Synthesis and Characterization of Hydrazine-Appended BODIPY Dyes and the Related Aminomethyl Complexes

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Supporting Information

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1) Multinuclear NMR of $BoNHNH_2$

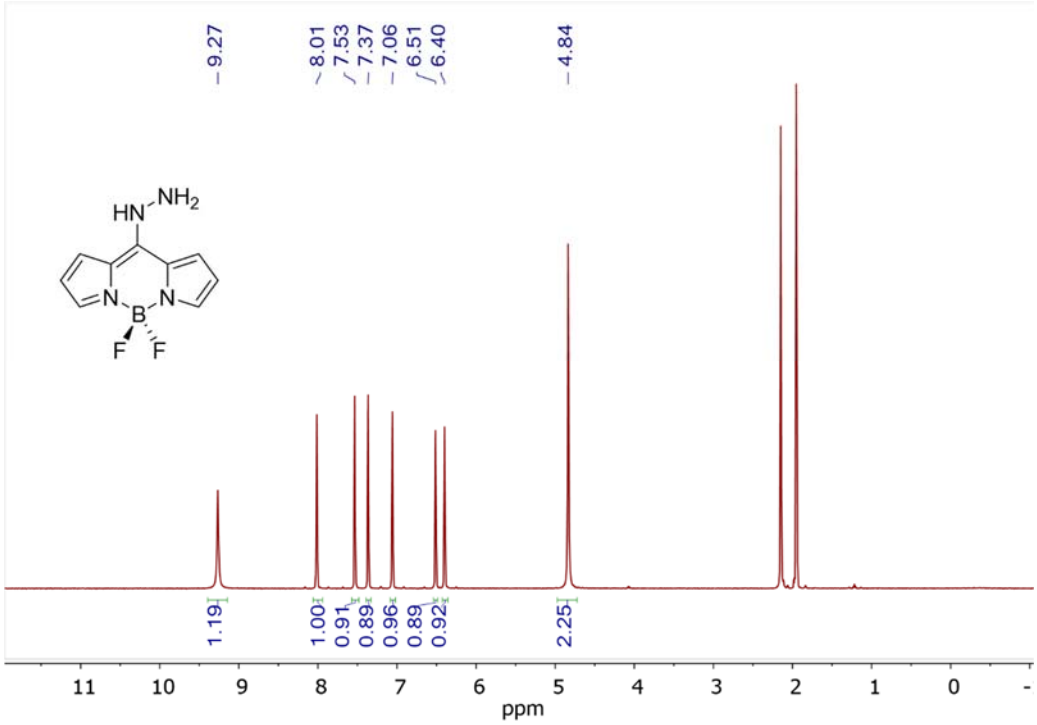


Figure S1. ^{1}H NMR spectrum of **$BoNHNH_2$** in CD_3CN

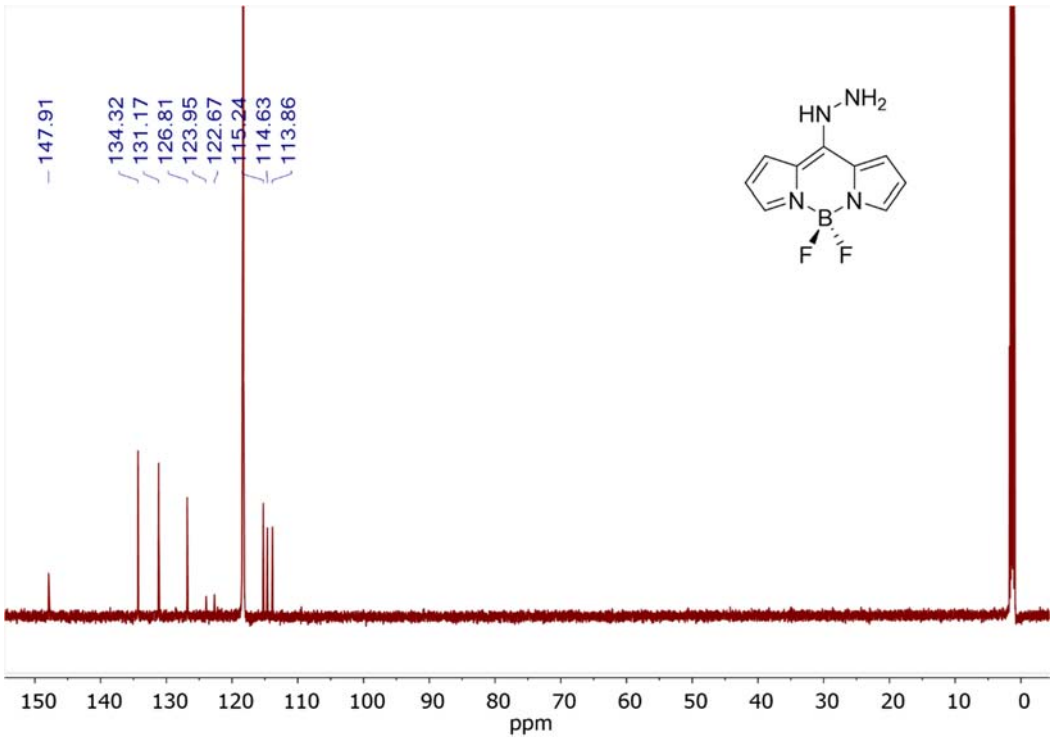


Figure S2 $^{13}C\{^{1}H\}$ spectrum of **$BoNHNH_2$** in CD_3CN

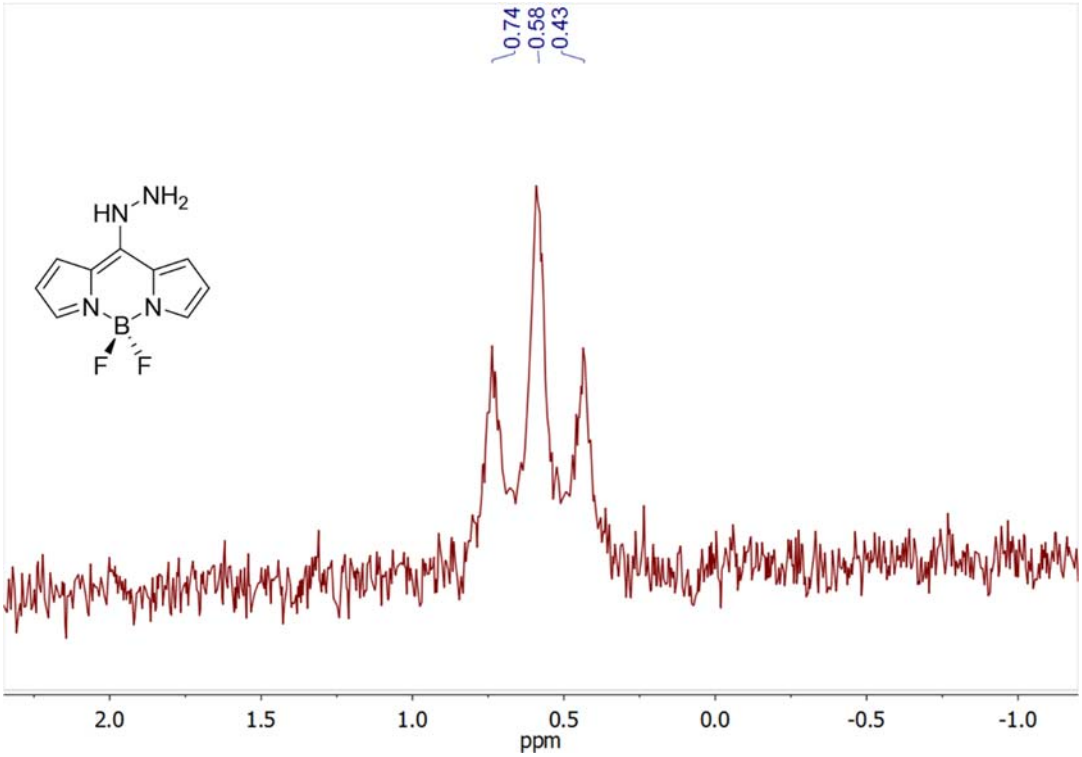


Figure S3. $^{11}B\{^{1}H\}$ NMR spectrum of **BoNHNH$_2$** in CD_3CN

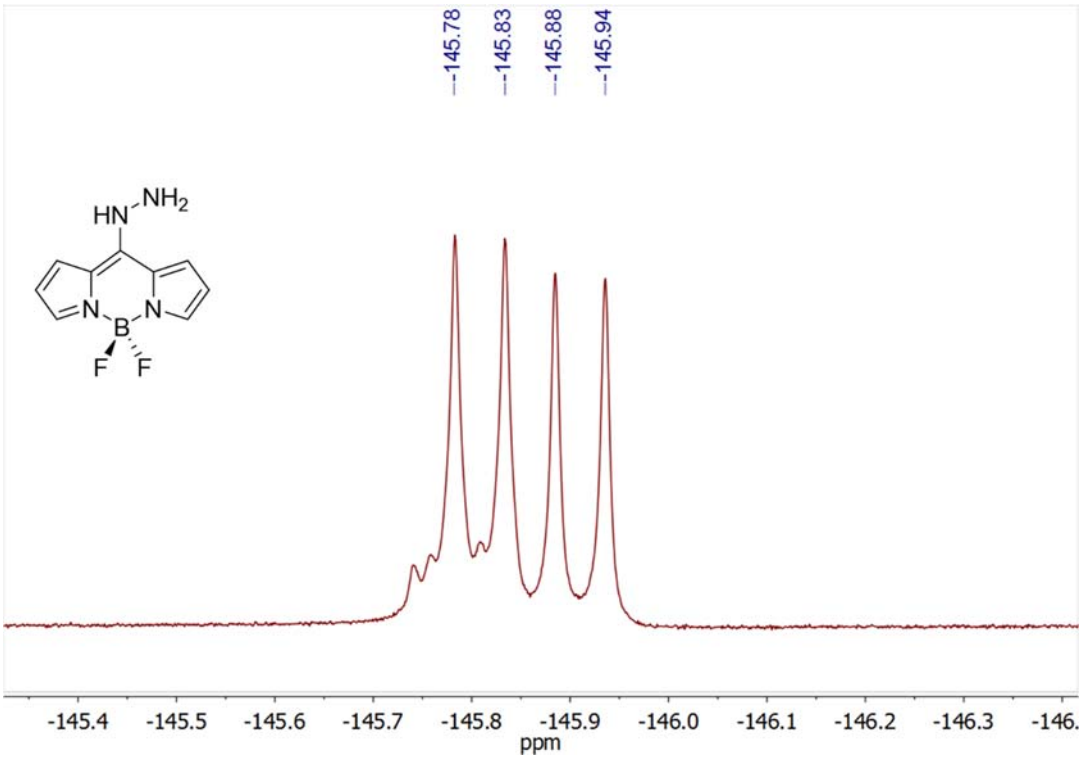


Figure S4. ^{19}F NMR spectrum of **BoNHNH$_2$** in CD_3CN

2) Multinuclear NMR of BoNHNHBo

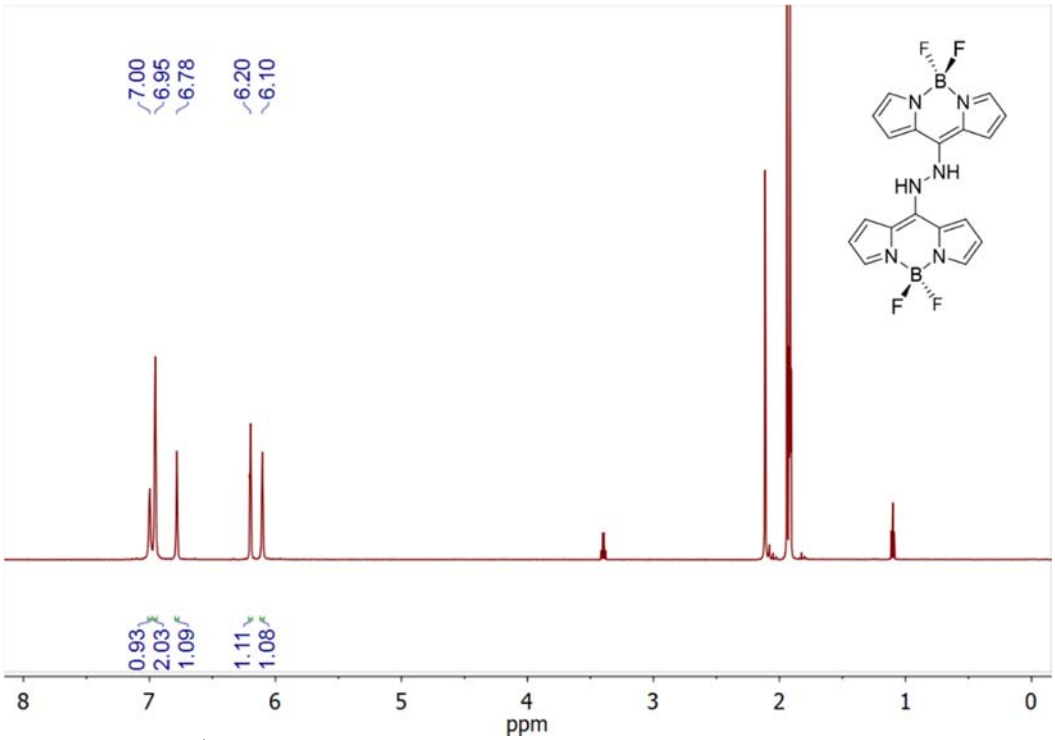


Figure S5. ^{1}H NMR spectrum of **BoNHNHBo** in CD_3CN. Unassigned signals are attributed to residual diethyl ether.

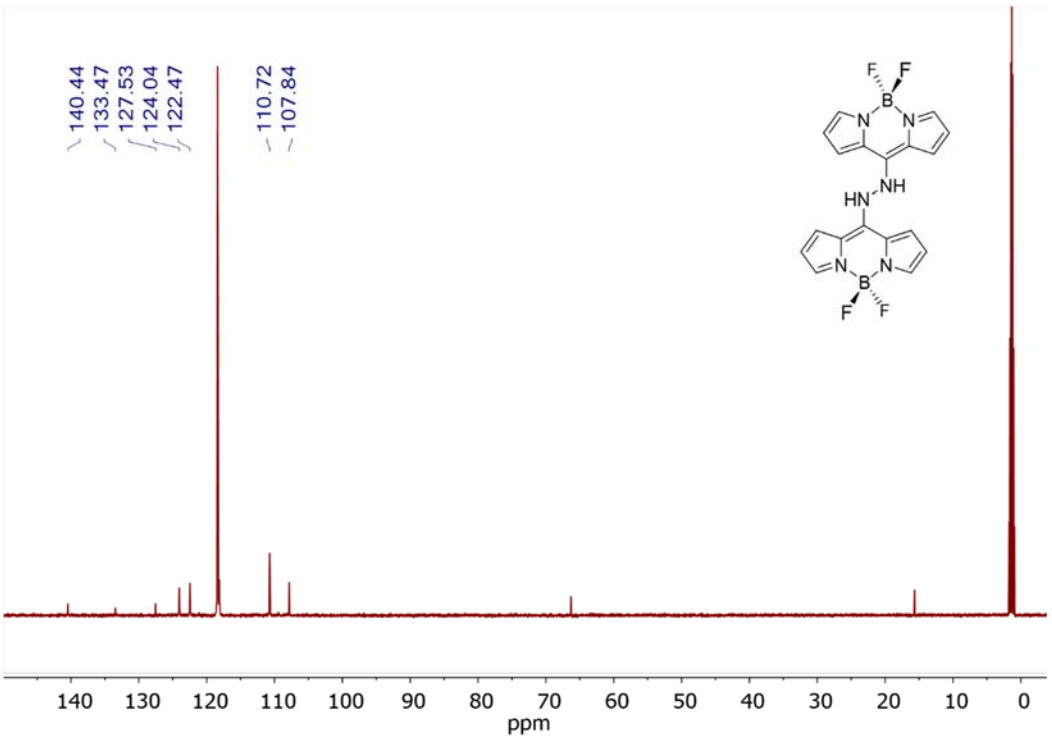


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of **BoNHNHBo** in CD_3CN. Unassigned signals are attributed to residual diethyl ether.

