.08070	4.82910	-0.88926
H	4.21313	3.22627	-0.89631
H	0.88890	1.00158	0.34588
H	-0.48418	4.48887	-0.11010
H	-1.64459	-5.05898	-0.28118
H	-3.76763	-3.58128	-1.03971
H	-0.71985	-0.97448	0.11332
H	-3.01380	-0.42489	-2.08714
H	-4.26953	-0.86852	-0.95401
H	4.94139	-1.77624	1.04283
H	3.35207	-3.91310	1.29967
H	1.27497	-0.90584	-0.71036
H	4.63601	0.68121	-0.10807
H	0.84170	-4.47119	0.59285
H	-1.12223	1.10686	-1.33768
H	-4.62157	0.42662	1.05144
H	-4.20457	2.54348	2.25370
H	-2.24748	3.93838	1.68793

10-BPhIH⁺

$\Delta G(\text{B3LYP}): -1013.131601$

$E(\text{B3LYP}): -1013.432829$

$E(\text{M06-2X}): -1013.007765$

$E(\text{B3LYP-D}): -1013.478271$

	X	Y	Z
C	-1.55256	4.01629	-0.58349
C	-0.26889	4.38827	-0.35495
C	0.51336	3.20968	-0.05651

N	-0.36890	2.11626	-0.18453
C	-1.66878	2.58085	-0.40237
C	-3.02042	0.45164	-0.07976
C	-2.30817	-1.88931	0.18818
C	-2.82827	1.85721	-0.36641
C	2.08804	-3.84400	-0.42125
C	0.78580	-4.21063	-0.15819
C	-0.00786	-3.02498	-0.05781
N	0.88235	-1.96619	-0.26787
C	2.12828	-2.43042	-0.48314
C	-1.36781	-2.97187	0.15477
C	3.64113	1.57892	1.26663
C	4.04925	0.25192	0.97013
C	3.25554	-0.21689	-0.05203
N	2.31454	0.76256	-0.33880
C	2.57498	1.89744	0.44244
C	1.82586	3.11816	0.29698
C	3.28536	-1.52383	-0.78717
C	-2.03261	-0.54548	-0.15636
C	-3.62013	-2.23665	0.58936
C	-4.61682	-1.27225	0.64380
C	-4.32300	0.04127	0.31019
H	-2.38252	4.65740	-0.84046
H	0.13925	5.38708	-0.39984
H	-0.22229	1.31279	0.40982
H	-3.73451	2.43810	-0.49075
H	2.93690	-4.49369	-0.56607
H	0.39517	-5.21277	-0.06241
H	0.68402	-0.98634	-0.13032
H	-1.80339	-3.95143	0.32744
H	4.06282	2.22751	2.01881
H	4.84122	-0.29931	1.45392
H	1.87092	0.85646	-1.24317
H	2.35143	4.04285	0.50275
H	3.31180	-1.36259	-1.87575
H	4.21031	-2.04872	-0.54291
H	-1.07679	-0.28768	-0.58754
H	-3.84299	-3.26372	0.85384
H	-5.62183	-1.54382	0.94251
H	-5.10904	0.78742	0.35029

5-BPhI-23,25-H $\Delta G(\text{B3LYP}): -1012.777147$ $E(\text{B3LYP}): -1013.063516$ $E(\text{M06-2X}): -1012.647658$ $E(\text{B3LYP-D}): -1013.110087$