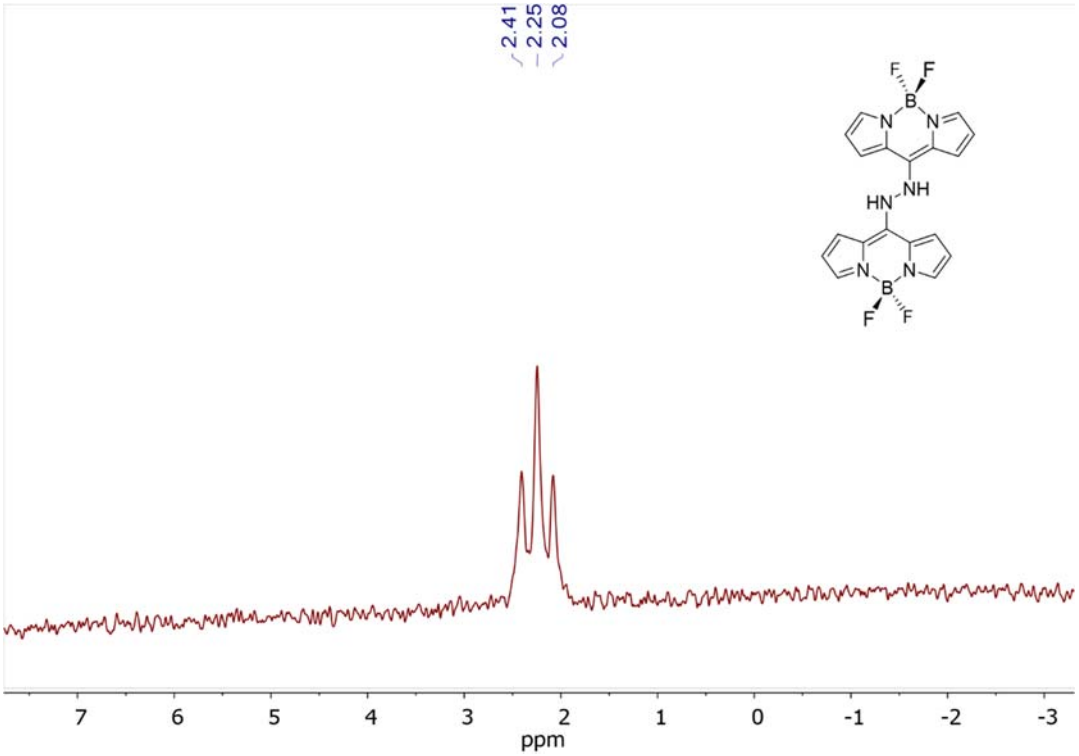


Figure S7. $^{11}B\{^{1}H\}$ NMR spectrum of **BoNHNHBo** in CD_3CN

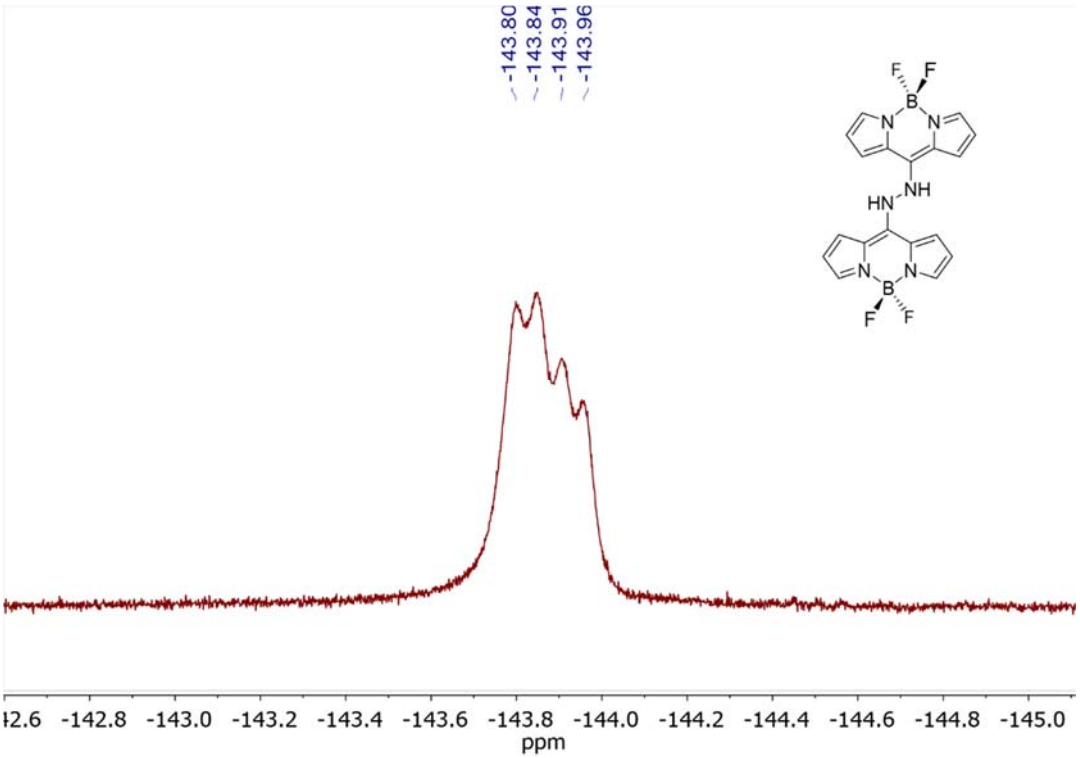


Figure S8. ^{19}F NMR spectrum of **BoNHNHBo** in CD_3CN

3) Multinuclear NMR of BoNHNHPh

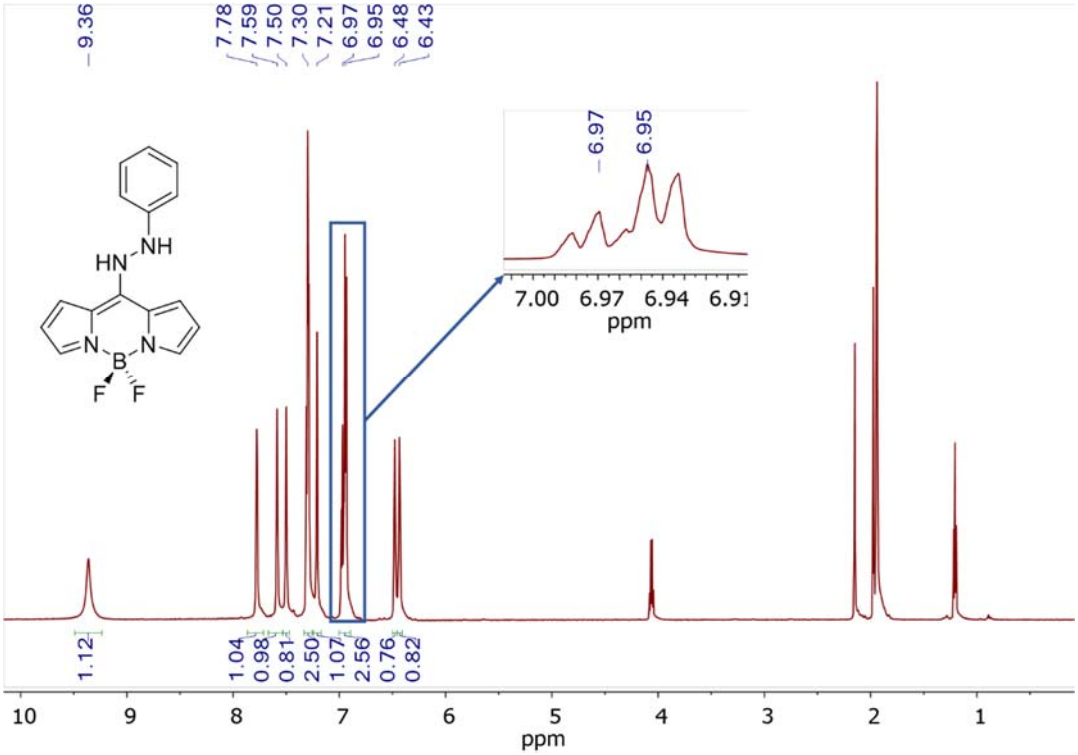


Figure S9. ^{1}H NMR spectrum of **BoNHNHPh** in CD_3CN

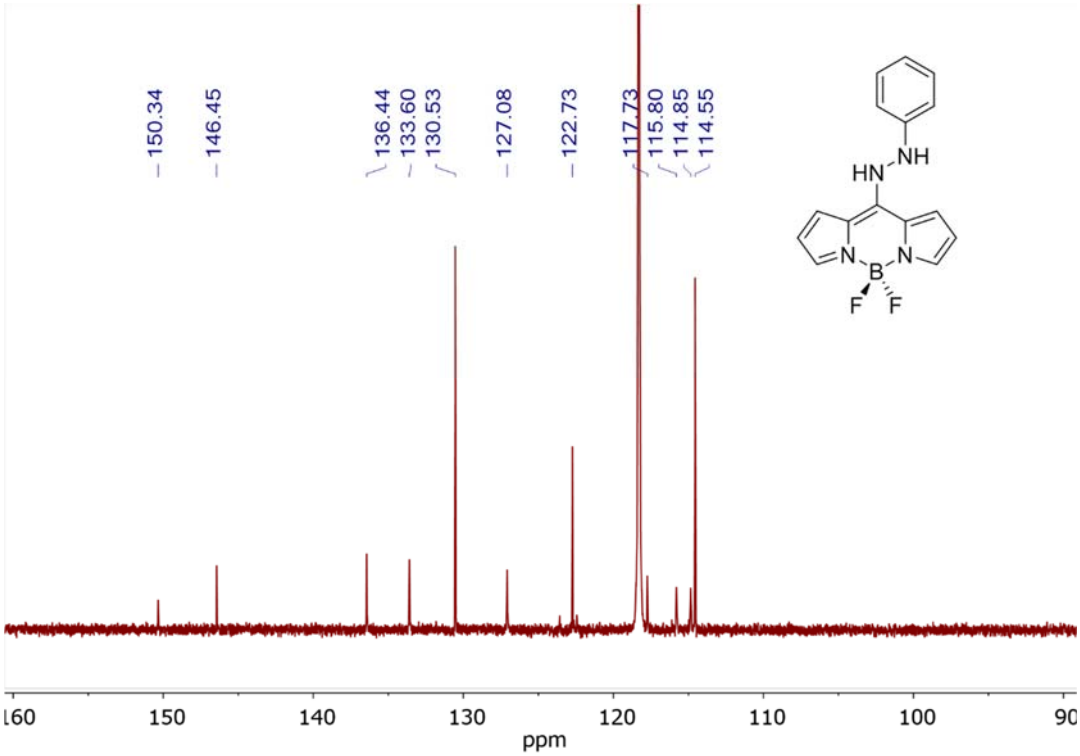


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of **BoNHNHPh** in CD_3CN

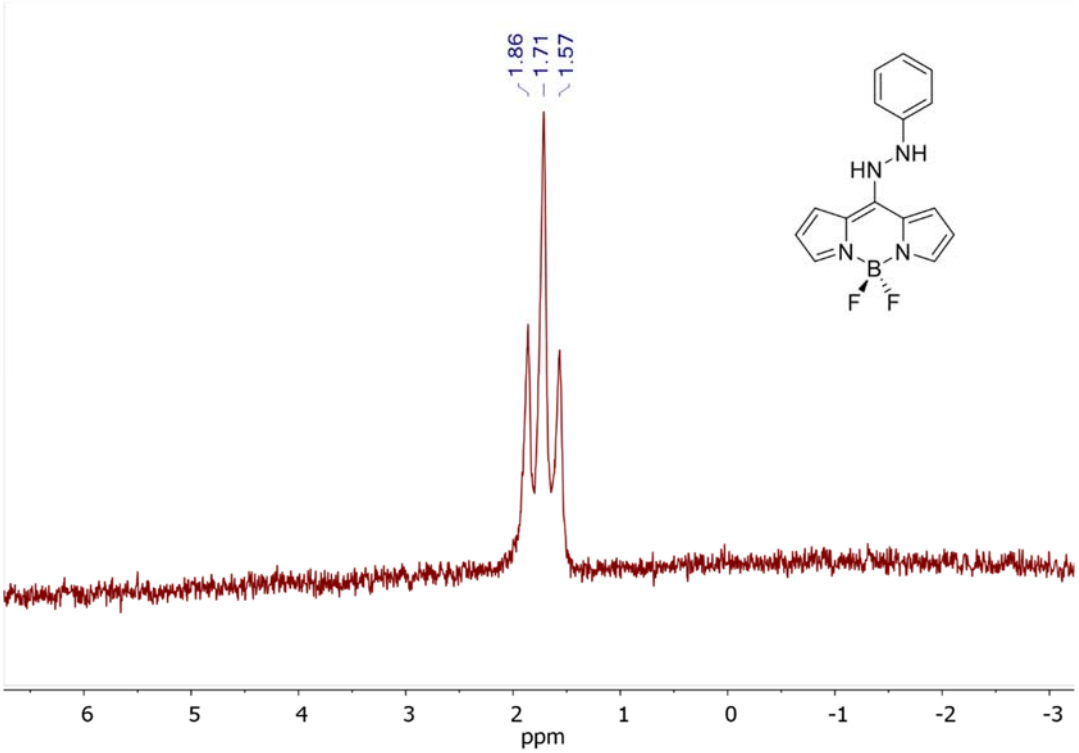


Figure S11. $^{11}B\{^{1}H\}$ NMR spectrum of **BoNHNHPh** in CD_3CN

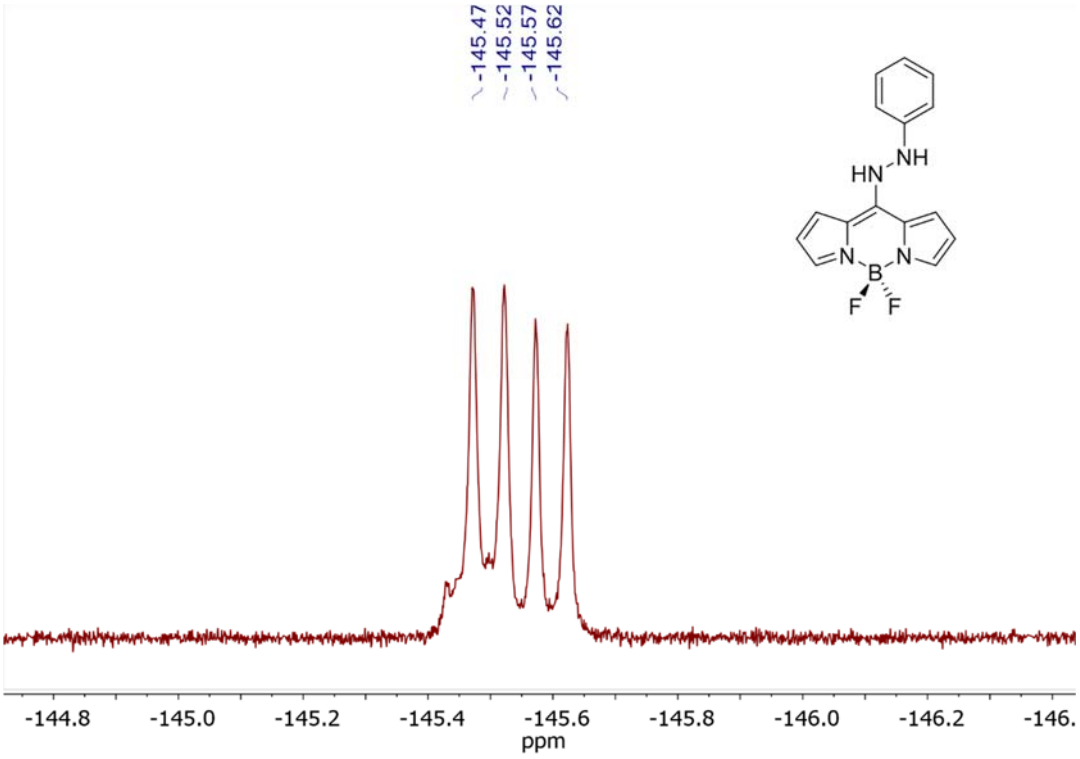


Figure S12. ^{19}F NMR spectrum of **BoNHNHPh** in CD_3CN

4) Multinuclear NMR of BoNHNHPy

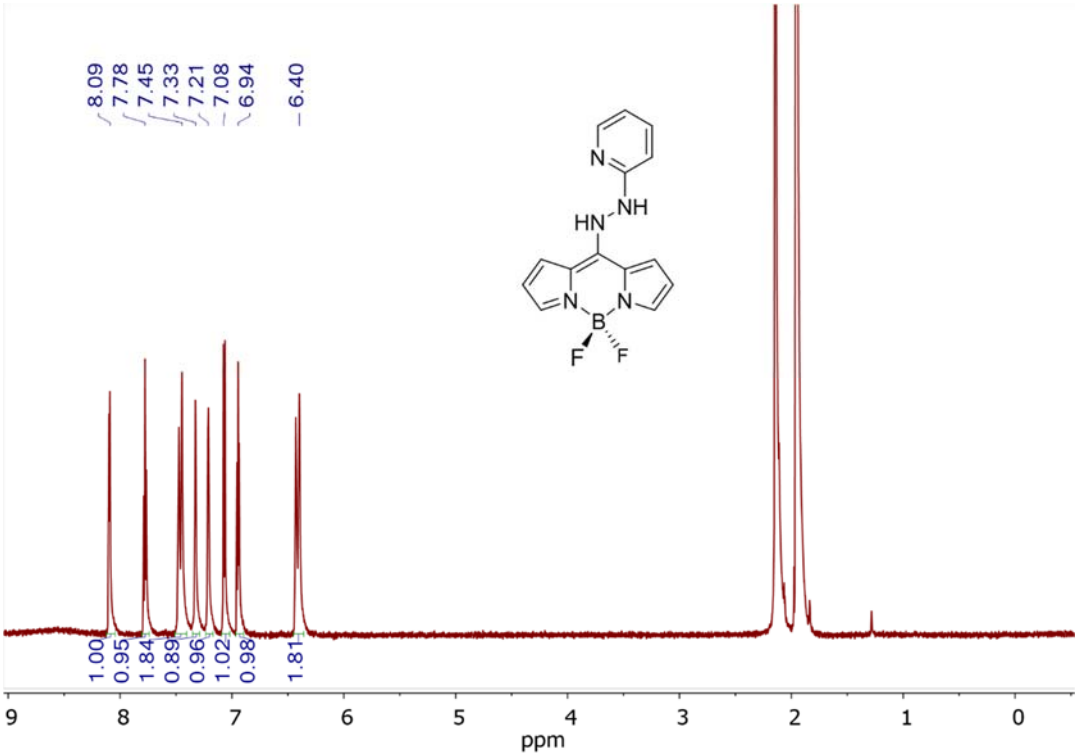


Figure S13. ^{1}H NMR spectrum of **BoNHNHPy** in CD_3CN

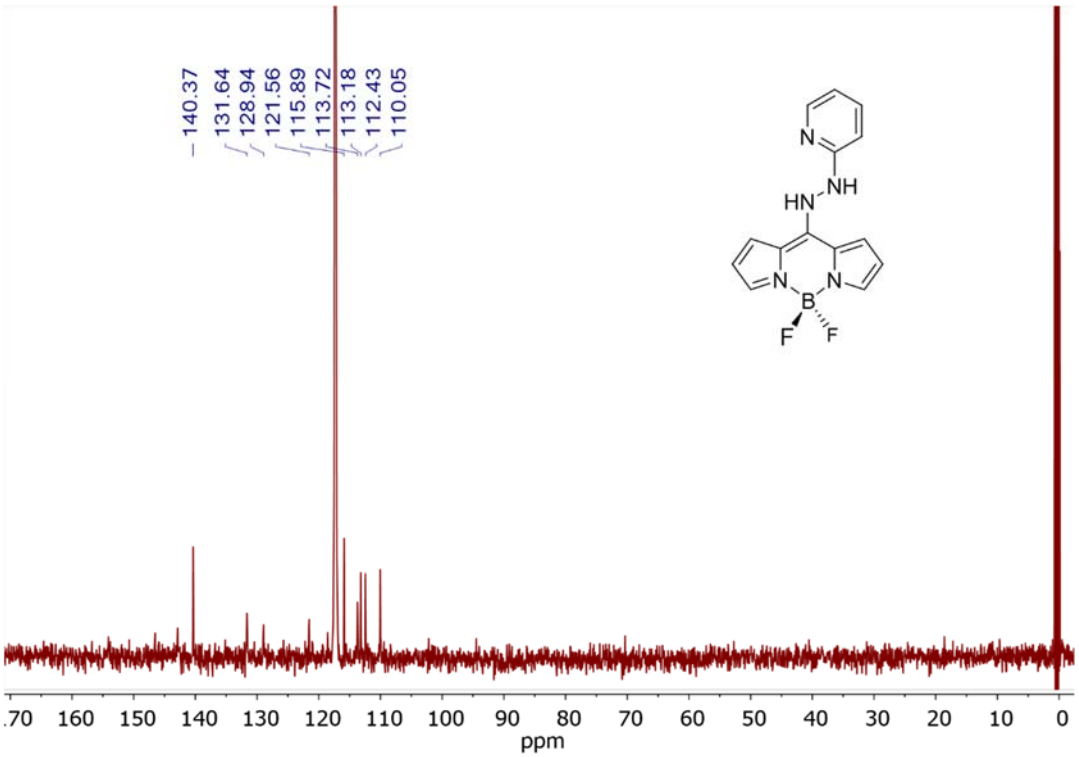


Figure S14. $^{13}C\{^{1}H\}$ NMR spectrum of **BoNHNHPy** in CD_3CN

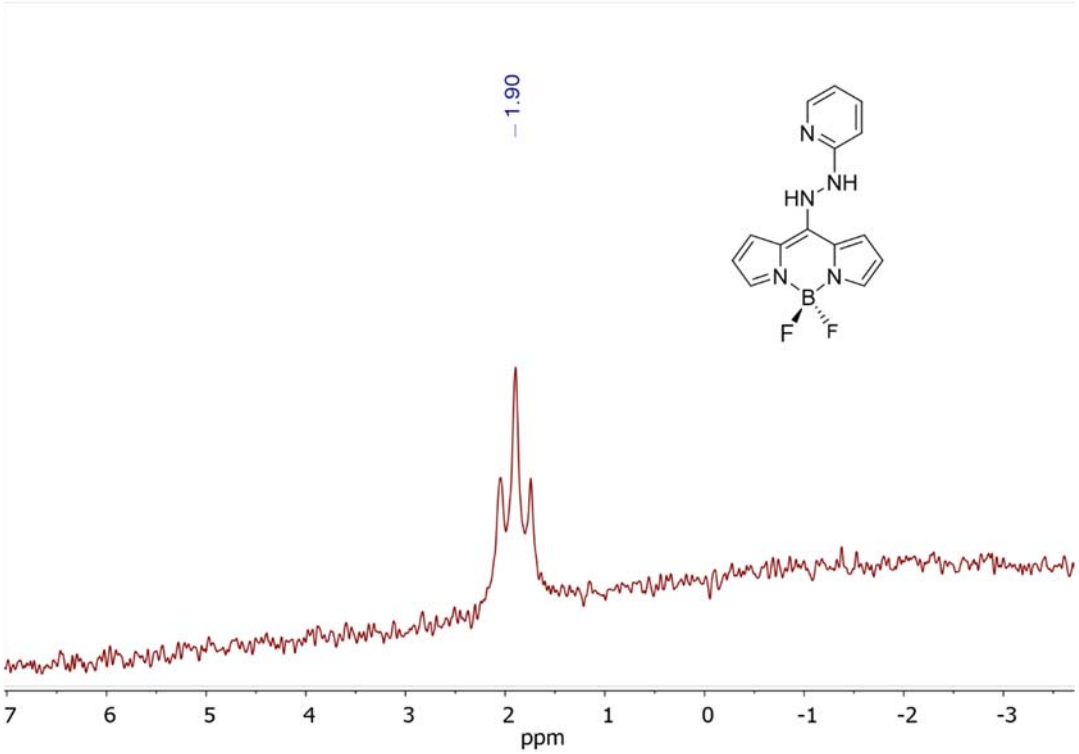


Figure S15. $^{11}B\{^{1}H\}$ NMR spectrum of **BoNHNHPy** in CD_3CN

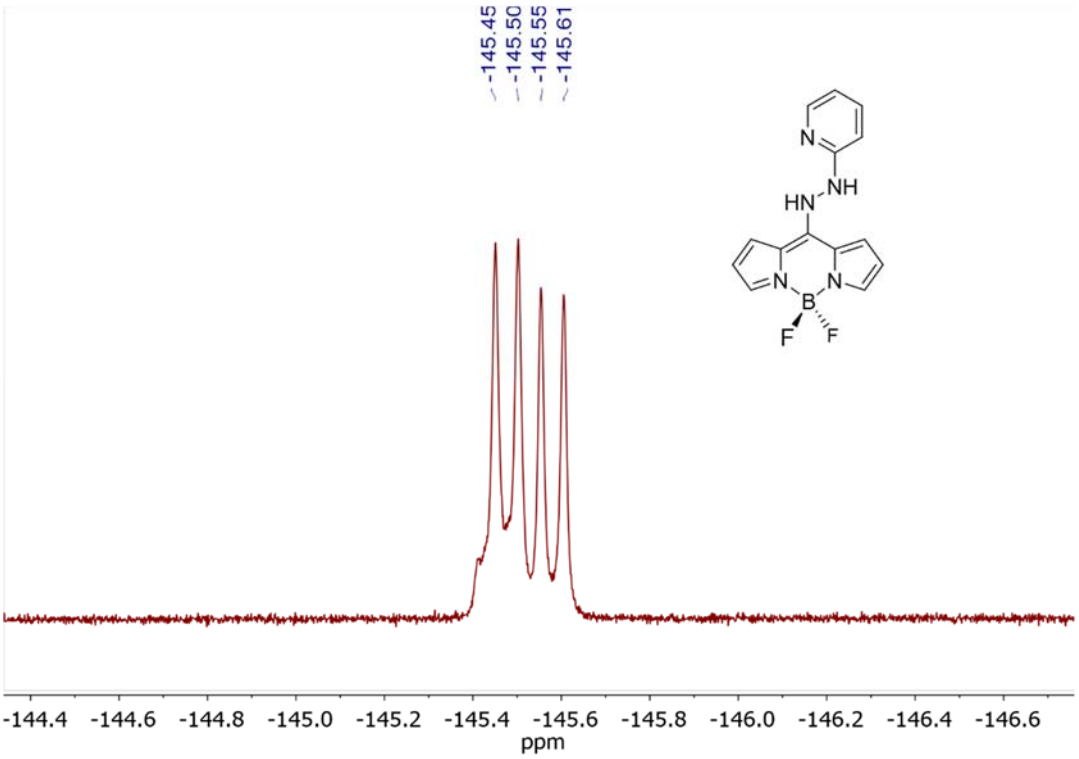


Figure S16. ^{19}F NMR spectrum of **BoNHNHPy** in CD_3CN

5) Multinuclear NMR of $BoNHCH_2Py$

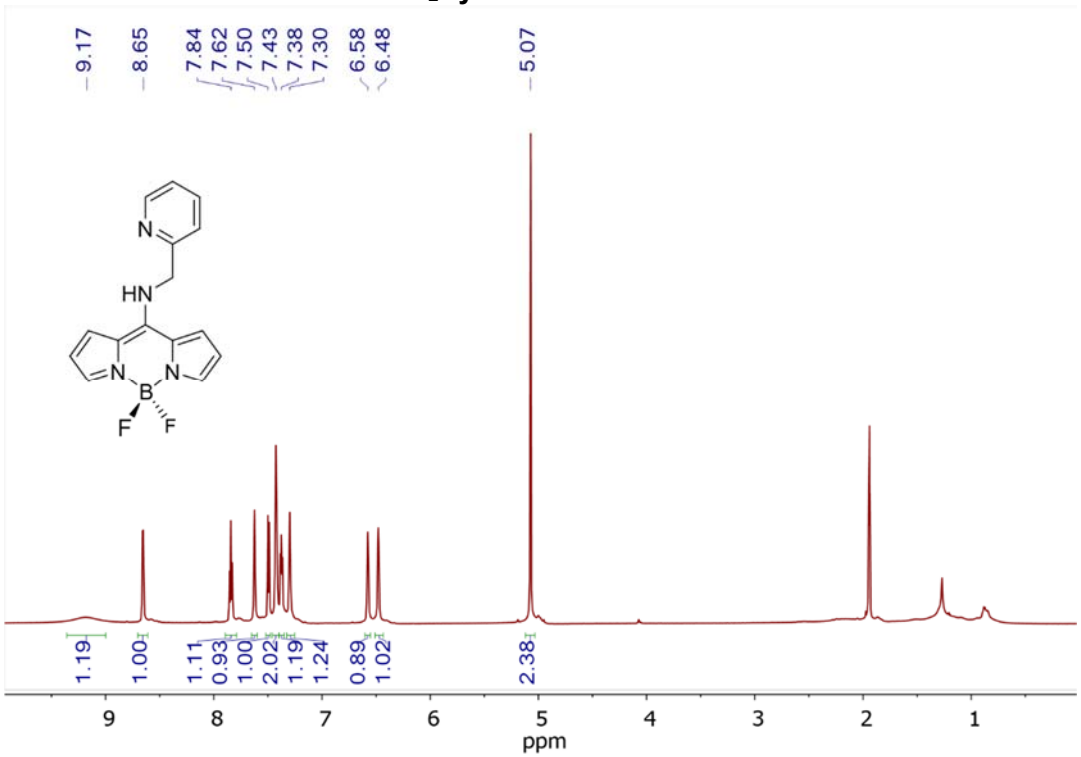


Figure S17. ^{1}H NMR spectrum of **$BoNHCH_2Py$** in CD_3CN.

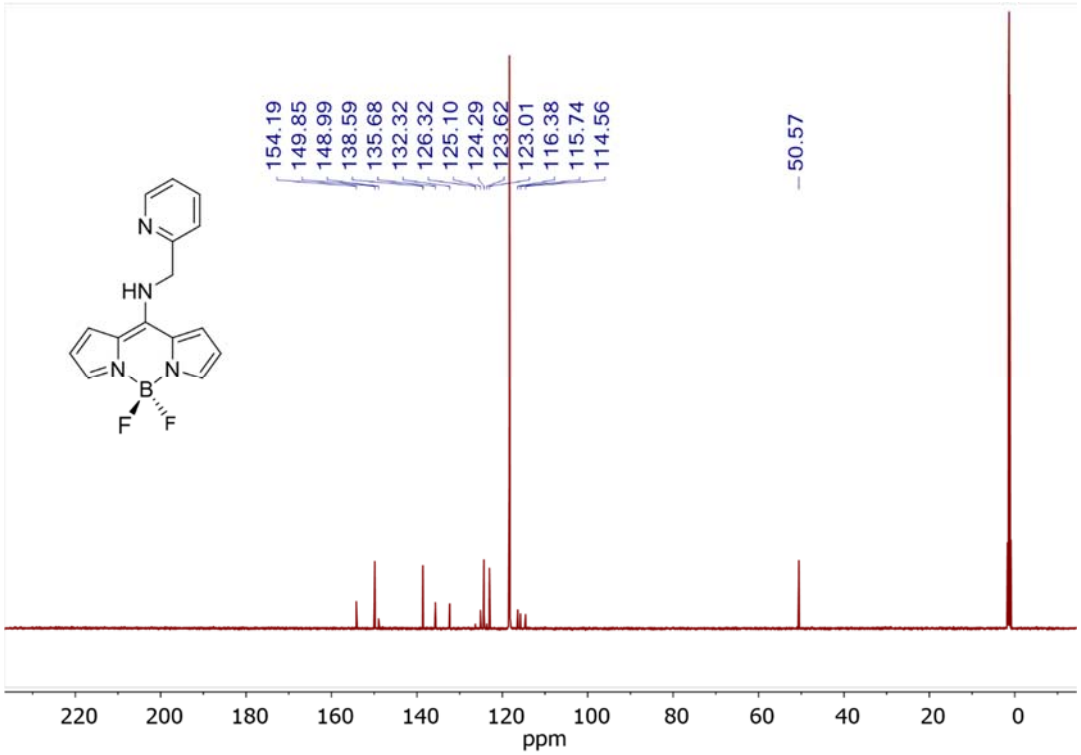


Figure S18. $^{13}C\{^{1}H\}$ NMR spectrum of **$BoNHCH_2Py$** in CD_3CN.

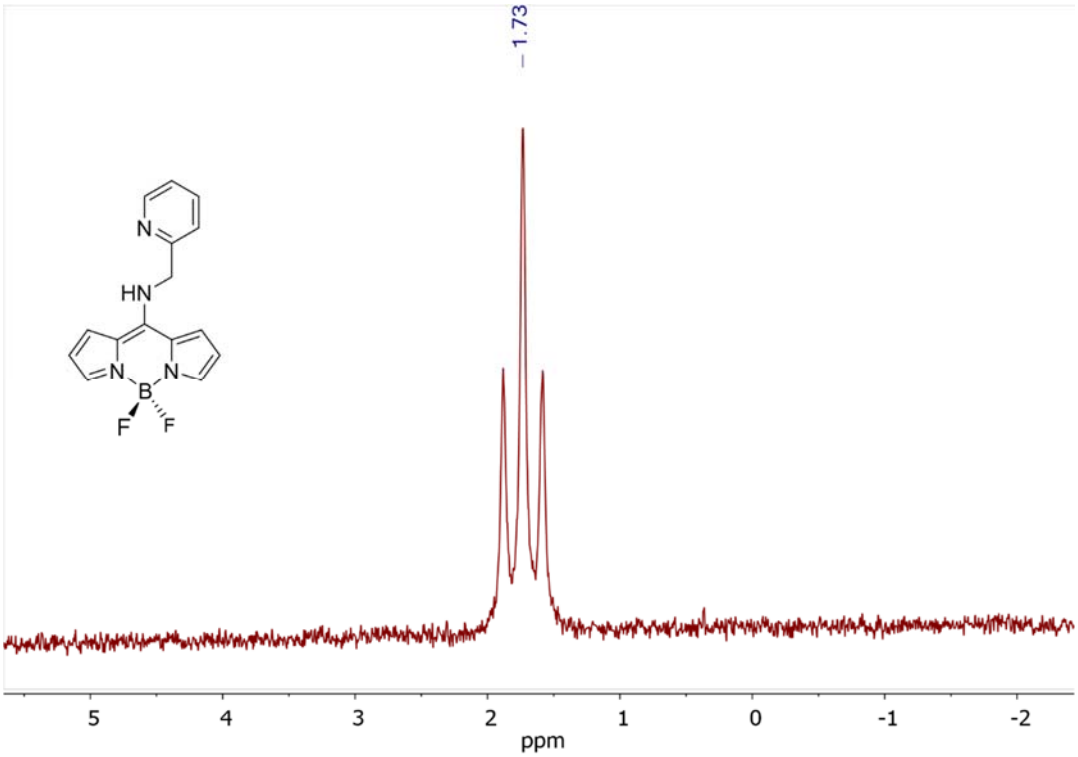


Figure S19. ^{11}B NMR of **BoNHCH$_2$Py** in CD_3CN.

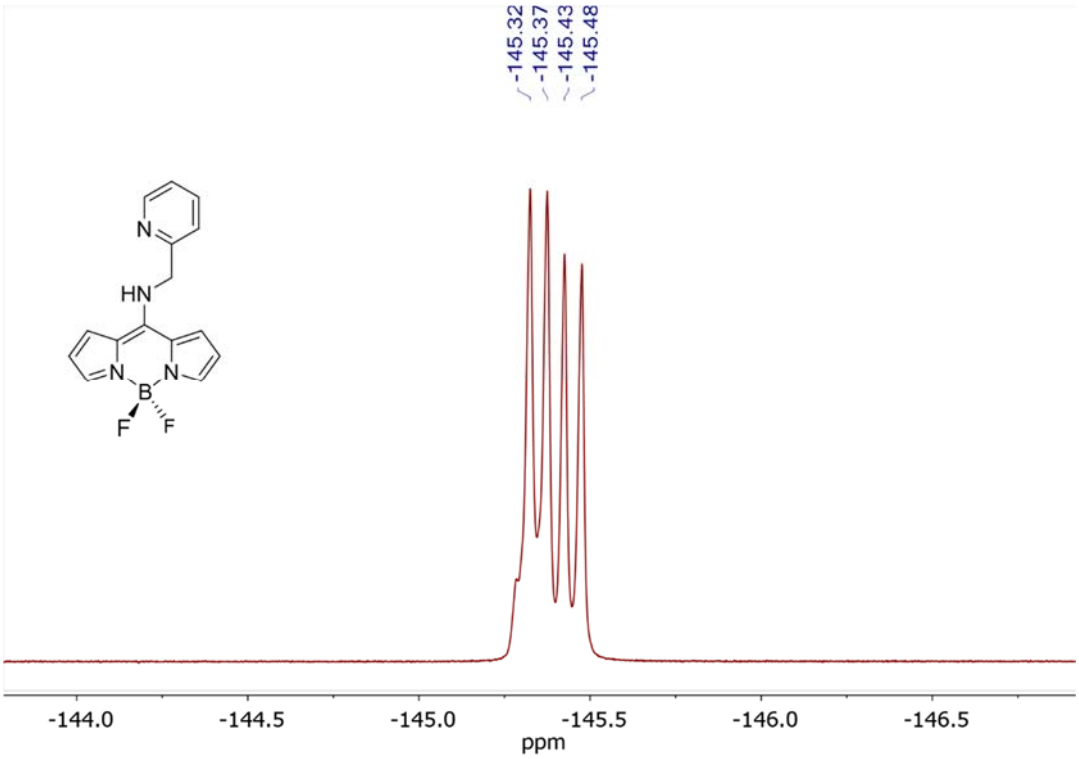


Figure S20. ^{19}F NMR spectrum of **BoNHCH$_2$Py** in CD_3CN.

6) Cyclic Voltammograms of the Hydrazine and Aminomethyl Complexes

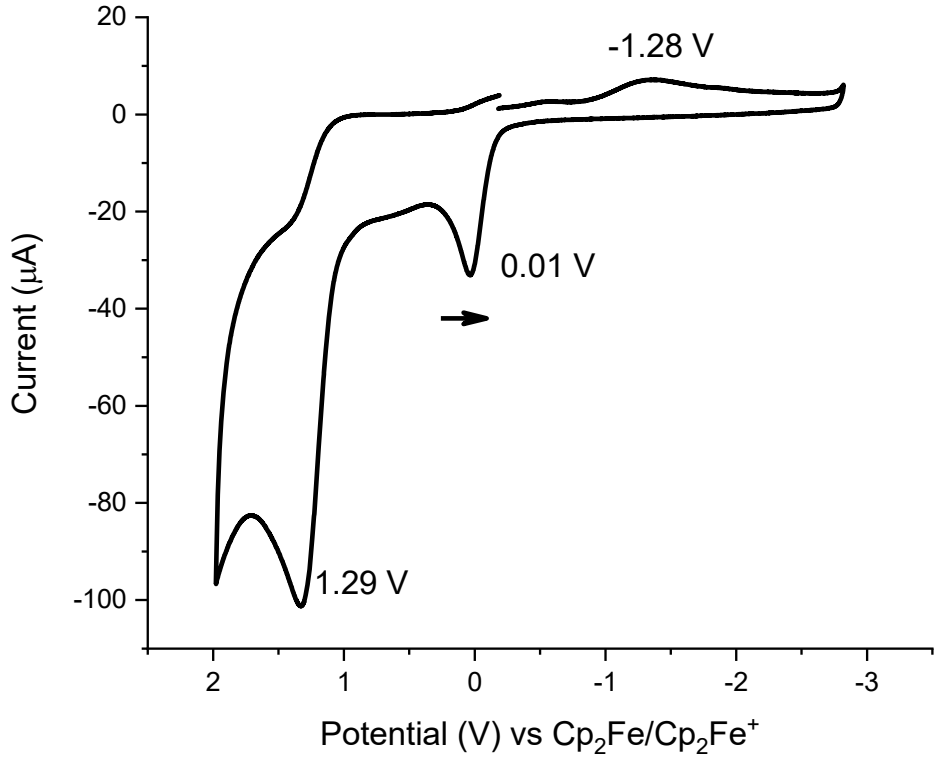


Figure S21. Cyclic voltammogram of **$PhNHNH_2$** in MeCN. Scan rate = 250 mV/s, electrolyte = Bu_4NPF_6. The irreversible reduction at -1.28 vs. Cp_2Fe/Cp_2Fe^+ only appears after the oxidation at 0.01 V occurs. The arrow indicates the direction of the initial scan.

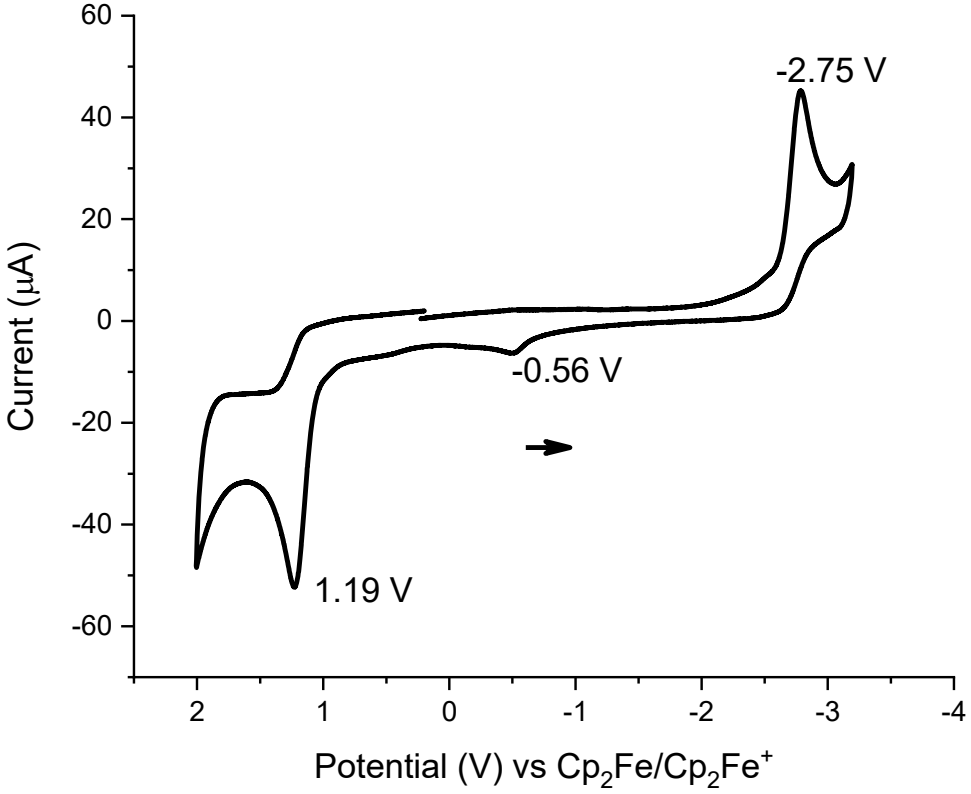


Figure S22. Cyclic voltammogram of **$PyNHNH_2$** in MeCN. Scan rate = 250 mV/s, electrolyte = Bu_4NPF_6. The irreversible oxidation at -0.56 vs. Cp_2Fe/Cp_2Fe^+ only appears after the reduction at -2.75 V occurs. The arrow indicates the direction of the initial scan.

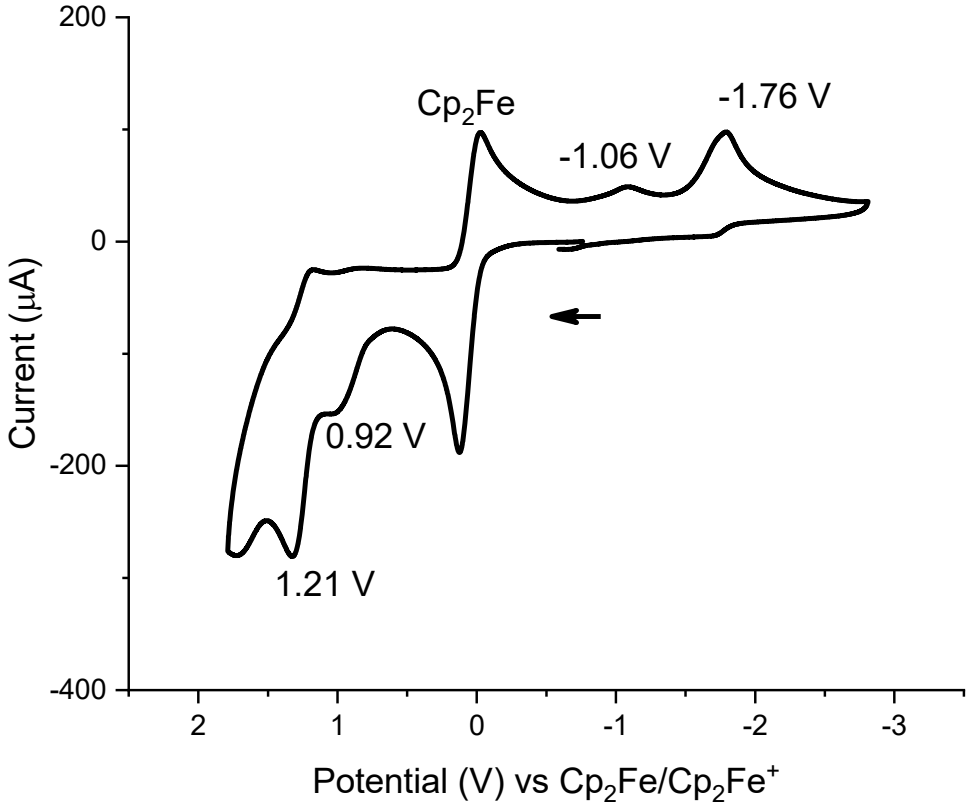


Figure S23. Cyclic voltammogram of **BoNHNH$_2$** in MeCN. Scan rate = 500 mV/s, electrolyte = Bu_4NPF_6. The reduction at -1.06 V occurs after an oxidation of **BoNHNH$_2$**. The arrow indicates the direction of the initial scan.

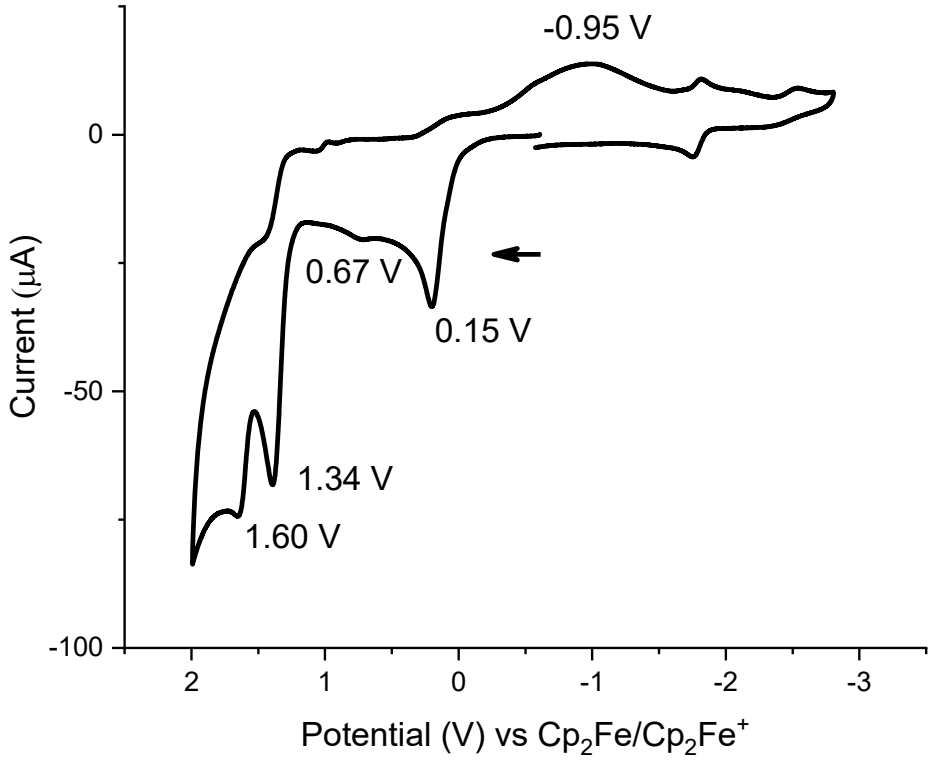


Figure S24. Cyclic voltammogram of **PhNHNHPh** in MeCN. Scan rate = 250 mV/s, electrolyte = Bu_4NPF_6. The reversible feature at -1.79 V and irreversible feature at -2.49 V are attributed to presence of a 10% azobenzene impurity in hydrazobenzene. The arrow indicates the direction of the initial scan.

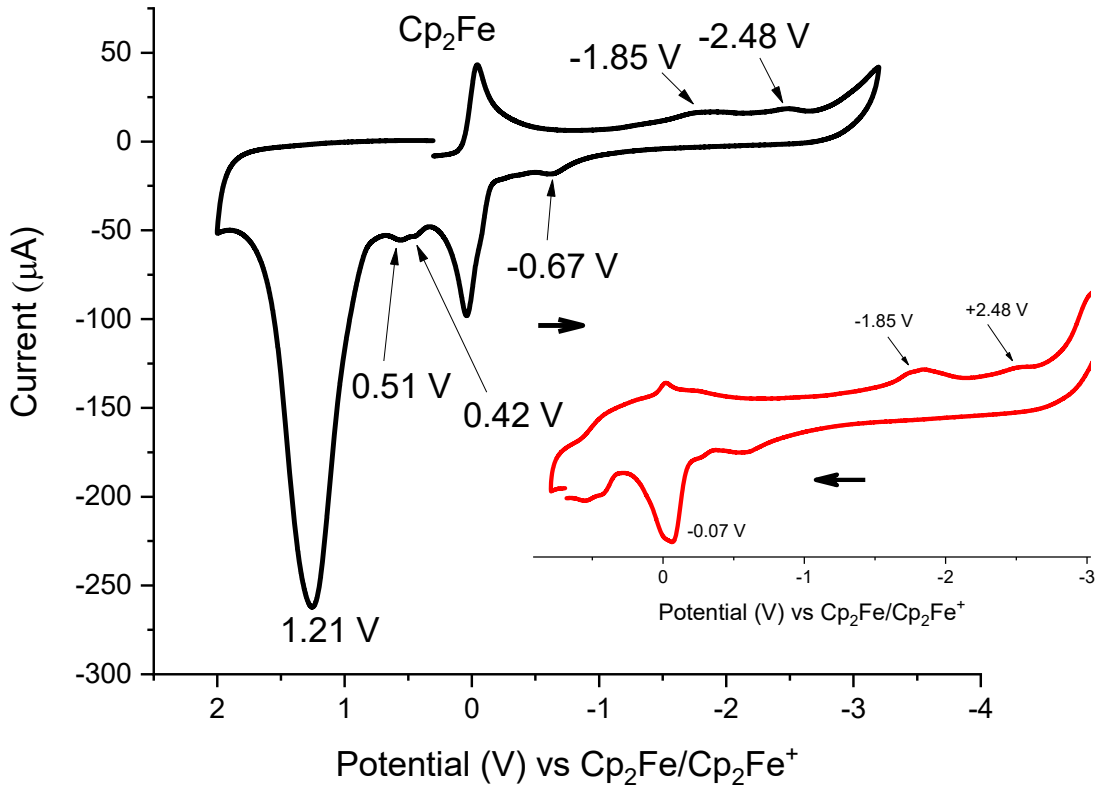


Figure S25. Cyclic voltammogram of **BoNHNHBo** in MeCN. Scan rate = 250 mV/s, electrolyte = Bu_4NPF_6. The oxidation events at -0.67, 0.42, and 0.51 V result from the reduction events at -1.85 and -2.48 V. The inset plot shows the oxidation wave that is occluded by the ferrocene standard and more intense reduction waves. The arrows indicate direction of the initial scan.

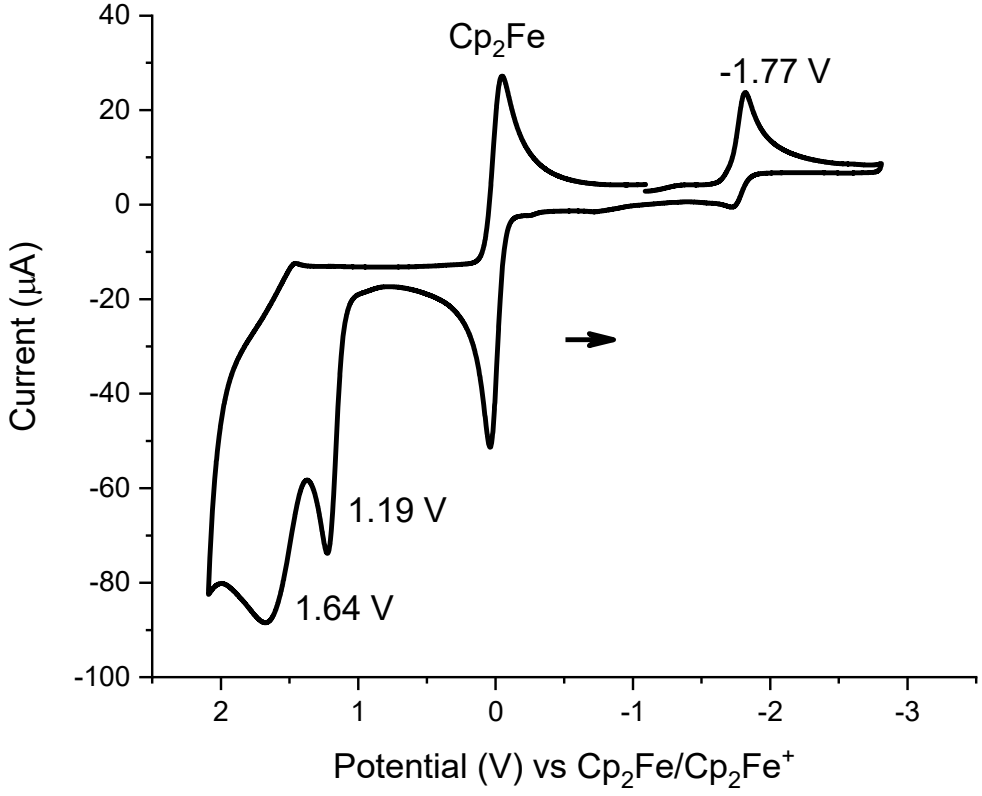


Figure S26. Cyclic voltammogram of **BoNHCH$_2$Ph** in MeCN. Scan rate = 100 mV/s, electrolyte = Bu_4NPF_6. The arrow indicates the direction of the initial scan.

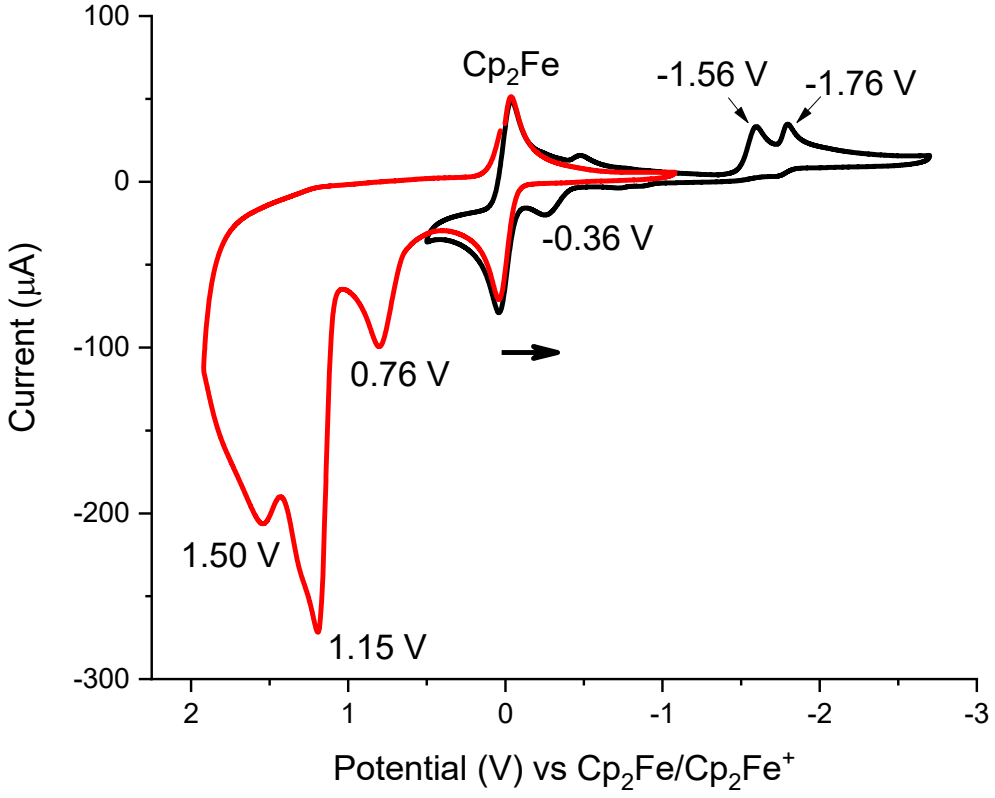


Figure S27. Cyclic voltammogram of **BoNHNHPh** in MeCN. Scan rate = 250 mV/s, electrolyte = Bu_4NPF_6. Separate scans showing the oxidation (red) and reduction (black) waves are shown for clarity. The arrow indicates the direction of the initial scan.

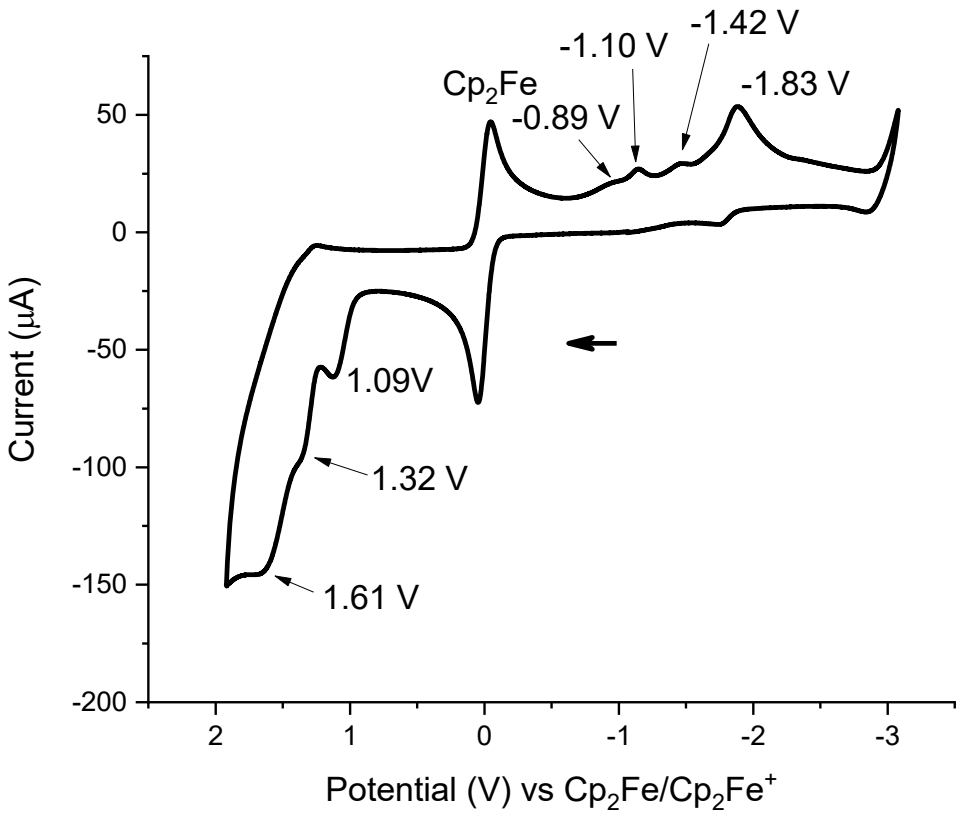


Figure S28. Cyclic voltammogram of **BoNHCH$_2$Py** in MeCN. Scan rate = 250 mV/s, electrolyte = Bu_4NPF_6. The reductions at -0.89 and -1.42 V result from the oxidation events. The arrow indicates the direction of the initial scan.

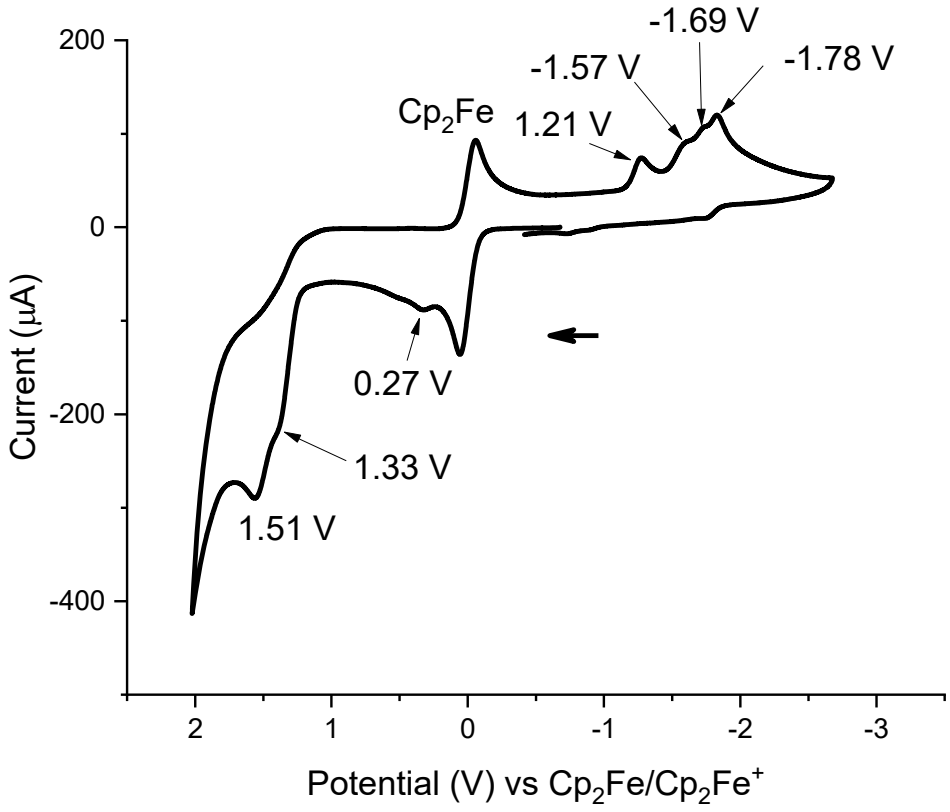


Figure S29. Cyclic voltammogram of **BoNHNHPy** in MeCN. Scan rate = 500 mV/s, electrolyte = Bu_4NPF_6. The reductions at -1.69 and −1.78 V occur from the oxidation waves of **BoNHNHPy**. The arrow indicates the direction of the initial scan.