	X	Y	Z
C	0.84125	4.25827	-0.24550
C	2.12483	3.83610	-0.35441
C	2.14156	2.38904	-0.26636
N	0.82174	1.99547	-0.17646
C	-0.02573	3.09894	-0.10724
C	-2.27260	1.97253	0.18175
C	-2.91878	-0.30705	-0.43882
C	-1.37568	3.11422	0.08877
C	-0.48290	-4.23455	0.23588
C	-1.73869	-3.82160	-0.23999
C	-1.63081	-2.48331	-0.62233
N	-0.35149	-2.09118	-0.37639
C	0.38607	-3.13705	0.14750
C	-2.65074	-1.57257	-1.23849
C	4.40653	-0.62495	0.31977
C	3.99205	-1.89633	0.55351
C	2.55331	-1.90284	0.36152
N	2.11046	-0.62446	0.03551
C	3.20951	0.14963	0.01772
C	3.23229	1.55879	-0.19924
C	1.76245	-3.02874	0.45136
C	-2.06030	0.78606	-0.54656
C	-4.02508	-0.21981	0.41013
C	-4.28020	0.96174	1.10790
C	-3.42280	2.04736	0.99140
H	0.47952	5.27572	-0.26070
H	3.01021	4.44372	-0.46801
H	0.59661	1.04028	0.06991
H	-1.81719	4.09482	0.23247
H	-0.21510	-5.21174	0.60801
H	-2.63517	-4.41793	-0.31416
H	0.07977	-1.18676	-0.53198
H	-2.32396	-1.29094	-2.24753
H	-3.57734	-2.13760	-1.35759

H	5.41233	-0.23183	0.36270
H	4.59135	-2.75686	0.81550
H	4.20571	2.03201	-0.24576
H	2.24904	-3.94697	0.76285
H	-1.23997	0.74666	-1.25566
H	-4.69569	-1.06631	0.51236
H	-5.15306	1.03161	1.74758
H	-3.62540	2.95992	1.54179

5-BPhl-24,25-H

$\Delta G(\text{B3LYP}): -1012.770991$

$E(\text{B3LYP}): -1013.059871$

$E(\text{M06-2X}): -1012.640486$

$E(\text{B3LYP-D}): -1013.103316$

	X	Y	Z
C	-0.48775	-4.31663	-0.32164
C	0.86491	-4.24995	-0.39532
C	1.27852	-2.86945	-0.24092
N	0.10398	-2.13508	-0.14810
C	-1.01384	-2.97857	-0.13660
C	-2.81072	-1.24236	0.17422
C	-2.68589	1.13717	-0.39294
C	-2.31133	-2.60581	0.04831
C	0.80989	4.23195	0.14173
C	-0.49035	4.16825	-0.27831
C	-0.74348	2.78190	-0.60360
N	0.31782	2.02190	-0.39062
C	1.31863	2.88401	0.07299
C	-2.03323	2.25673	-1.18317
C	4.36072	-0.71364	0.41732
C	4.38583	0.66263	0.60314
C	3.09247	1.15750	0.33862
N	2.30616	0.06781	0.00882
C	3.04358	-1.08702	0.05104
C	2.56968	-2.41170	-0.16222
C	2.60011	2.47482	0.38279
C	-2.22405	-0.17069	-0.52451
C	-3.76718	1.38721	0.45672

C	-4.39054	0.33445	1.12992
C	-3.92767	-0.96685	0.98662
H	-1.10607	-5.19870	-0.39730
H	1.55519	-5.06825	-0.53726
H	0.05470	-1.20378	0.23584
H	-3.03000	-3.41220	0.14912
H	1.36426	5.10033	0.46853
H	-1.20046	4.97822	-0.36694
H	-2.73448	3.08887	-1.28056
H	-1.83150	1.89598	-2.19882
H	5.17627	-1.40709	0.55394
H	5.22916	1.26568	0.90413
H	1.36327	0.24063	-0.33741
H	3.34006	-3.17195	-0.20401
H	3.30753	3.23680	0.69312
H	-1.42026	-0.36739	-1.22300
H	-4.13575	2.40039	0.57803
H	-5.24232	0.53499	1.77057
H	-4.41522	-1.77856	1.51613

5-BPhl-23,24-H

$\Delta G(\text{B3LYP}): -1012.76864$

$E(\text{B3LYP}): -1013.057423$

$E(\text{M06-2X}): -1012.638265$

$E(\text{B3LYP-D}): -1013.100889$

	X	Y	Z
C	-0.90315	4.21780	-0.05199
C	-2.18425	3.81630	-0.18508
C	-2.15574	2.34917	-0.20530
N	-0.89782	1.88296	-0.13113
C	-0.08047	3.00354	-0.02197
C	2.24535	1.96185	0.14829
C	2.98433	-0.27682	-0.49714
C	1.27800	3.04332	0.14151
C	0.57881	-4.10618	0.51493
C	1.84980	-3.72106	0.04035
C	1.72288	-2.47004	-0.54834
N	0.41511	-2.08986	-0.41673
C	-0.32153	-3.07738	0.22304