7) Normalized UV-Vis and Fluorescence Spectra of the BODIPY-Appended Hydrazine and Aminomethyl Complexes

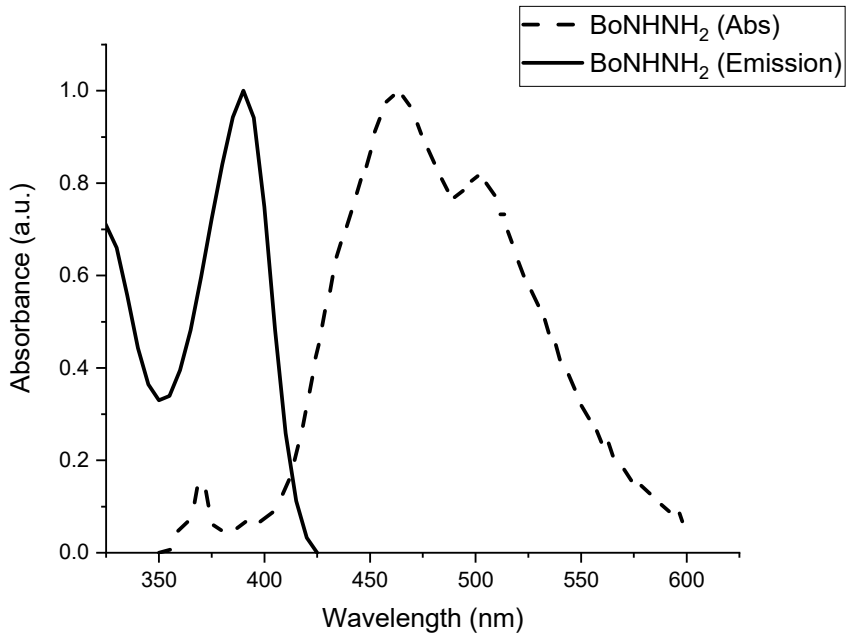


Figure S30. Normalized UV-Vis and fluorescence spectra of **$BoNHNH_2$** in MeCN.

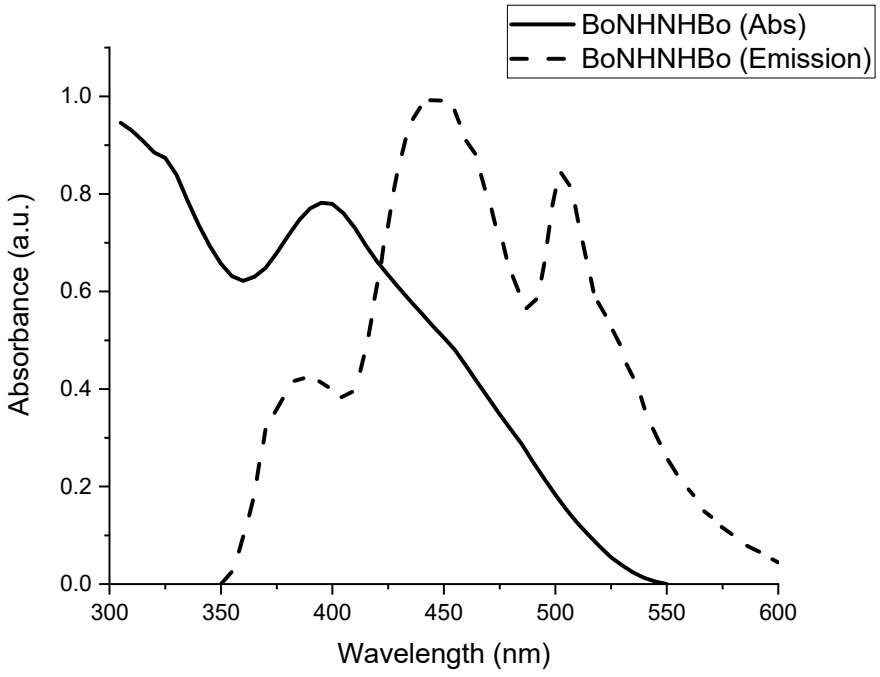


Figure S31. Normalized UV-Vis and fluorescence spectra of **BoNHNHBo** in MeCN.

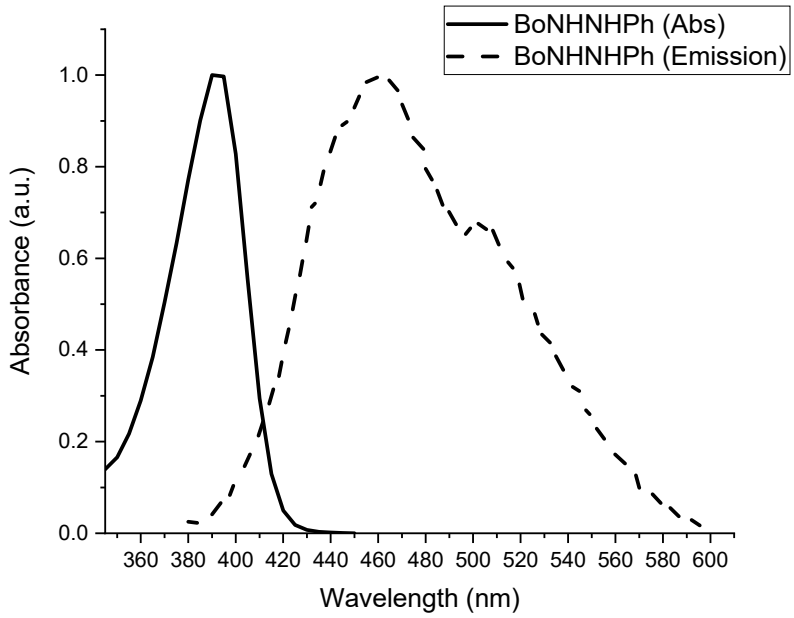


Figure S32. Normalized UV-Vis and fluorescence spectra of **BoNHNHPh** in MeCN.

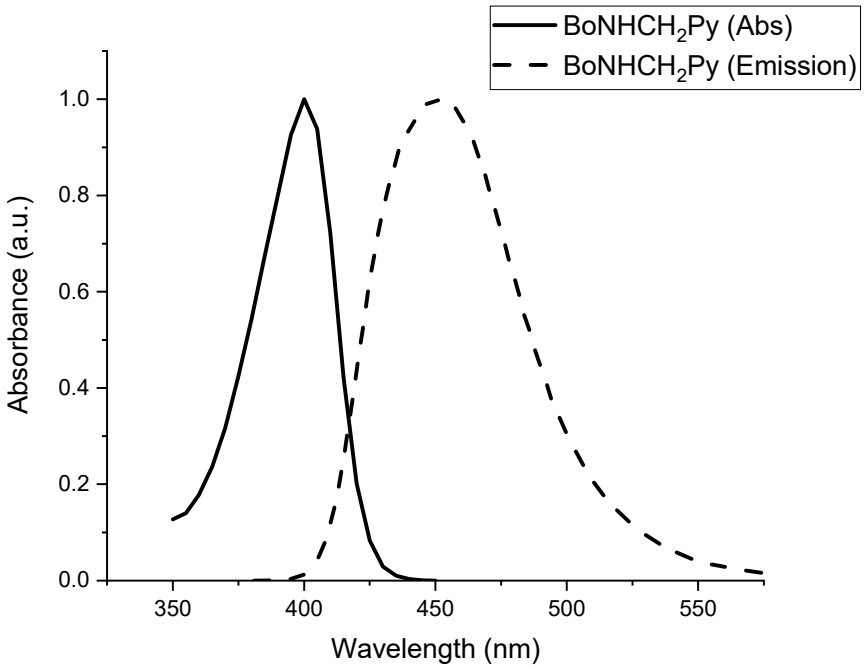


Figure S33. Normalized UV-Vis and fluorescence spectra of **BoNHCH$_2$Py** in MeCN.

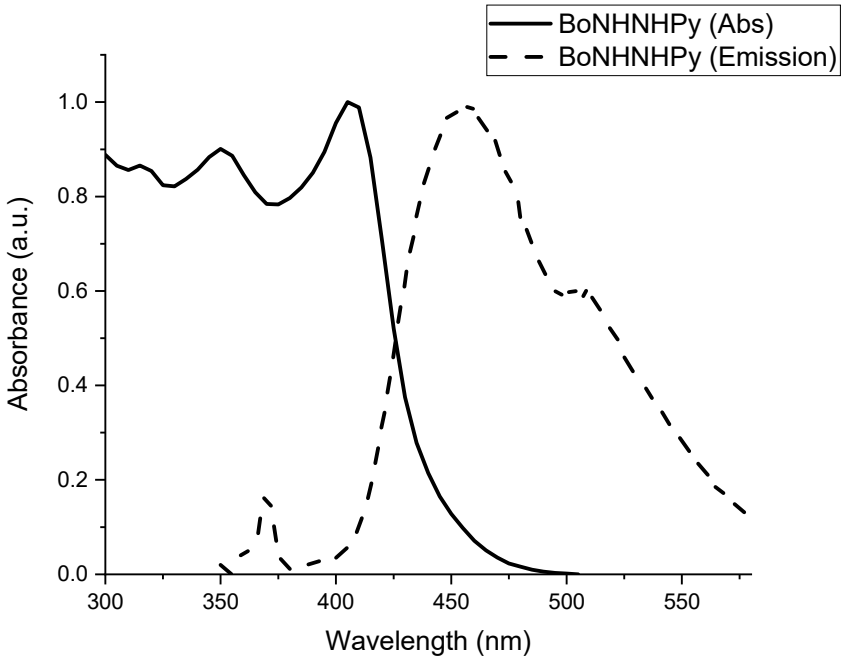
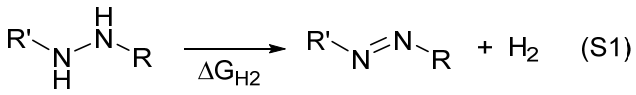


Figure S34. Normalized UV-Vis and fluorescence spectra of **BoNHNHPy** in MeCN.

8) Computed Free Energies for H_2 Transfer from the Examined Hydrazines and Aminomethyl Complexes

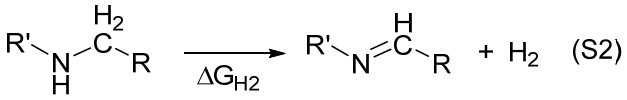
The ability of a organic hydrazine to lose H_2 is described by the following equation:



R' = BODIPY, Ph, H
R = BODIPY, Ph, Py, H

Table S1. Computed free energies for H_2 loss from the hydrazines examined in this study. The reported values were obtained at the M06-2X/6-31G(d,p)//M06-2X/6-311++G(d,p) level of theory in MeCN.

Hydrazine	ΔG_{H2} (kcal/mol)
H_2N-NH_2	**20.81**
HN=NH	**-49.98**
PhNHNH_2	**19.65**
PyNHNH_2	**25.04**
BoNHNH_2	**38.32**
PhNHNHPh	**9.59**
BoNHNHBo	**39.24**
BoNHNHPh	**27.62**
BoNHNHPy	**32.55**



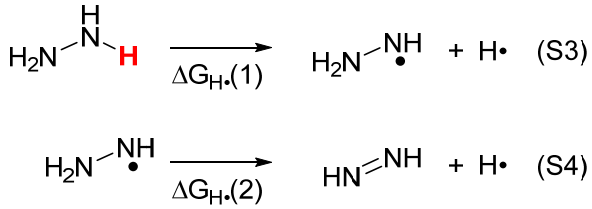
R' = BODIPY, Ph, H
R = BODIPY, Ph, Py, H

Table S2. Computed free energies for H_2 loss from the aminomethyl complexes examined in this study. The reported values were obtained at the M06-2X/6-31G(d,p)//M06-2X/6-311++G(d,p) level of theory in MeCN.

Complex	ΔG_{H2} (kcal/mol)
BoNHCH_2Ph	**23.44**
BoNHCH_2Py	**24.40**

9) Computed Free Energies for H-atom Transfer from the Examined Hydrazines and Aminomethyl Complexes

The ability of a organic hydrazine to lose H-atoms is described by the following equations:



where $\Delta G_{H\bullet}(1)$ describes free energy for the loss of the first H-atom, and $\Delta G_{H\bullet}(2)$ describes the free energy for the loss of the second H-atom.

Table S3. Computed free energies for H-atom loss from the hydrazine and aminomethyl complexes examined in this study. The values were reported at the M06-2X/6-31G(d,p)//M06-2X/6-311++G(d,p) level of theory in MeCN, using TEMPOH ($\Delta G_{H\bullet}$ = 66.5 kcal/mol) as an anchor for the scale. The first H-atom that is removed is highlighted in red (Equation S3), with the second H-atom that is removed is the H-atom that remains after the first H-atom loss.

Hydrazine	$\Delta G_{H\bullet}(1)$ (kcal/mol)	$\Delta G_{H\bullet}(2)$ (kcal/mol)
H_2N-NH_2	80.24	52.33
HN=NH	62.53	-0.75
PhNHNH_2	78.21	57.29
PhNHNH_2	75.85	55.55
PyNHNH_2	79.44	57.21
PyNHNH_2	74.29	62.51
BoNHNH_2	84.15	65.93
BoNHNH_2	80.09	70.00
PhNHNHPh	66.53	65.31
BoNHNHBo	83.04	67.96
BoNHNHPh	75.37	64.01
BoNHNHPh	85.73	53.65
BoNHNHPy	79.38	64.93
BoNHNHPy	74.79	69.52
BoNHCH_2Ph	100.70	31.51
BoNHCH_2Ph	81.54	50.67
BoNHCH_2Py	100.33	37.23
BoNHCH_2Py	80.91	56.65

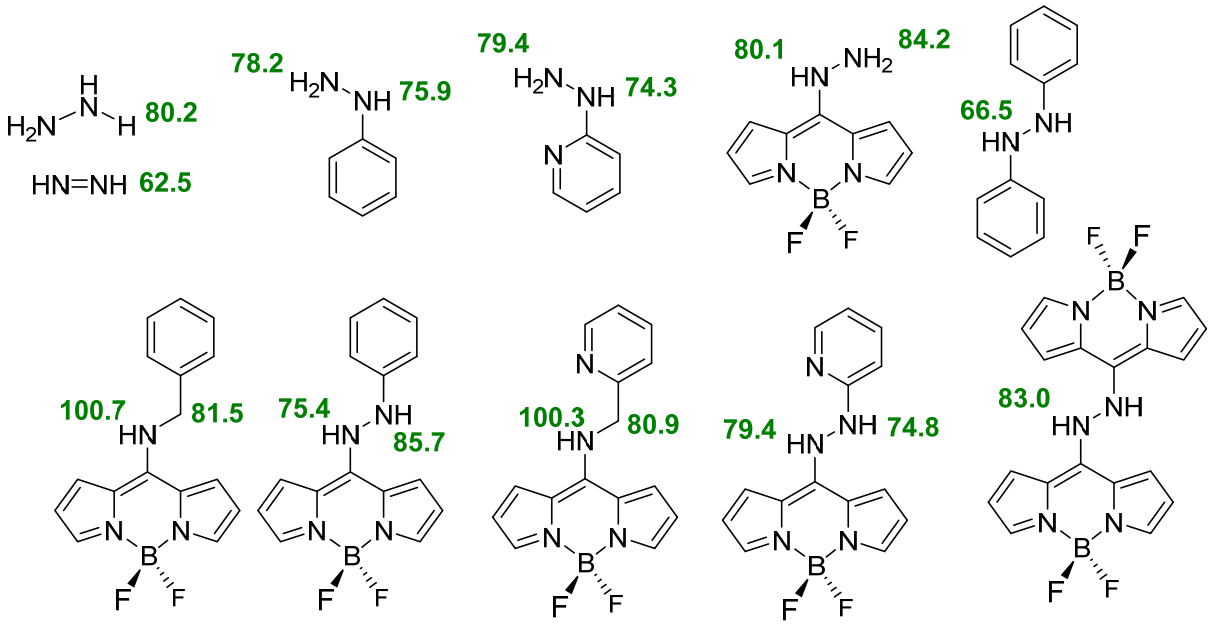


Figure S35. Computed free energies for H-atom loss ($\Delta G_{H\bullet}$(1)) from the examined hydrazine and aminomethyl complexes. The values were reported at the M06-2X/6-31G(d,p)//M06-2X/6-311++G(d,p) level of theory in MeCN, using TEMPOH ($\Delta G_{H\bullet}$ = 66.5 kcal/mol) as an anchor for the scale.[1]

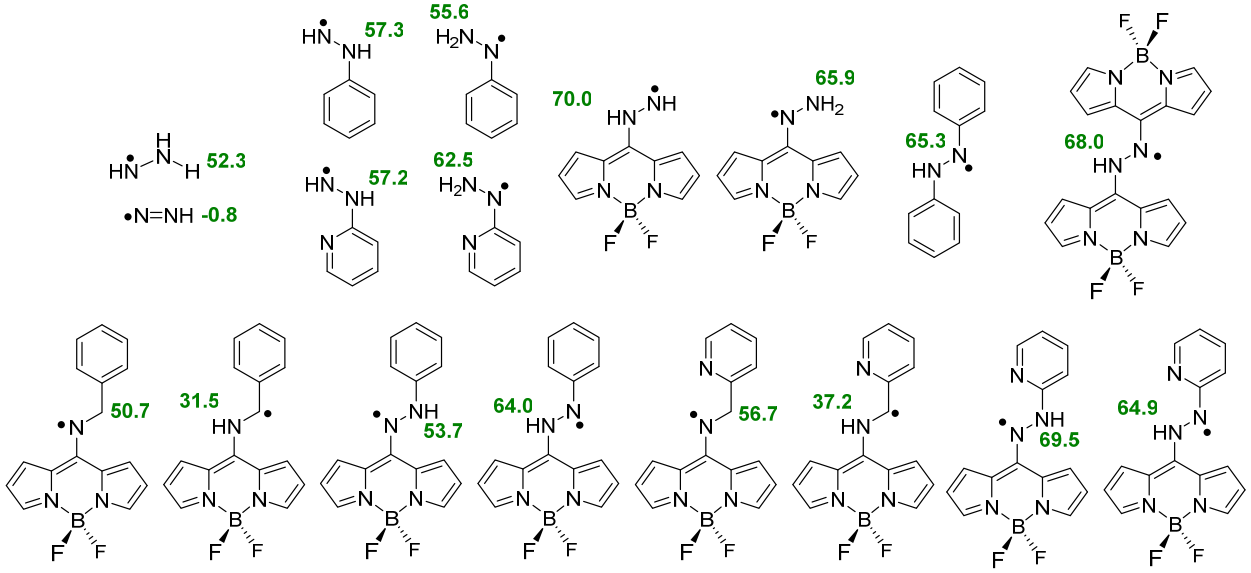
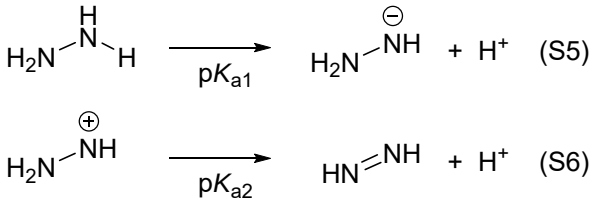


Figure S36. Computed free energies for H-atom loss ($\Delta G_{H\bullet}$(2)) from the examined hydrazine and aminomethyl complexes. The values were reported at the M06-2X/6-31G(d,p)//M06-2X/6-311++G(d,p) level of theory in MeCN, using TEMPOH ($\Delta G_{H\bullet}$ = 66.5 kcal/mol) as an anchor for the scale.[1]

10) Computed pK_a's of the Examined Hydrazines and Aminomethyl Complexes

The ability of a organic hydrazine to lose protons is described by the following equations:



where pK_{a1} describes the acidity of the hydrazine, and pK_{a2} describes the acidity of the hydrazine after an initial hydride transfer.

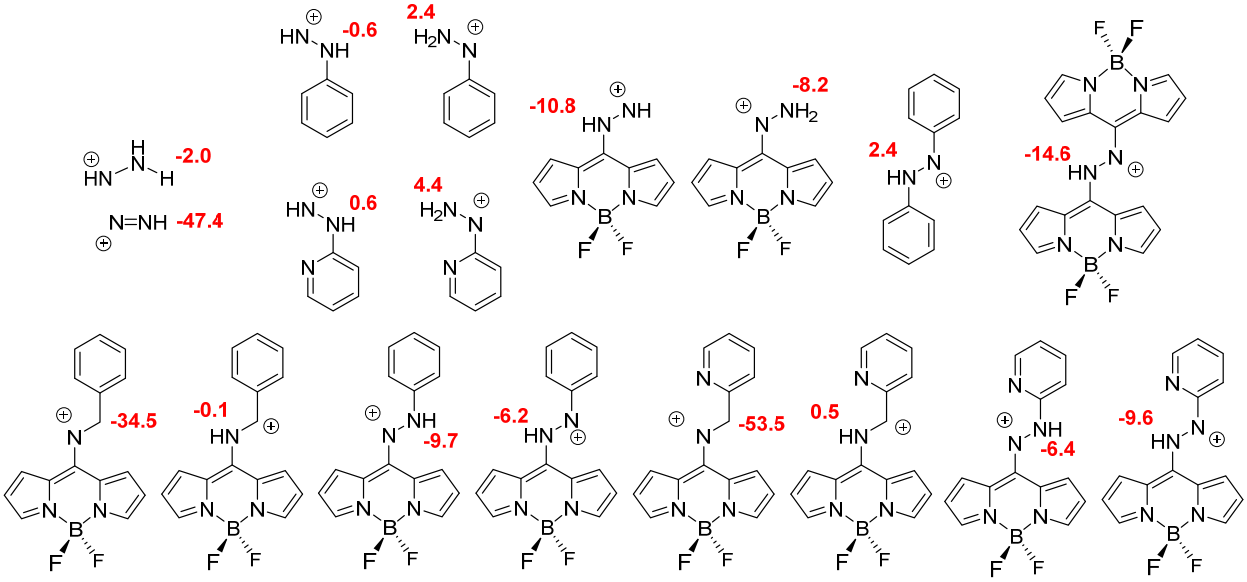
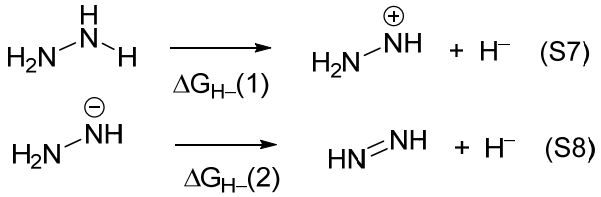


Figure S37. Computed pK_{a2} from the examined hydrazine and aminomethyl complexes after an initial hydride transfer. The values were reported at the M06-2X/6-31G(d,p)//M06-2X/6-311++G(d,p) level of theory in MeCN, using pyridinium (pK_a = 12.33) as an anchor for the scale.

11) Computed Free Energies for Hydride Transfer from the Examined Hydrazines and Aminomethyl Complexes

The ability of a organic hydrazine to lose hydrides is described by the following equations:



where $\Delta G_{H-}(1)$ describes the hydride donor ability of the hydrazine, and $\Delta G_{H-}(2)$ describes the hydride donor ability of the hydrazine after an initial deprotonation.

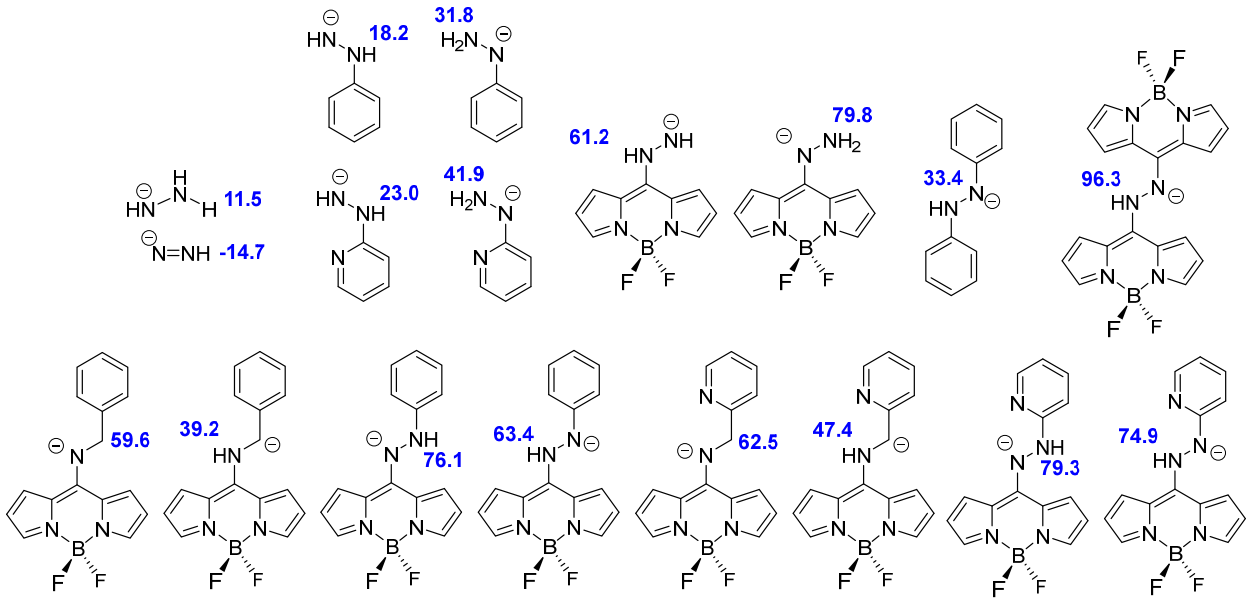


Figure S38. Computed hydride donor abilities ($\Delta G_{H-}(2)$) for the examined hydrazine and aminomethyl complexes after an initial proton transfer. The values were reported at the M06-2X/6-31G(d,p)//M06-2X/6-311++G(d,p) level of theory in MeCN.