C	2.72899	-1.58966	-1.22574
C	-4.47353	-0.70588	0.08761
C	-4.00452	-1.95894	0.33952
C	-2.56149	-1.93276	0.31244
N	-2.21386	-0.60717	0.03702
C	-3.34154	0.17718	-0.06591
C	-3.32579	1.55079	-0.21368
C	-1.72325	-3.00881	0.45131
C	2.03714	0.74522	-0.52592
C	4.17138	-0.08354	0.21580
C	4.41625	1.12965	0.86052
C	3.47097	2.14455	0.82039
H	-0.52080	5.22673	0.01404
H	-3.07555	4.42536	-0.24082
H	1.69135	4.03180	0.32270
H	0.32628	-5.02105	1.02887
H	2.76791	-4.28334	0.11502
H	0.01590	-1.27495	-0.85397
H	3.66221	-2.14835	-1.31748
H	2.39496	-1.36993	-2.24814
H	-5.50376	-0.38987	0.02363
H	-4.58466	-2.85546	0.50189
H	-1.32285	-0.13458	0.18580
H	-4.28193	2.05581	-0.26835
H	-2.19270	-3.93941	0.74869
H	1.12369	0.63727	-1.09742
H	4.91143	-0.87599	0.25506
H	5.34809	1.27890	1.39454
H	3.66453	3.08578	1.32400

10-BPhl-24,25-H

$\Delta G(\text{B3LYP}): -1012.754143$

$E(\text{B3LYP}): -1013.04192$

$E(\text{M06-2X}): -1012.624628$

$E(\text{B3LYP-D}): -1013.084703$

	X	Y	Z
C	0.75493	-4.23017	-0.33040
C	-0.58743	-4.32864	-0.16294

C	-1.13370	-3.00922	0.04904
N	-0.03945	-2.12153	-0.03023
C	1.15022	-2.83972	-0.20007
C	2.93862	-1.01852	-0.06240
C	2.72240	1.42151	0.10675
C	2.43182	-2.36790	-0.21662
C	-1.24400	4.18042	-0.09087
C	0.09443	4.28392	0.08614
C	0.63077	2.92876	-0.00786
N	-0.42340	2.02700	-0.24826
C	-1.51203	2.75893	-0.29571
C	1.95929	2.65618	0.12785
C	-4.30600	-0.98151	0.64830
C	-4.43445	0.41056	0.44371
C	-3.23907	0.86734	-0.08872
N	-2.39675	-0.20508	-0.19356
C	-3.02440	-1.36042	0.24845
C	-2.44122	-2.66749	0.22537
C	-2.88468	2.22423	-0.61194
C	2.15404	0.15009	-0.08720
C	4.11261	1.52902	0.30684
C	4.90903	0.38882	0.30407
C	4.33407	-0.85964	0.12445
H	1.45025	-5.03153	-0.53206
H	-1.18842	-5.22493	-0.21347
H	-0.03906	-1.27632	0.52225
H	3.19030	-3.13655	-0.31928
H	-1.98404	4.96789	-0.08244
H	0.67943	5.17334	0.27258
H	2.57006	3.53962	0.29792
H	-5.05058	-1.65046	1.05222
H	-5.30210	1.01942	0.64778
H	-1.46453	-0.12615	-0.57204
H	-3.13846	-3.48878	0.34476
H	-2.98245	2.23044	-1.70987
H	-3.63187	2.93462	-0.25021
H	1.09634	0.11164	-0.29321
H	4.55822	2.50558	0.46063
H	5.98017	0.47441	0.44857
H	4.96224	-1.74417	0.13262