12) Computed Energy Gaps Between the Frontier Molecular Orbitals of the Examined Hydrazines and Aminomethyl Complexes

Table S4. Computed energy gaps between the frontier molecular orbitals in kcal for the complexes descrbied within. The values were reported at the M06-2X/6-31G(d,p)//M06-2X/6-311++G(d,p) level of theory.

Complex	HOMO-1 to HOMO	HOMO-LUMO Gap	LUMO to LUMO+1
H_2N-NH_2	3.53	207.18	12.89
HN=NH	94.32	191.50	16.04
N_2	16.30	336.64	0.00
$PhNHNH_2$	30.55	166.73	7.40
trans-PhN=NH	0.70	168.52	31.27
$PyNHNH_2$	38.12	177.11	15.14
cis-PyN=NH	17.20	165.19	22.62
$BoNHNH_2$	18.49	132.38	35.65
trans-BoNH=NH	33.94	108.73	45.68
PhNHNHPh	24.00	159.96	5.12
trans-PhN=NPh	14.36	142.16	41.03
BoNHNHBo	1.44	124.00	3.74
trans-BoN=NBo	0.59	87.35	32.33
BoNHNHPh	5.33	129.21	40.81
trans-BoN=NPh	26.11	102.52	41.50
BoNHNHPy	5.08	131.64	32.61
trans-BoN=NPy	31.60	101.37	40.10
$BoNHCH_2Ph$	16.52	132.76	35.48
trans-BoN=CHPh	24.85	114.41	32.48
$BoNHCH_2Py$	16.07	133.16	32.15
trans-BoN=CHPy	30.27	113.92	28.51

13) Frontier Molecular Orbitals of the Examined Hydrazines and Aminomethyl Complexes

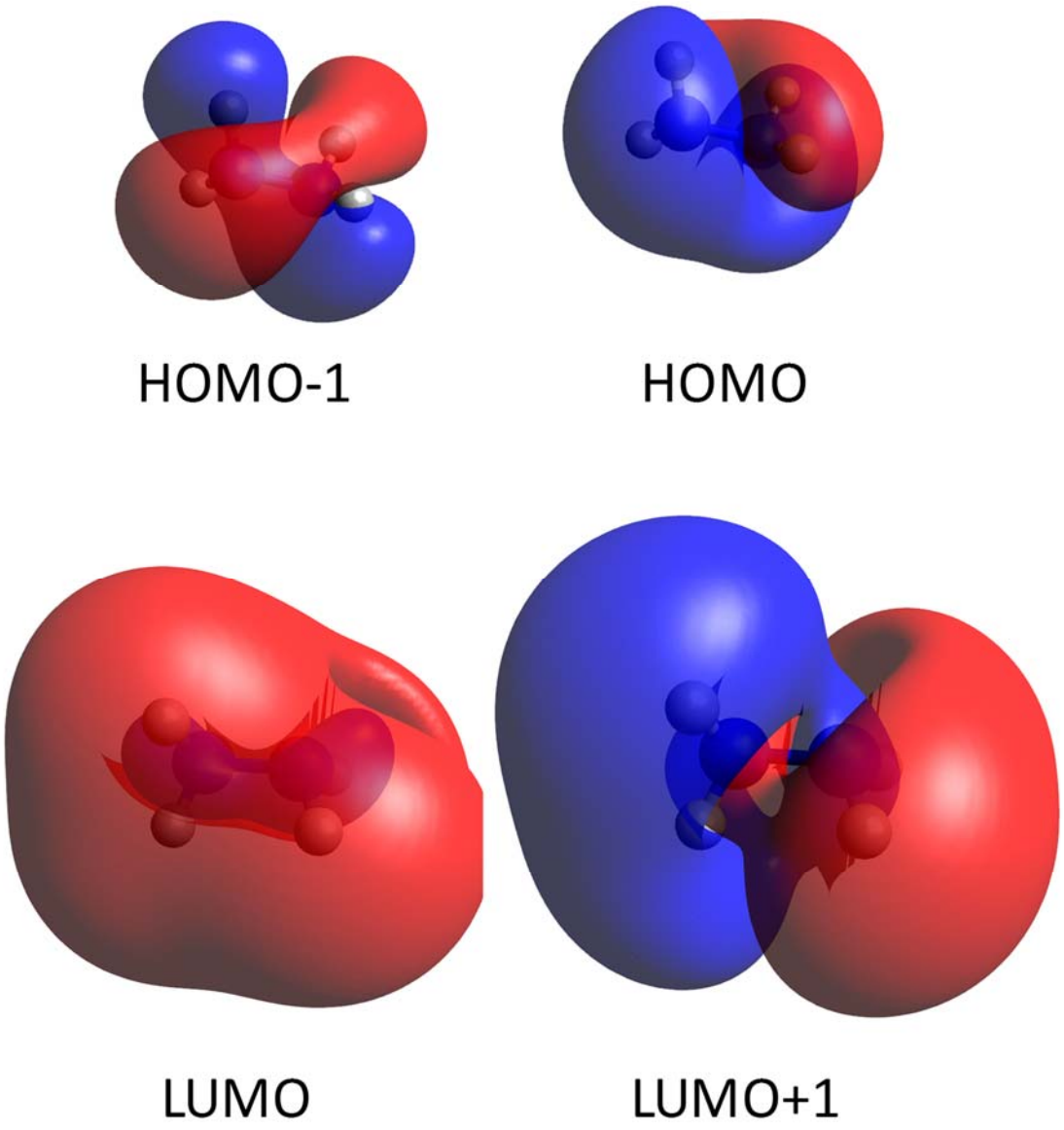


Figure S39. Frontier molecular orbitals for hydrazine.

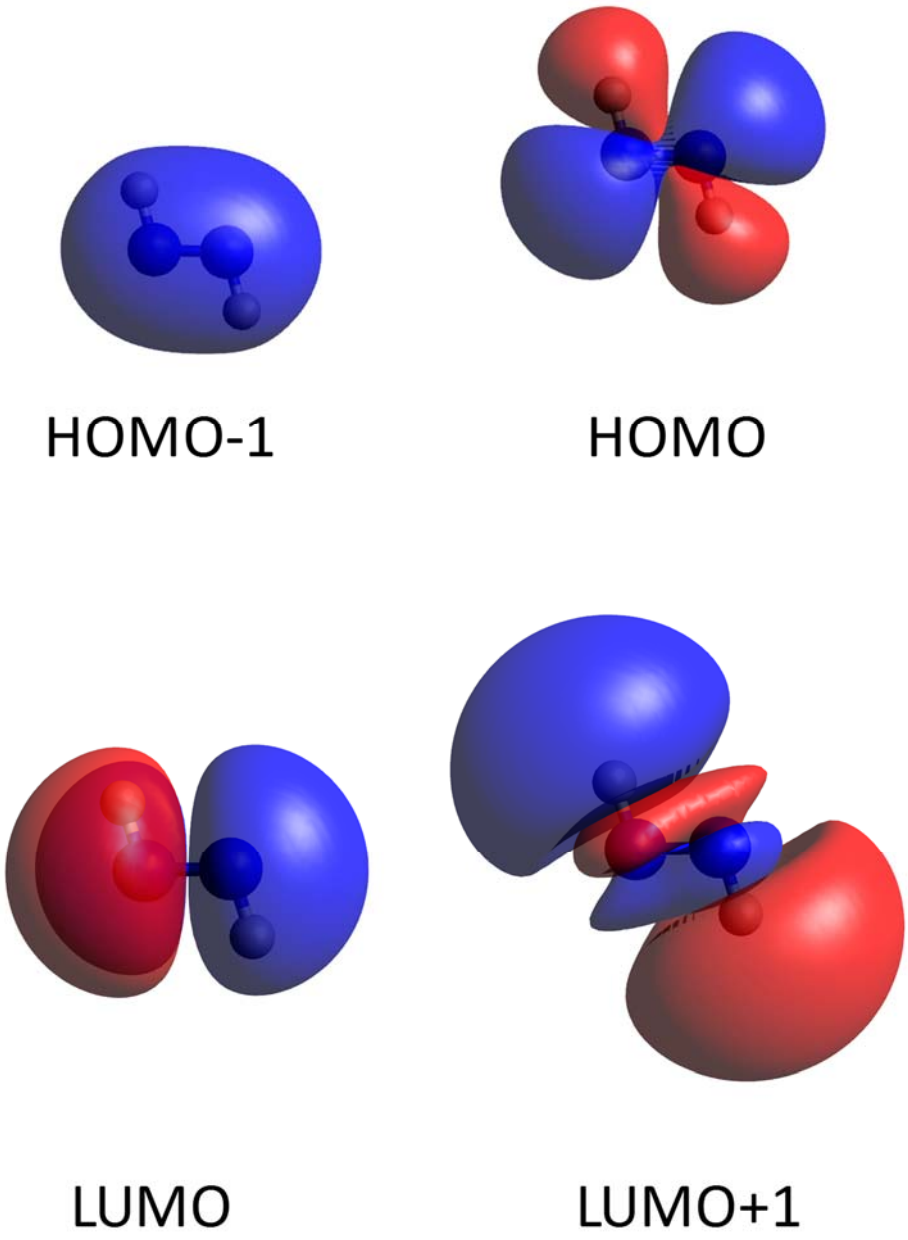


Figure S40. Frontier molecular orbitals for diazene.

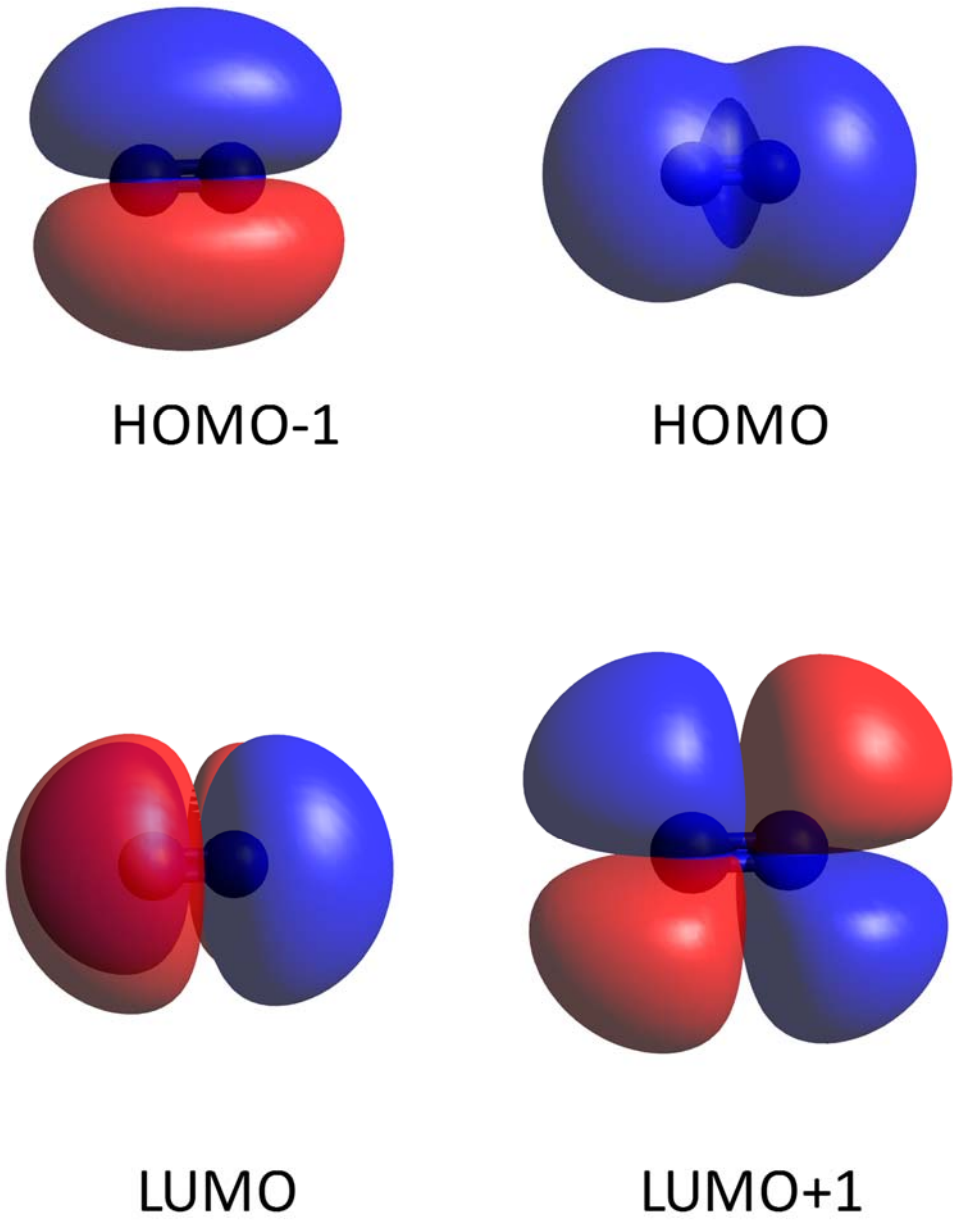


Figure S41. Frontier molecular orbitals for N_2.

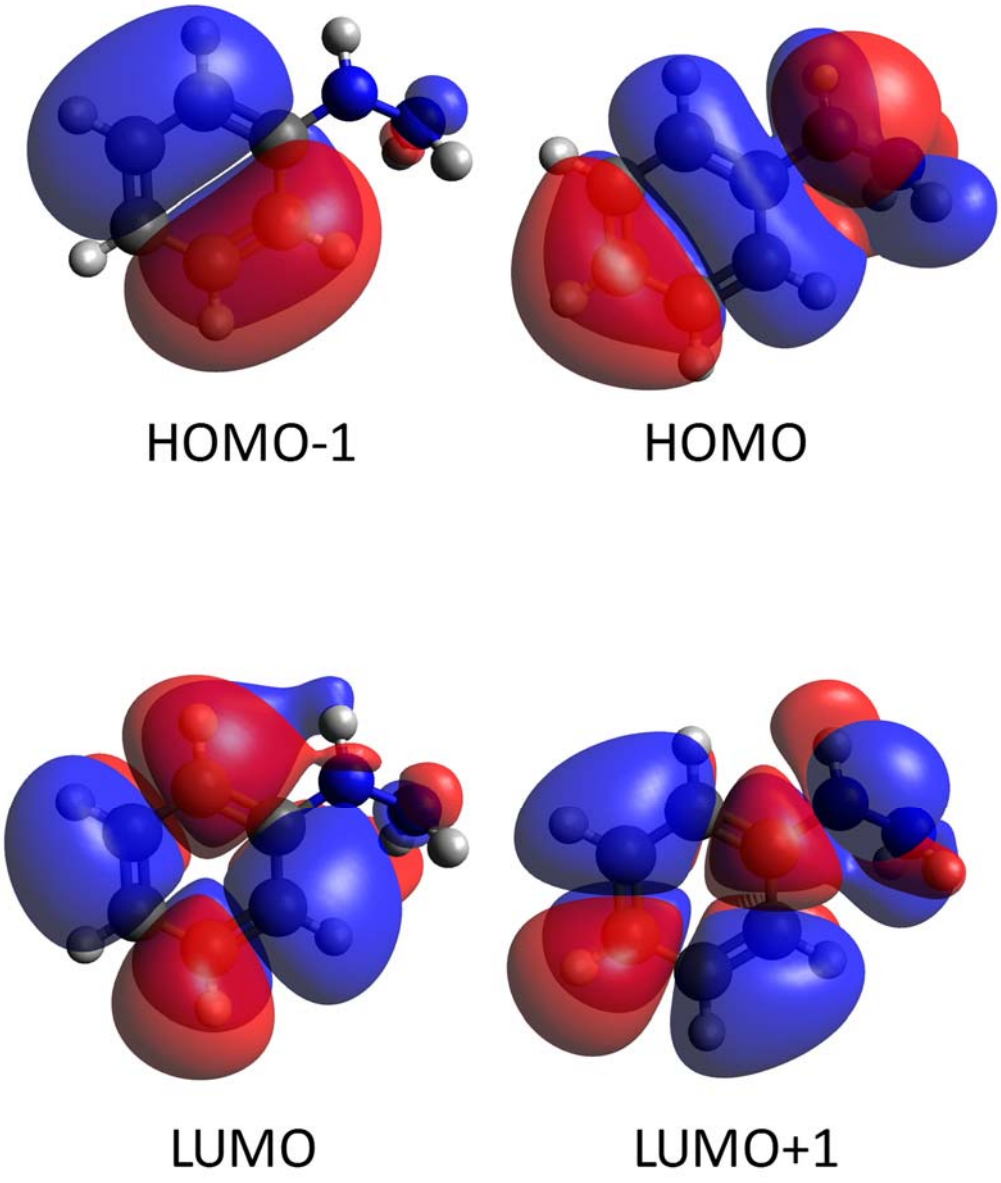


Figure S42. Frontier molecular orbitals for $PhNHNH_2$.

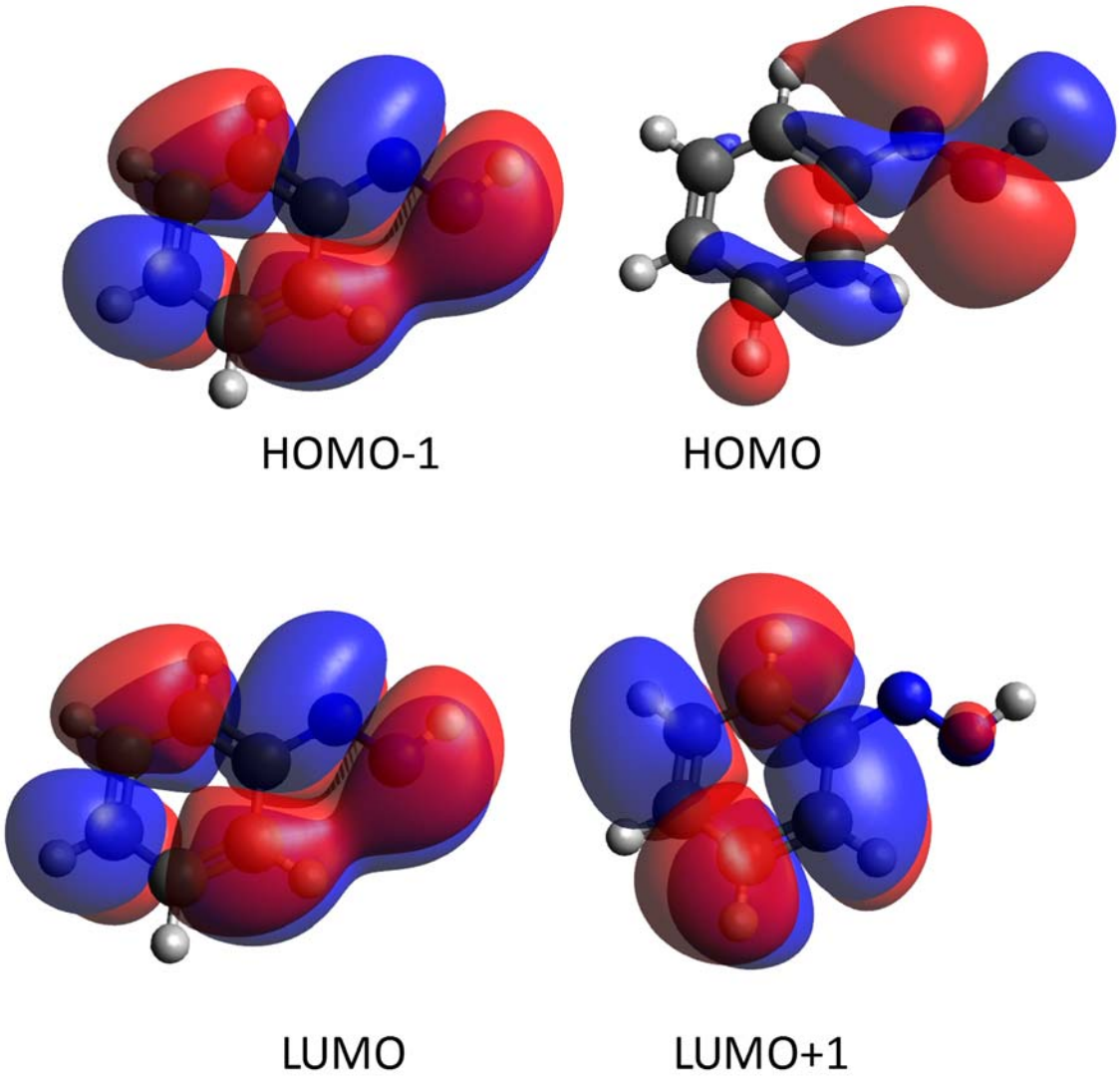


Figure S43. Frontier molecular orbitals for PhN=NH.

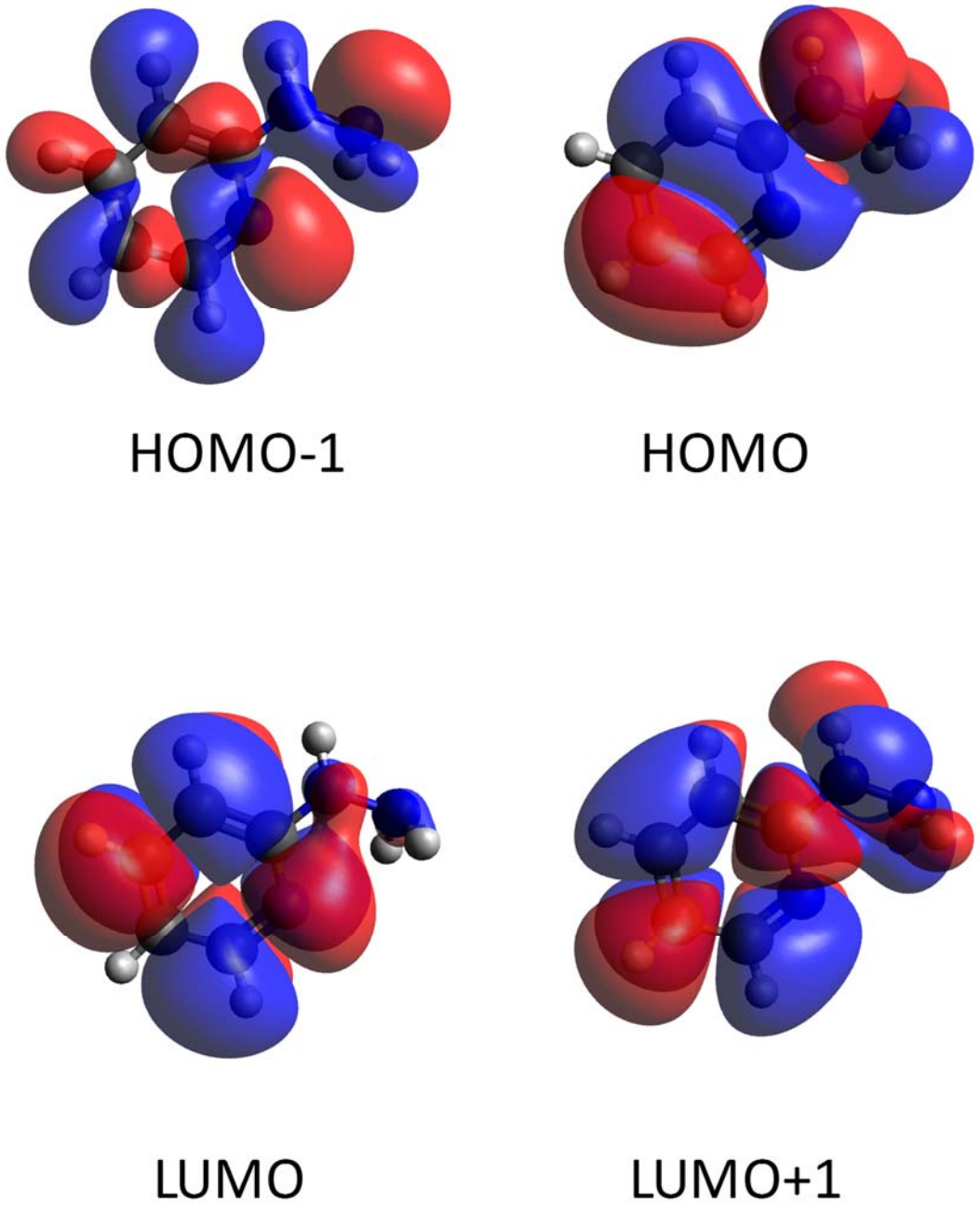


Figure S44. Frontier molecular orbitals for $PyNHNH_2$.

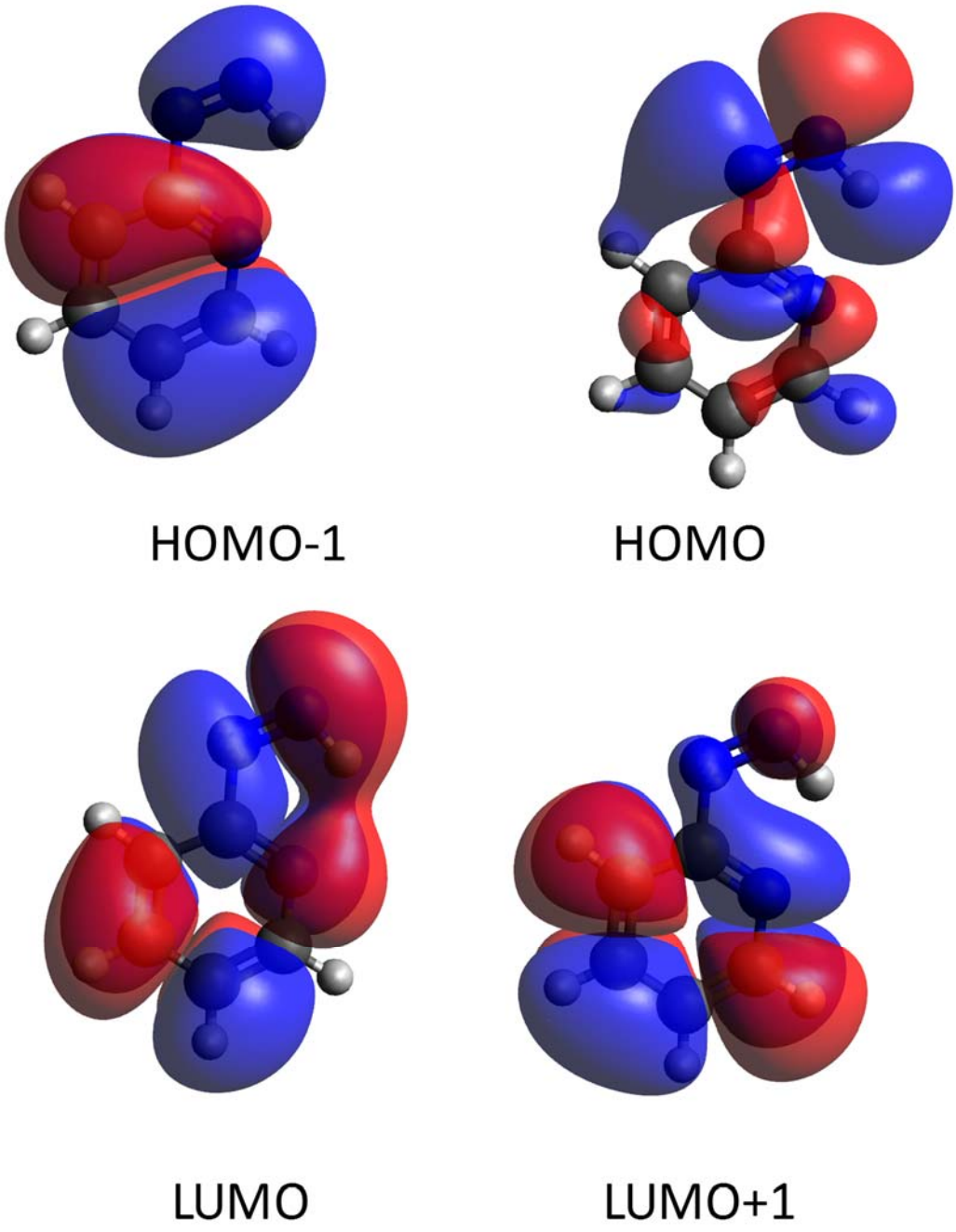


Figure S45. Frontier molecular orbitals for cis-PyN=NH.

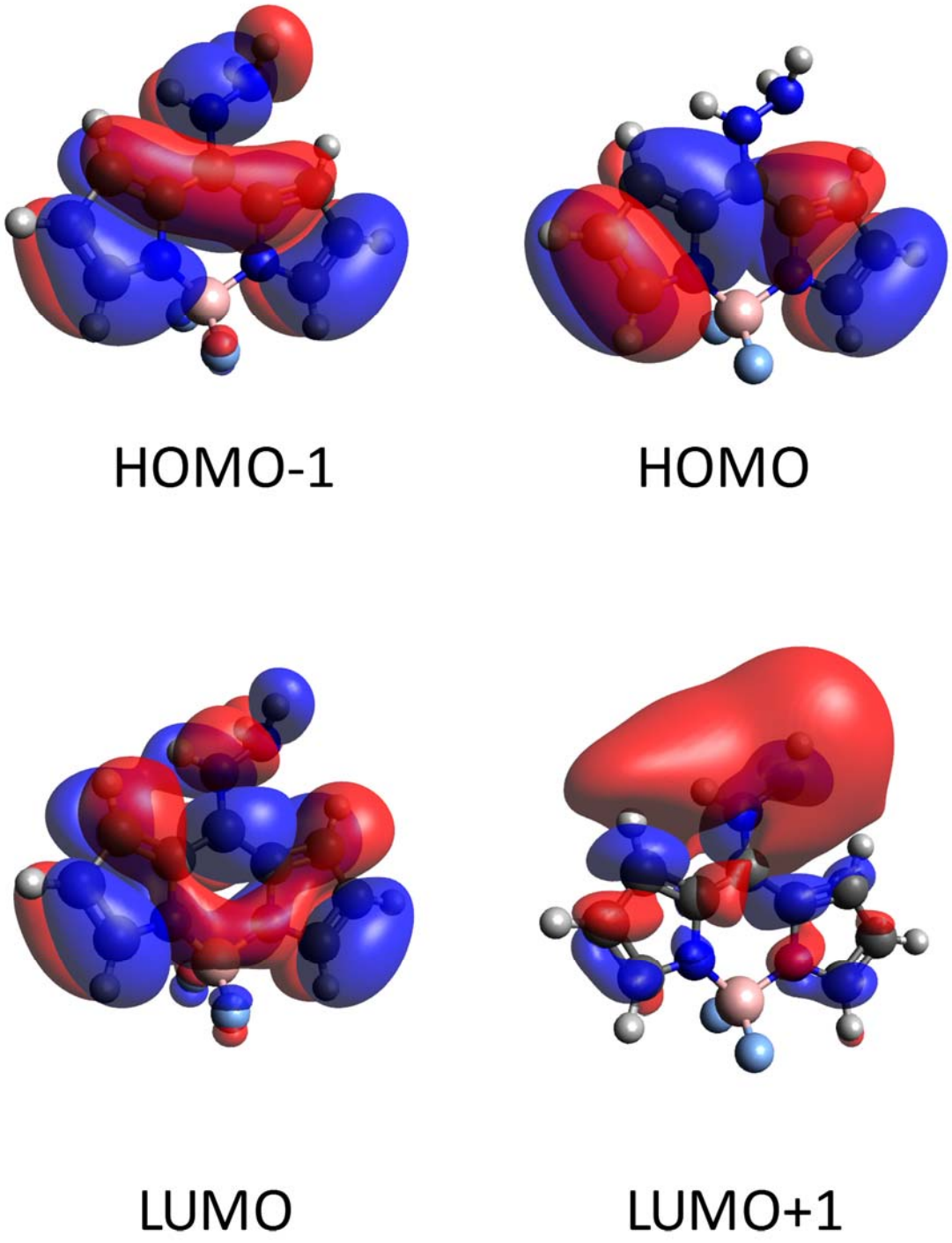


Figure S46. Frontier molecular orbitals for $BoNHNH_2$.

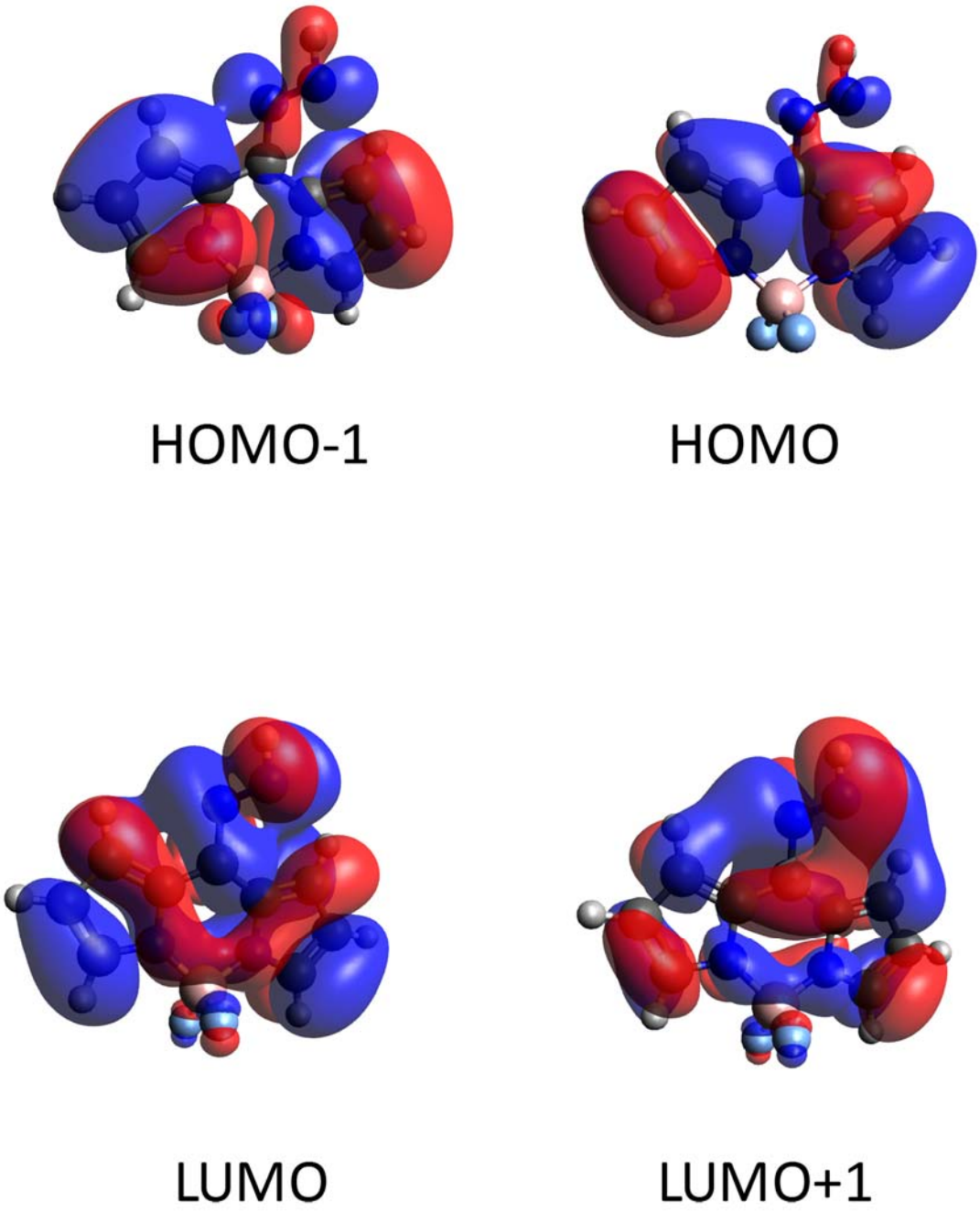


Figure S47. Frontier molecular orbitals for BoN=NH.

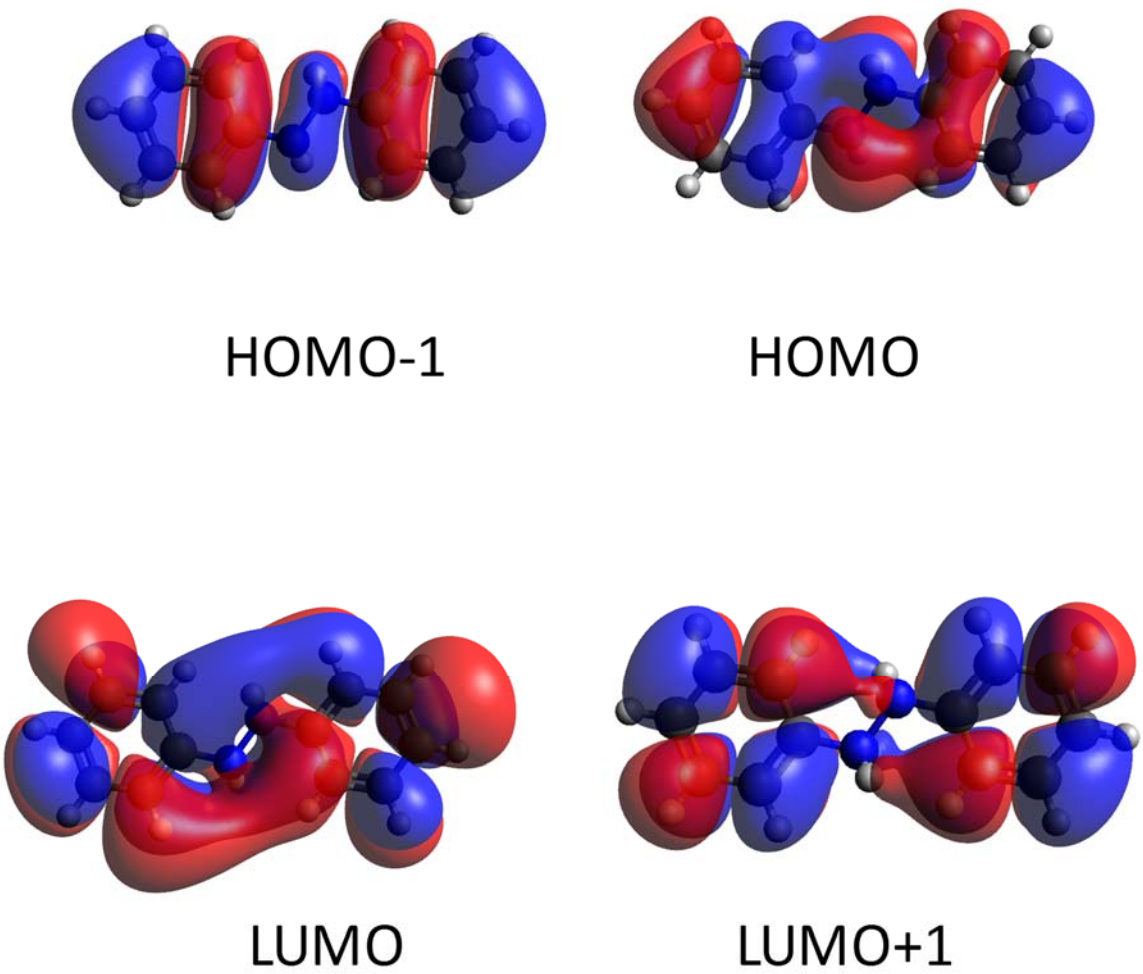


Figure S48. Frontier molecular orbitals for PhNHNHPh.

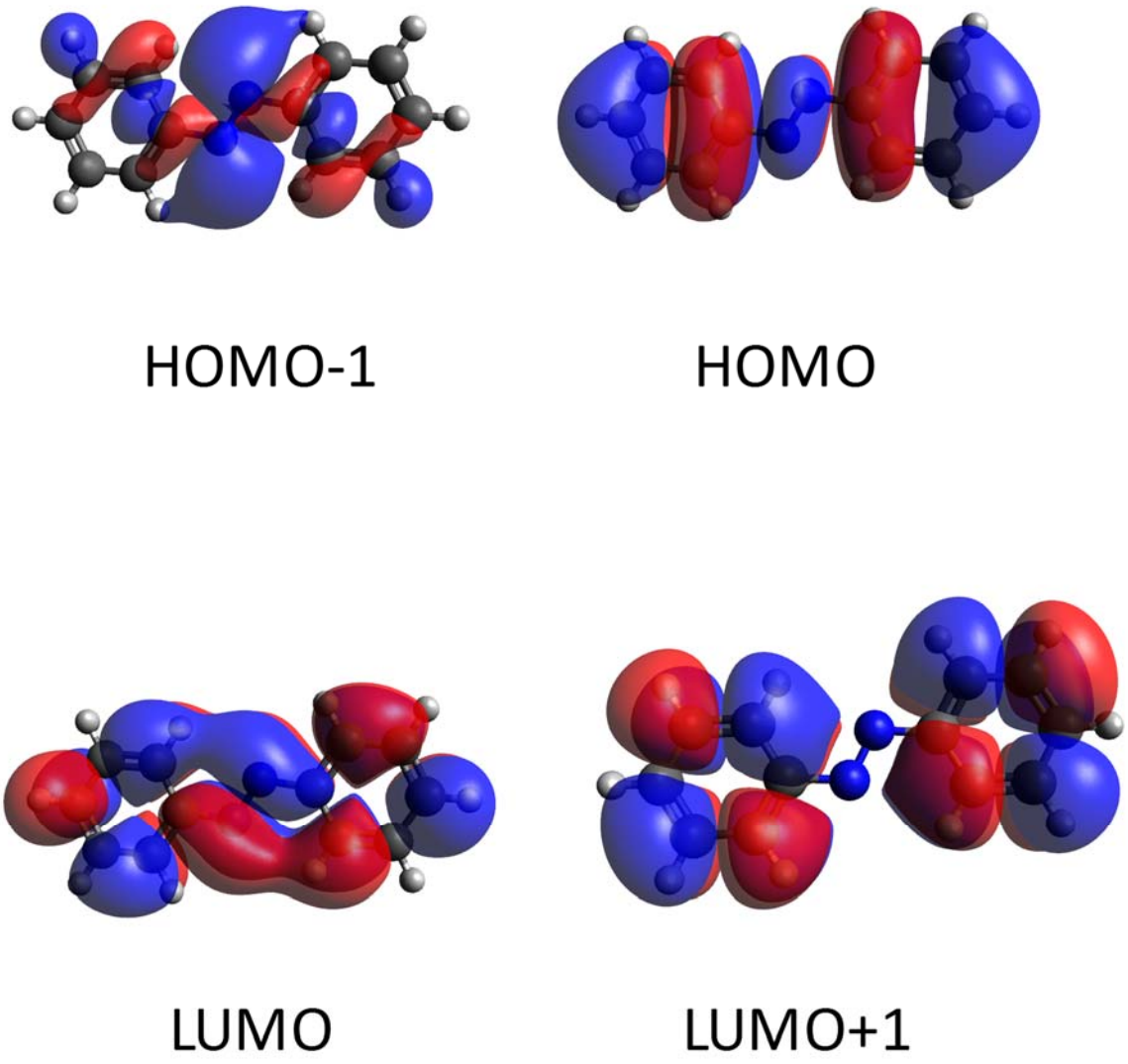


Figure S49. Frontier molecular orbitals for PhN=NPh.

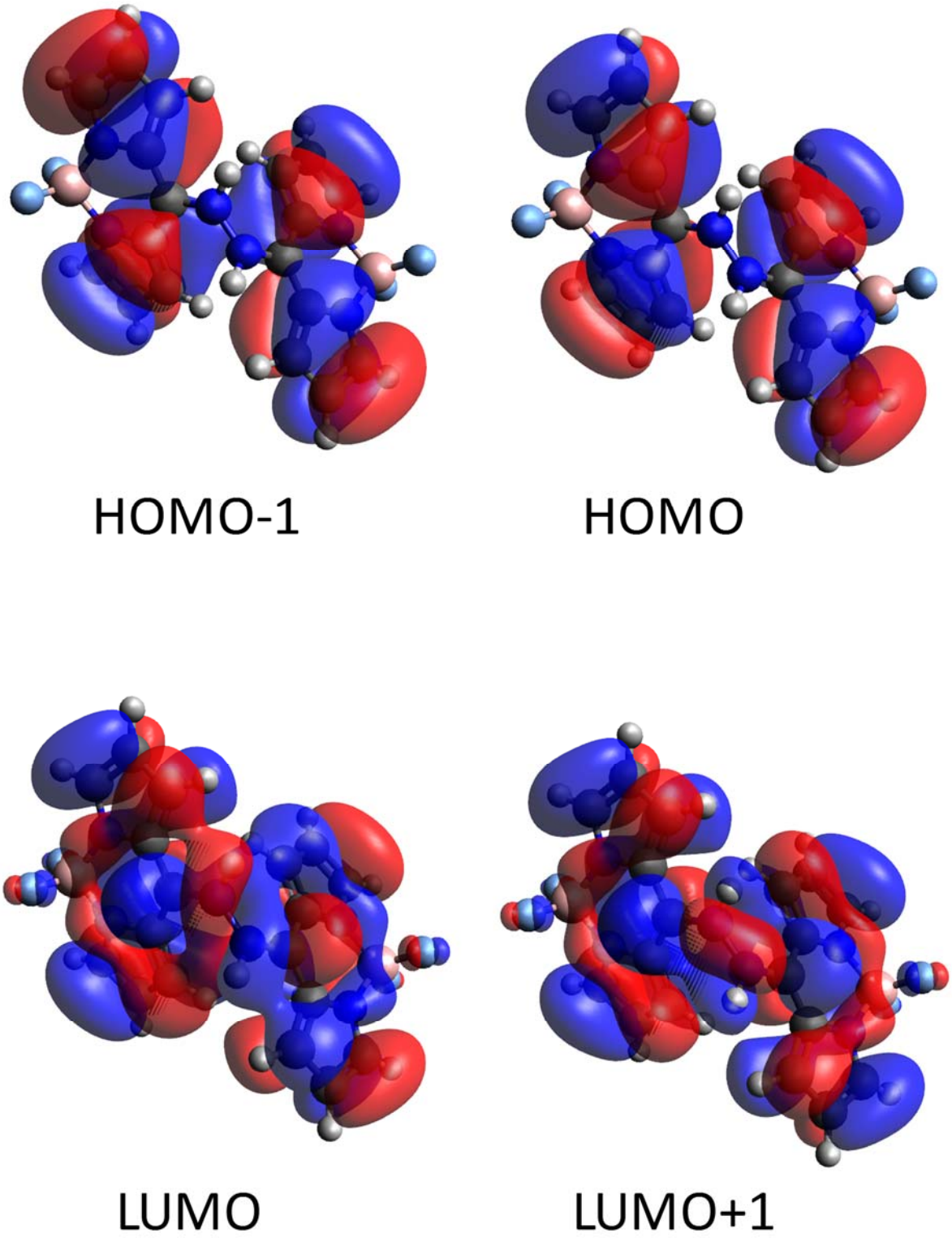


Figure S50. Frontier molecular orbitals for BoNHNHBo.

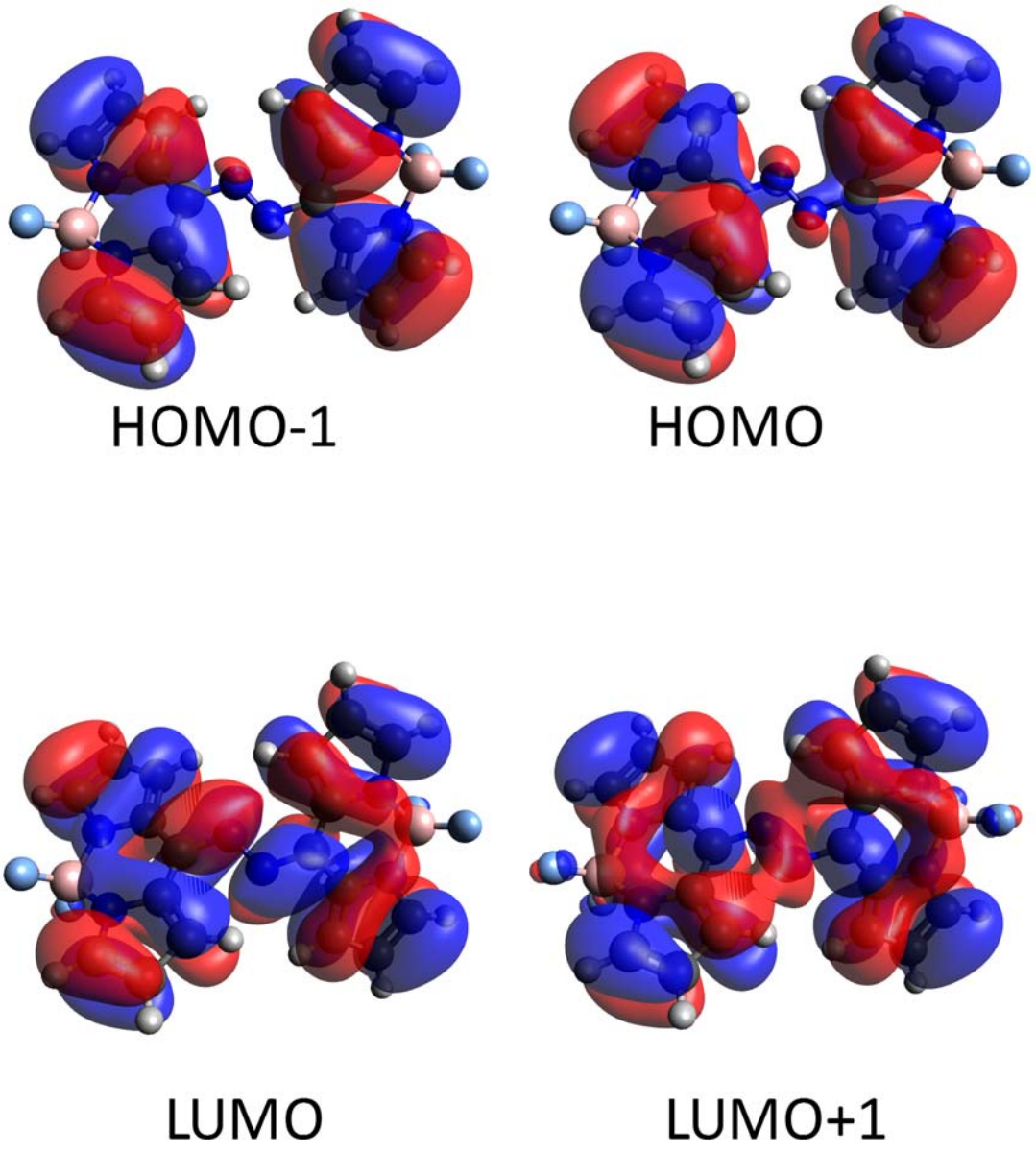


Figure S51. Frontier molecular orbitals for BoN=NBo.

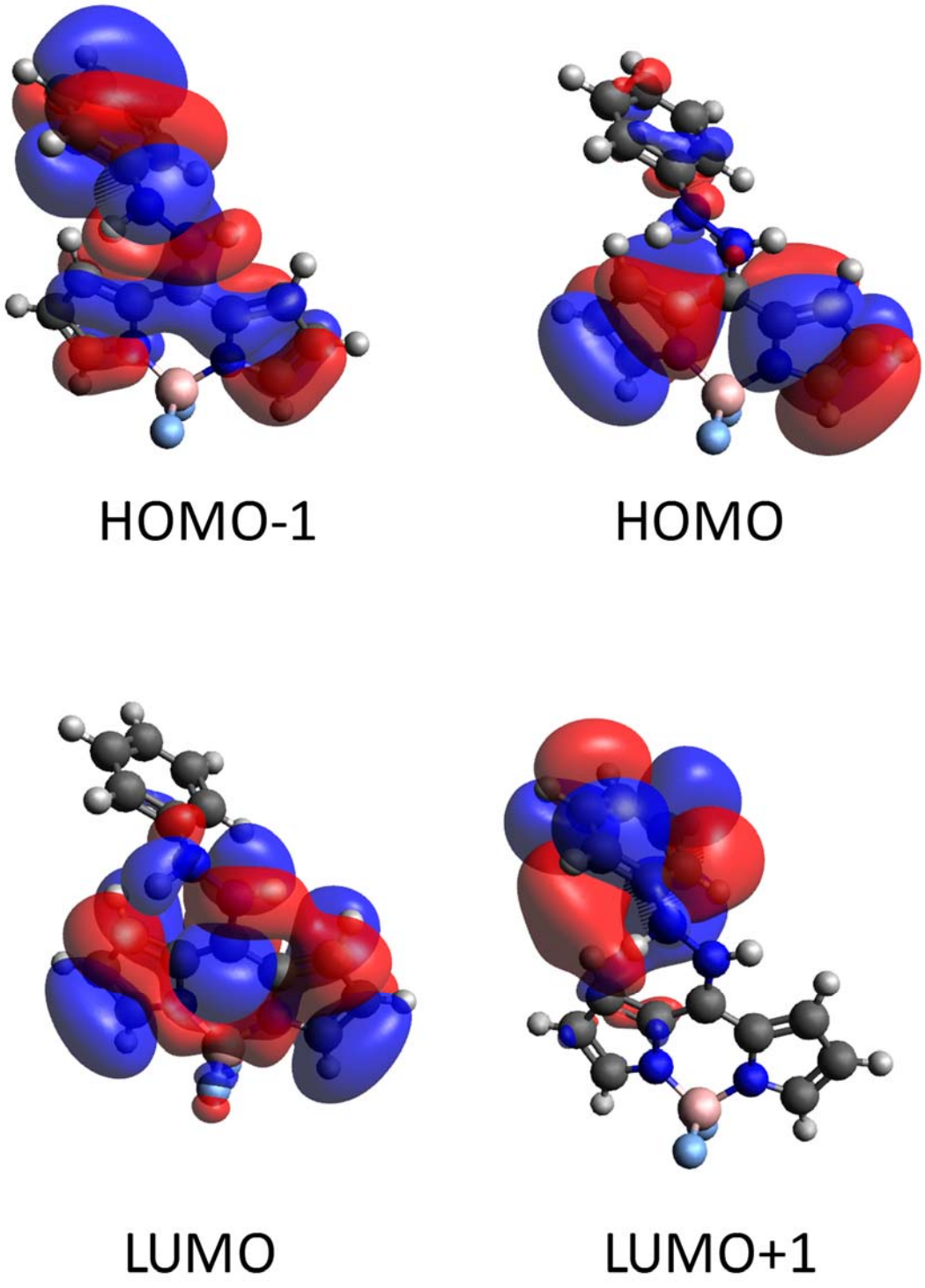


Figure S52. Frontier molecular orbitals for BoNHNHPh.

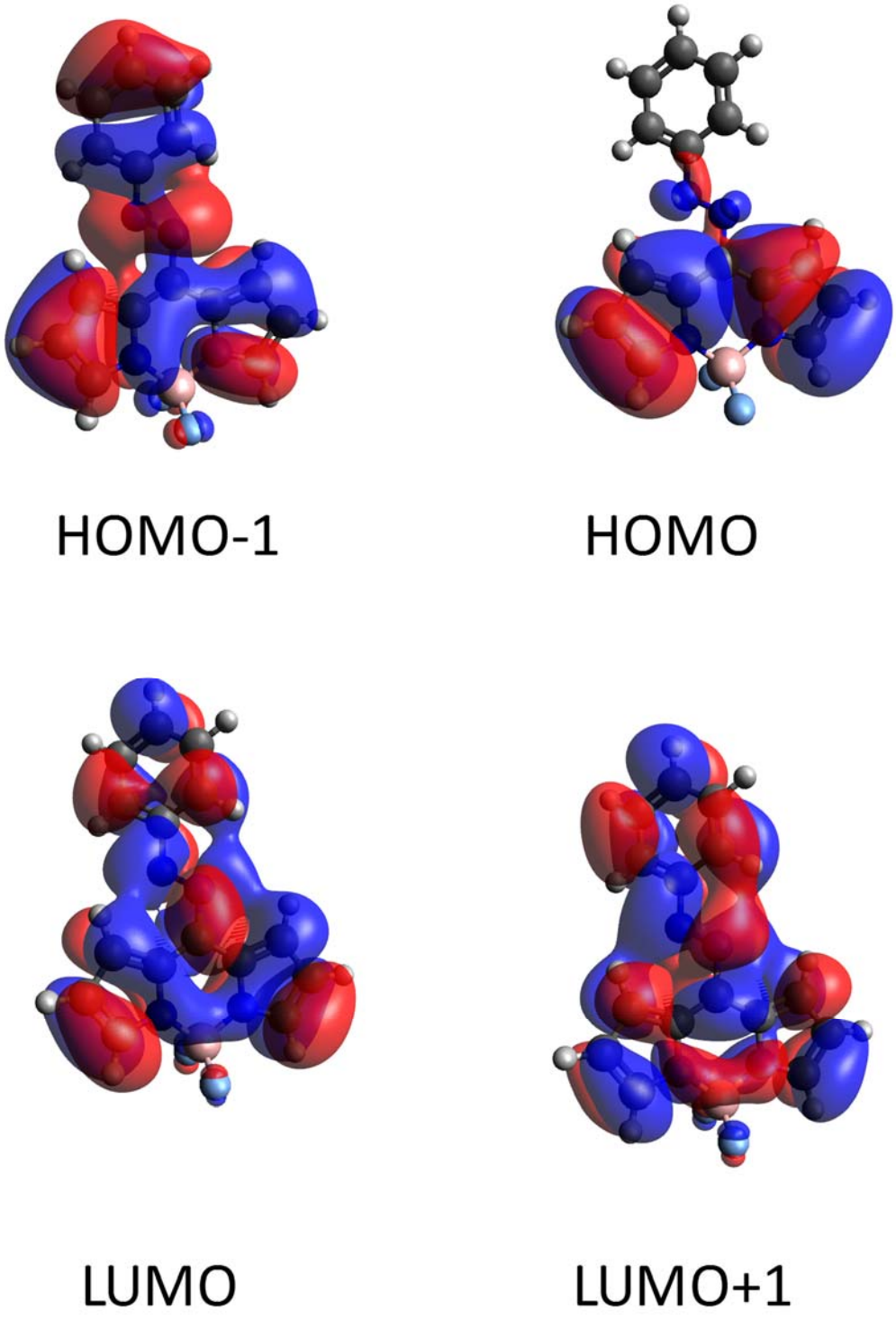


Figure S53. Frontier molecular orbitals for BoN=NPh.

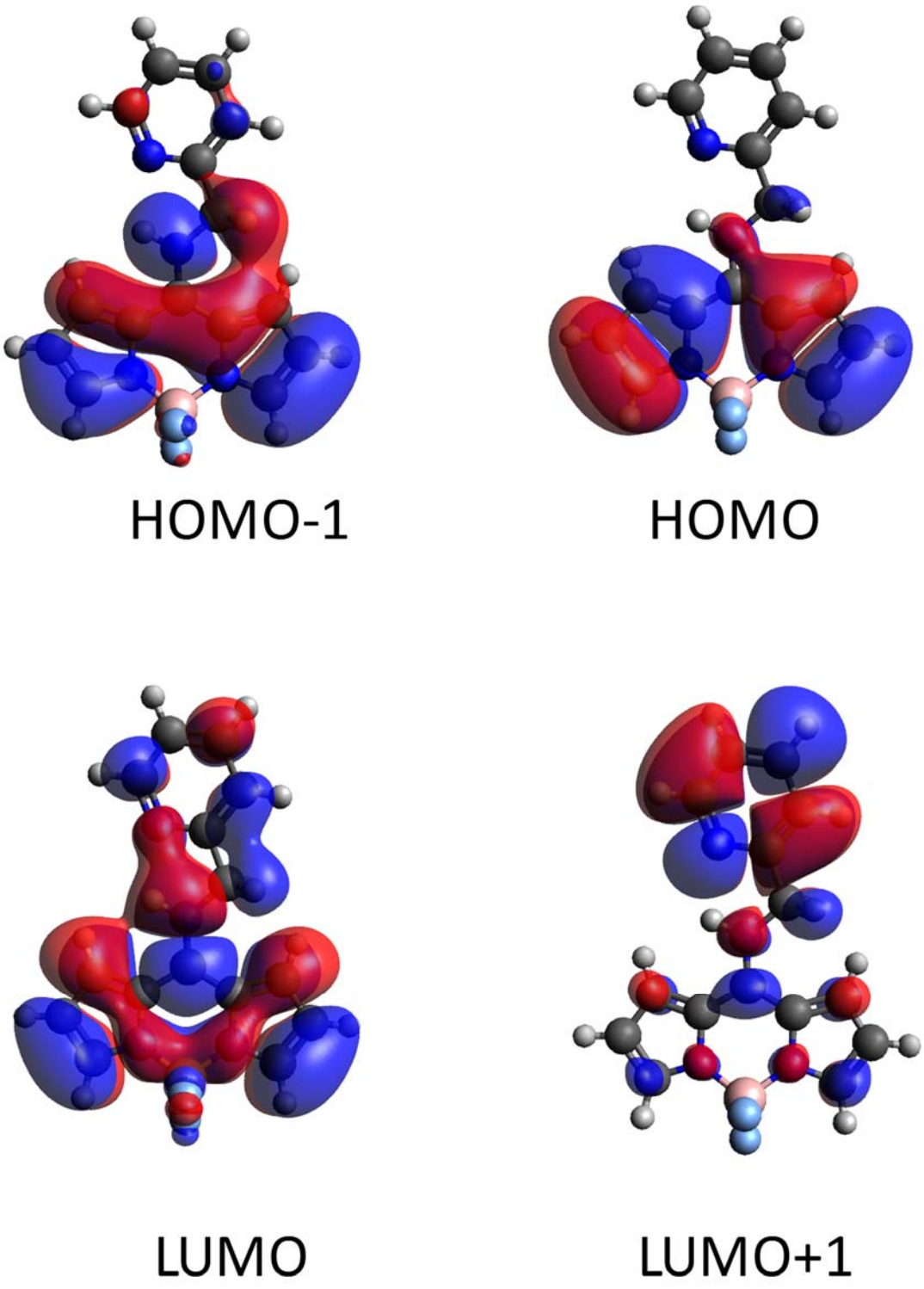


Figure S54. Frontier molecular orbitals for BoNHNHPy.

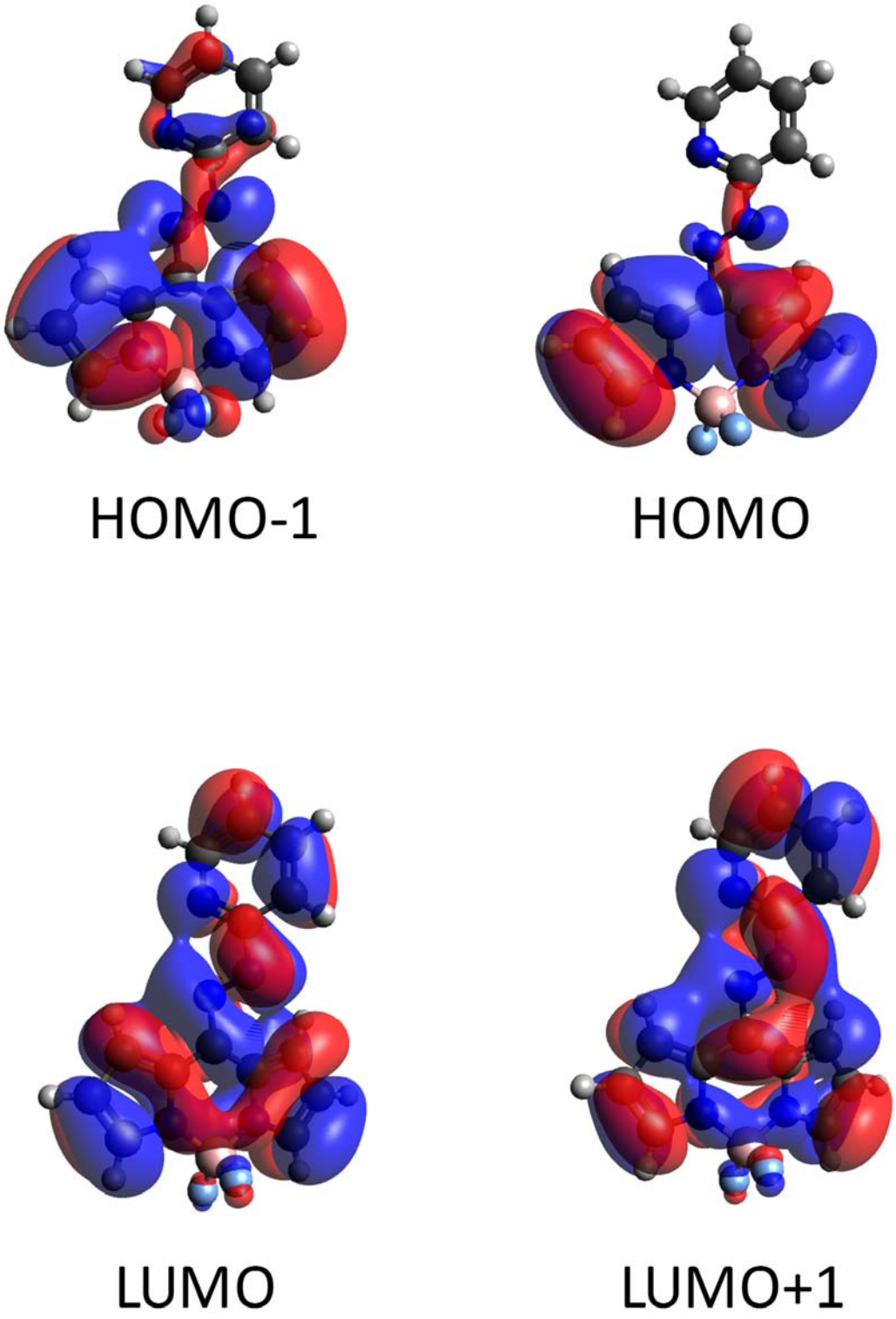


Figure S55. Frontier molecular orbitals for BoN=NPy.

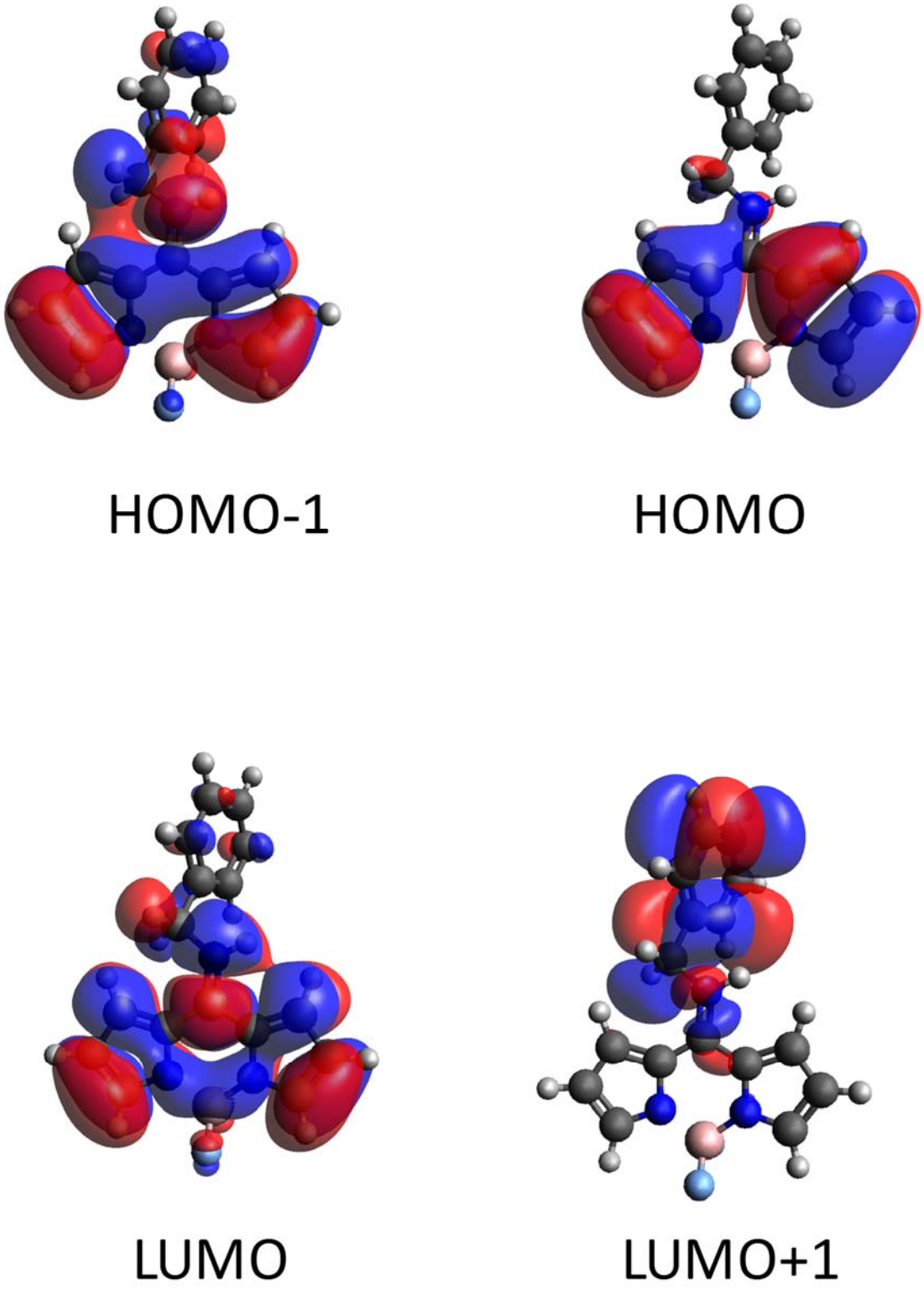


Figure S56. Frontier molecular orbitals for $BoNHCH_2Ph$.

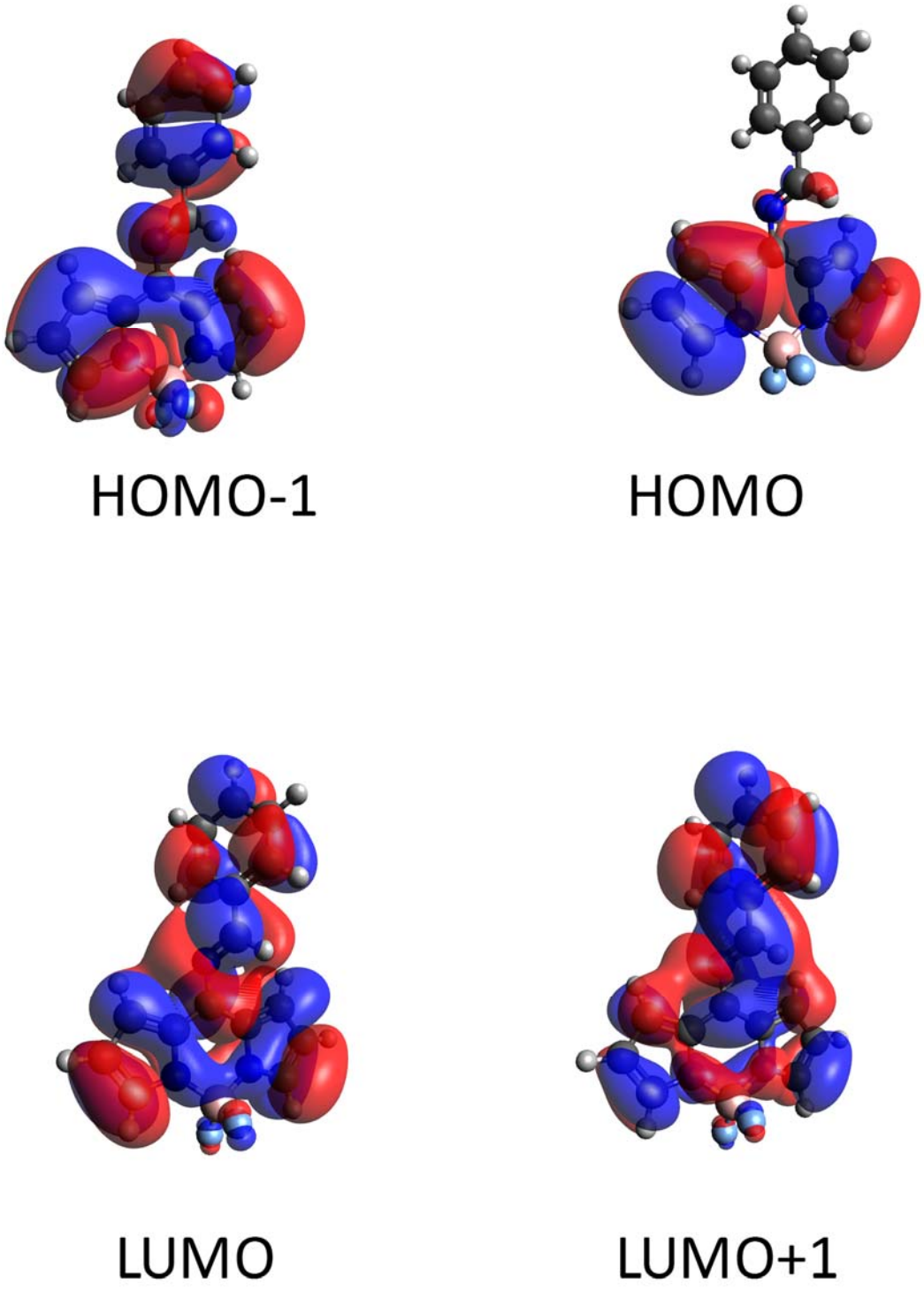


Figure S57. Frontier molecular orbitals for BoN=CHPh.

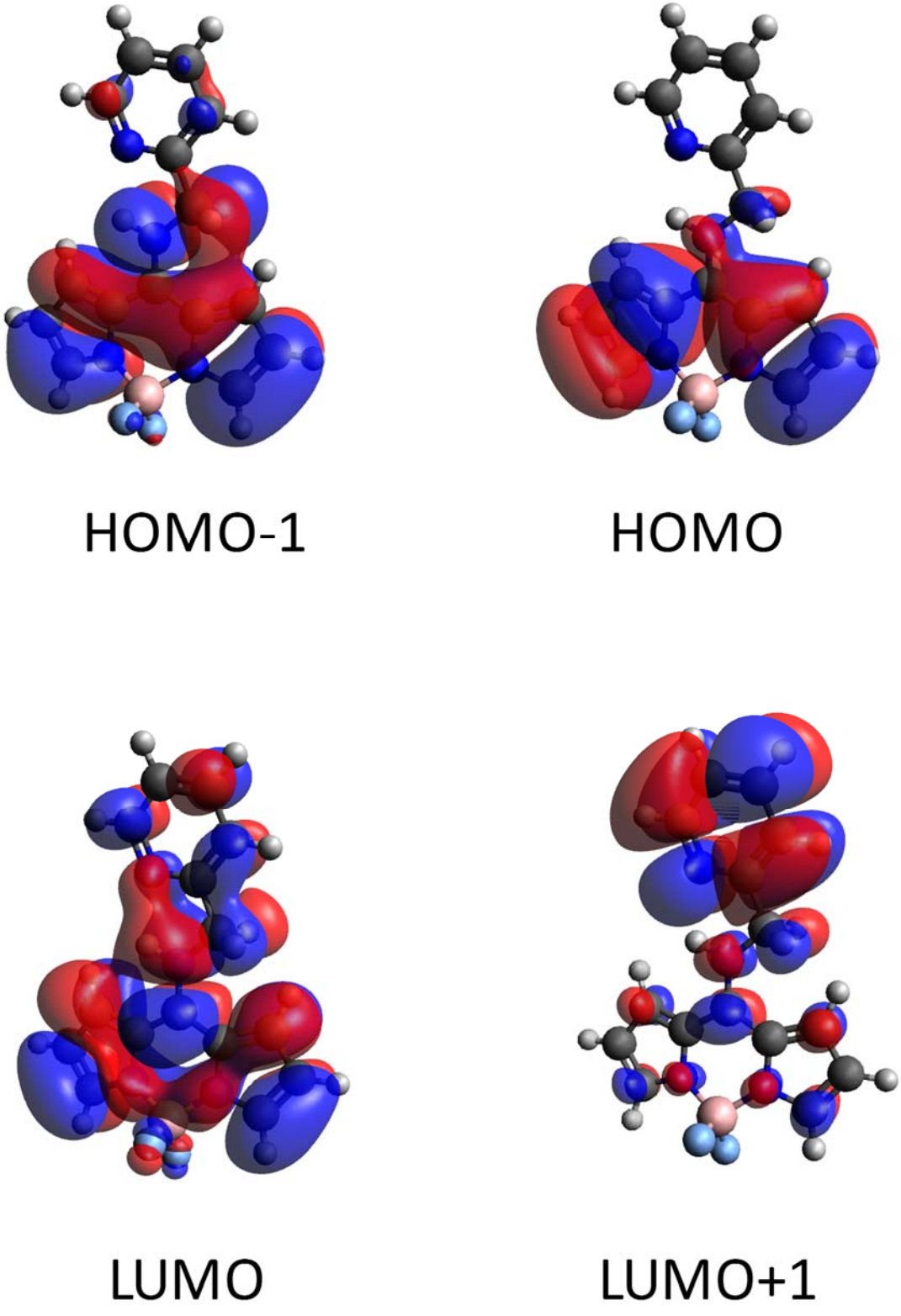


Figure S58. Frontier molecular orbitals for BoNHCH$_2$Py.

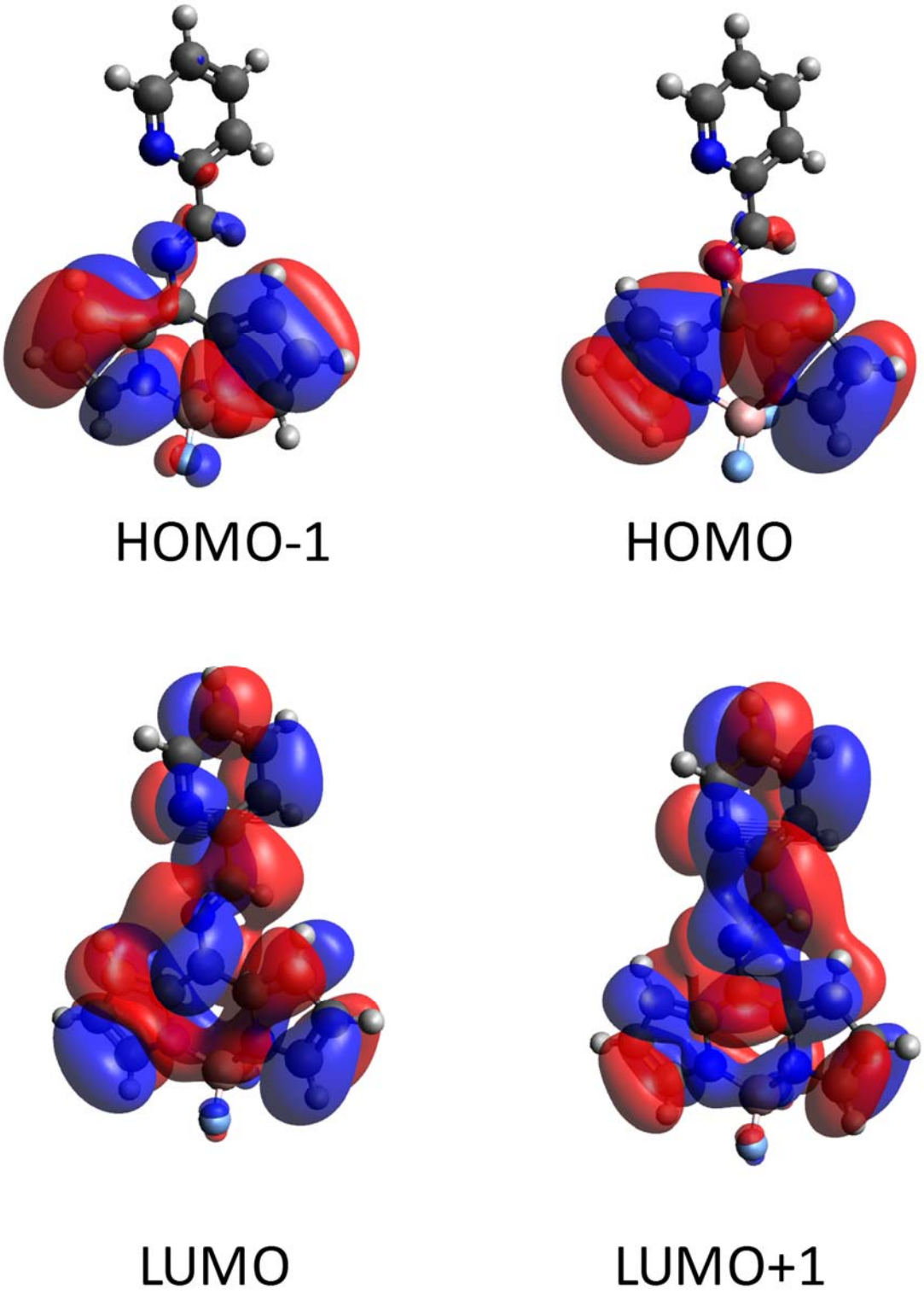


Figure S59. Frontier molecular orbitals for BoN=CHPy.

14) Summary of H_2, Proton, Hydride, and H-atom Transfer from the Investigated Hydrazine and Aminomethyl Complexes

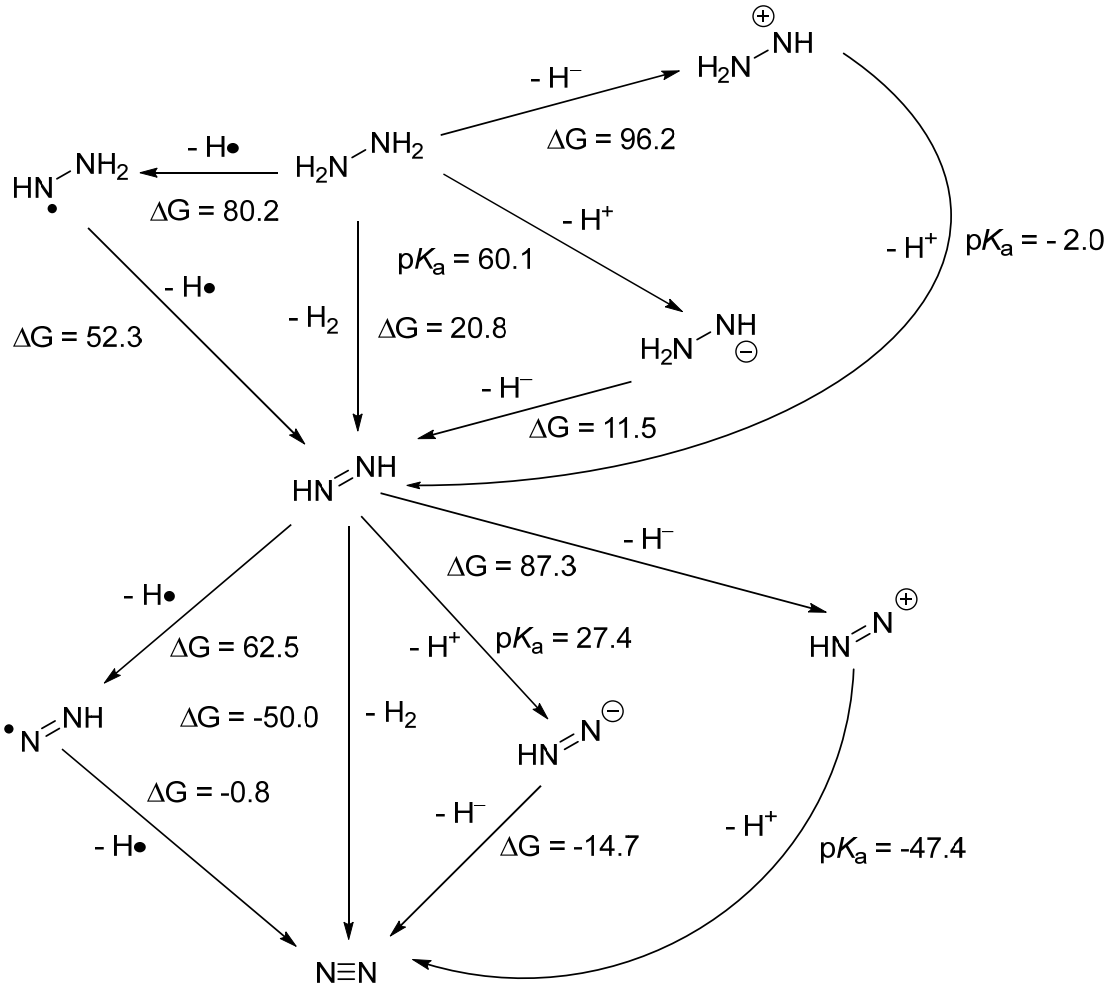


Figure S60. Summary of the computed thermodynamics for H_2, proton, hydride, and H-atom loss from hydrazine in MeCN.

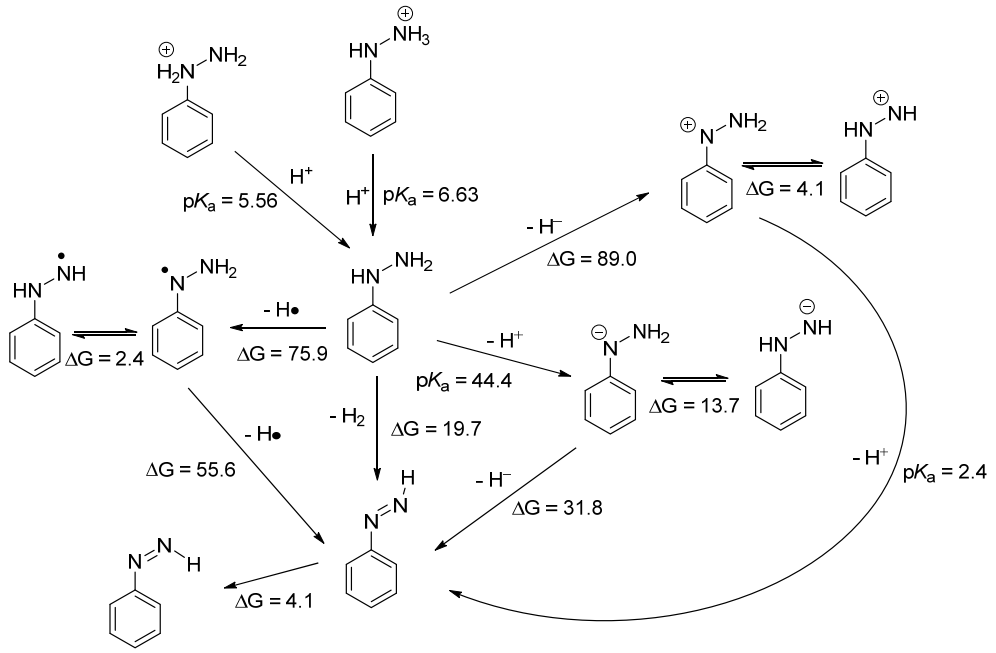


Figure S61. Summary of the computed thermodynamics of H_2, proton, hydride, and H-atom loss from **PhNHNH$_2$** in MeCN.

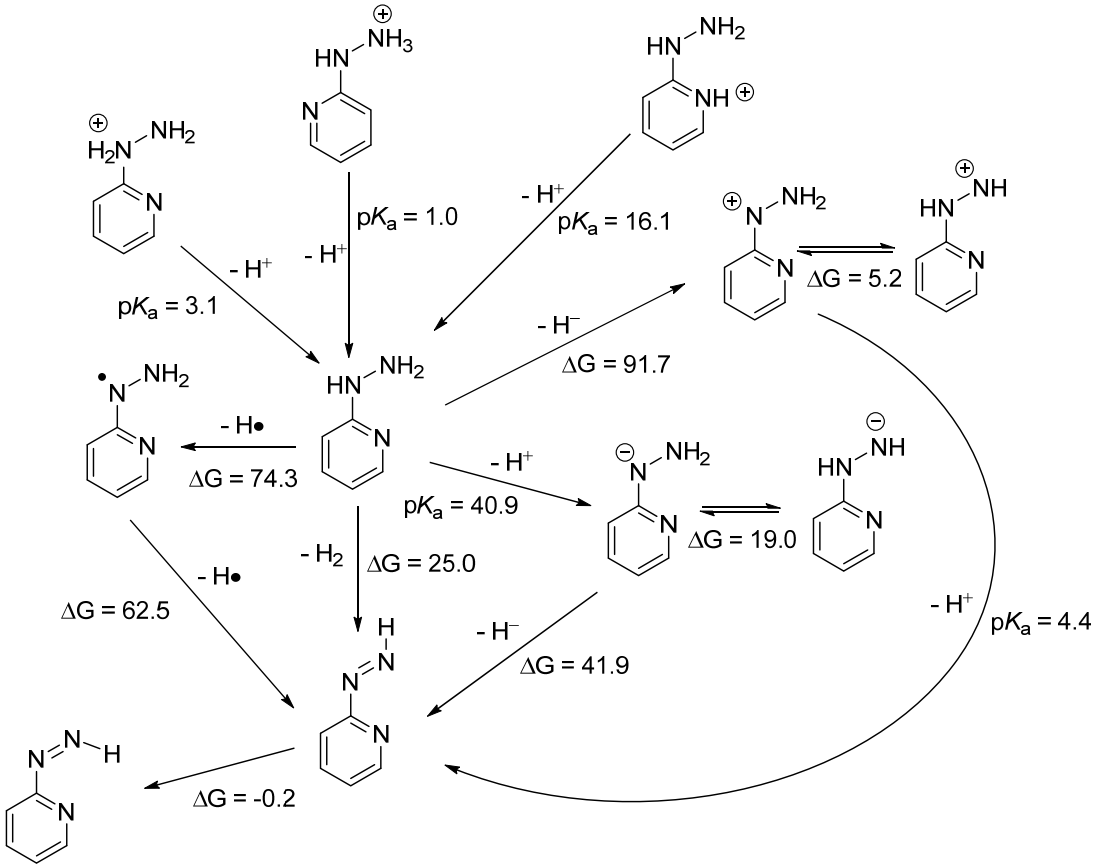


Figure S62. Summary of the computed thermodynamics of H_2, proton, hydride, and H-atom loss from **PyNHNH$_2$** in MeCN.

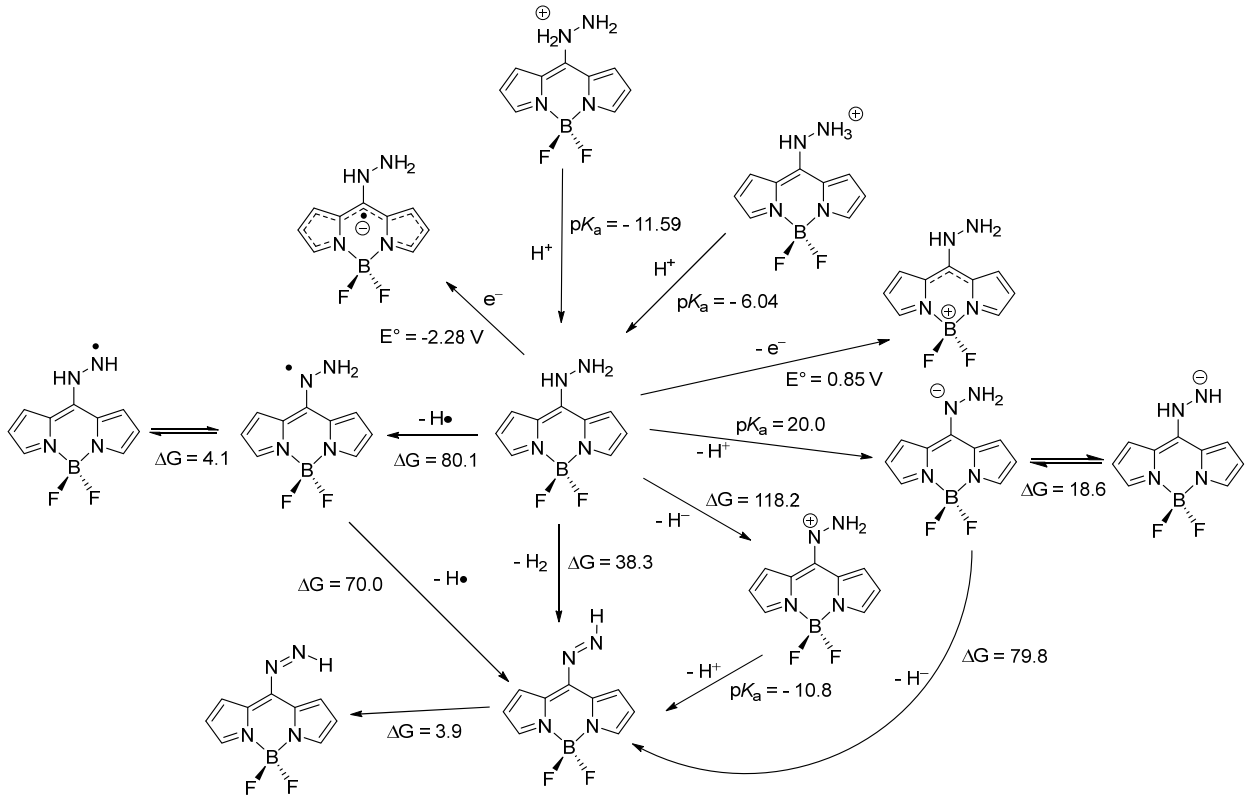


Figure S63. Summary of the computed thermodynamics of H_2, proton, hydride, and H-atom loss from **BoNHNH$_2$** in MeCN.

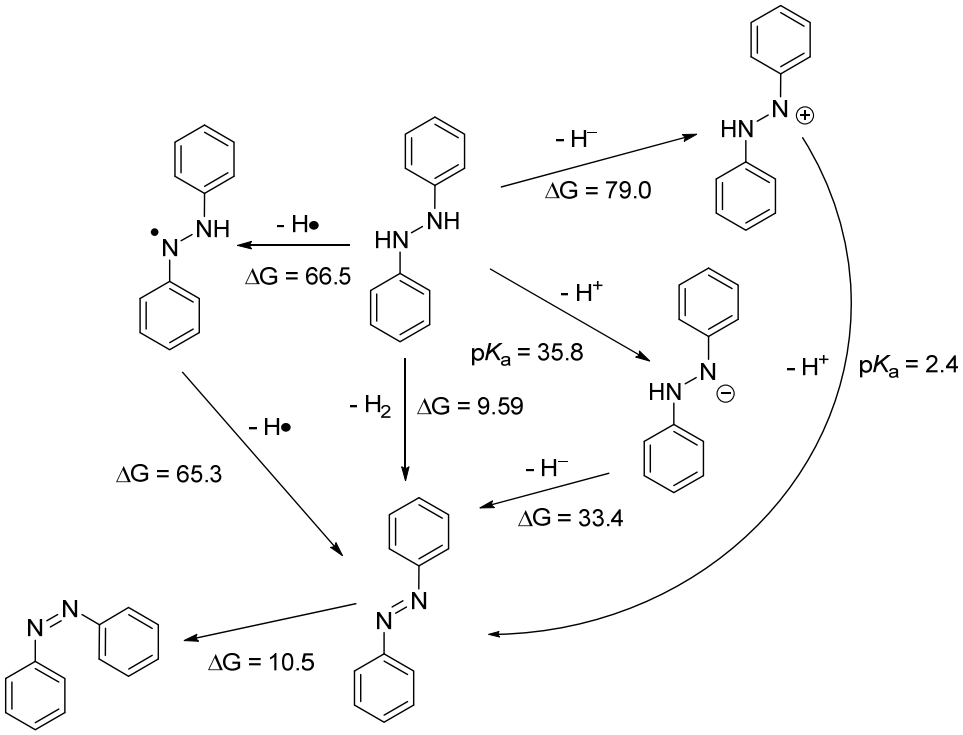


Figure S64. Summary of the computed thermodynamics of H_2, proton, hydride, and H-atom loss from **PhNHNHPh** in MeCN.

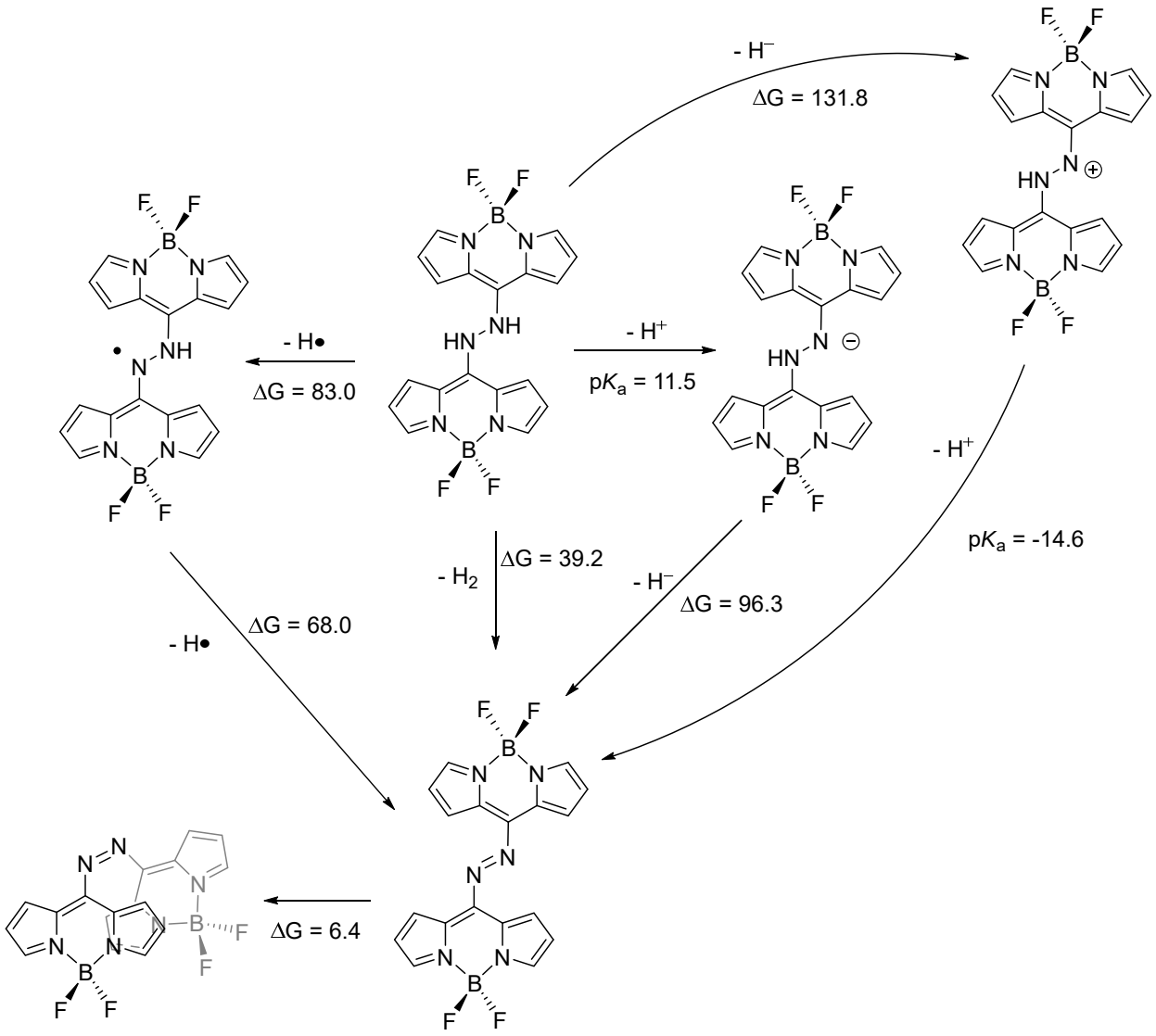


Figure S65. Summary of the computed thermodynamics of H_2, proton, hydride, and H-atom loss from **BoNHNHBo** in MeCN.

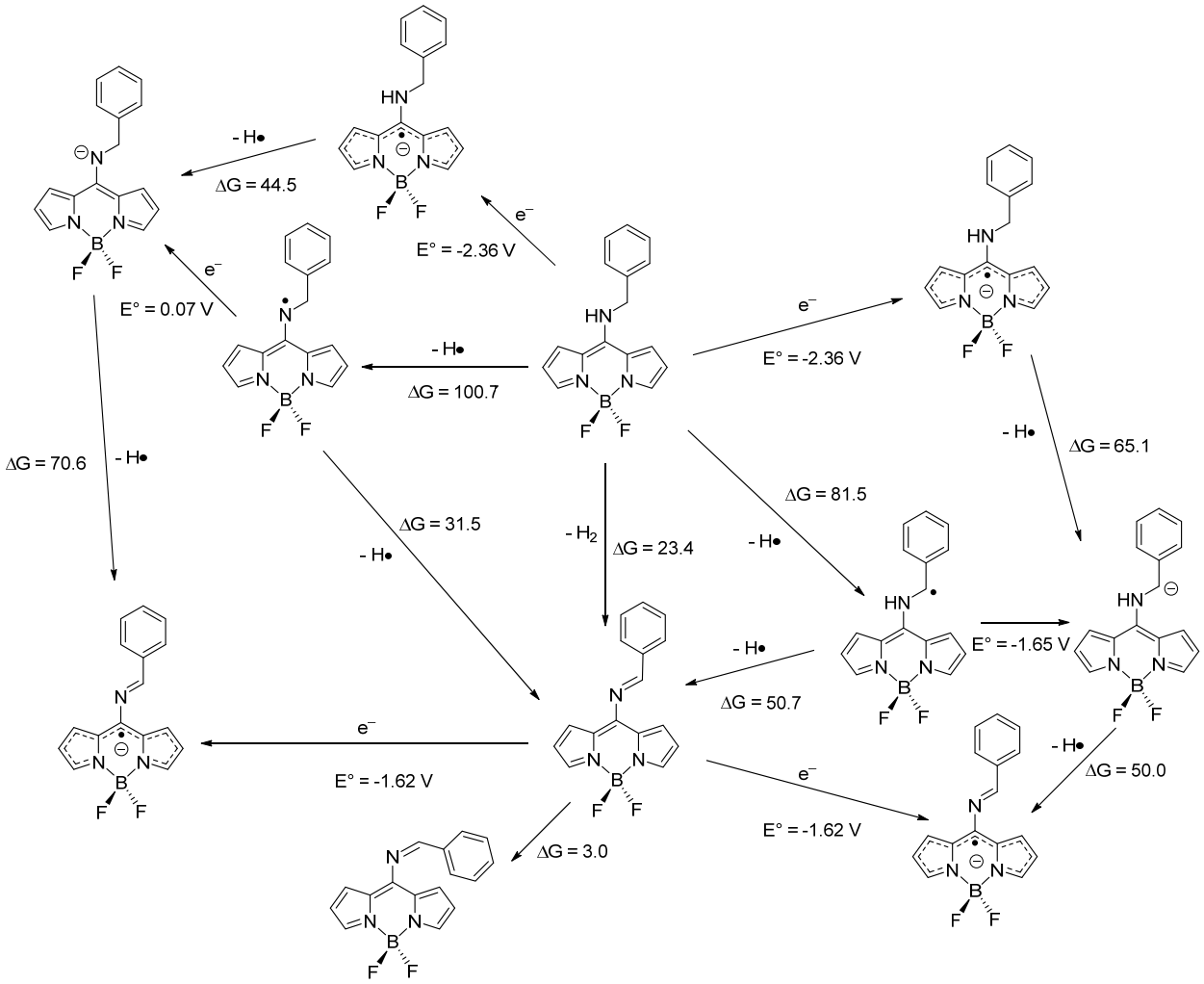


Figure S66. Summary of the influence of a reduction on H-atom loss from **BoNHCH$_2$Ph** in MeCN.

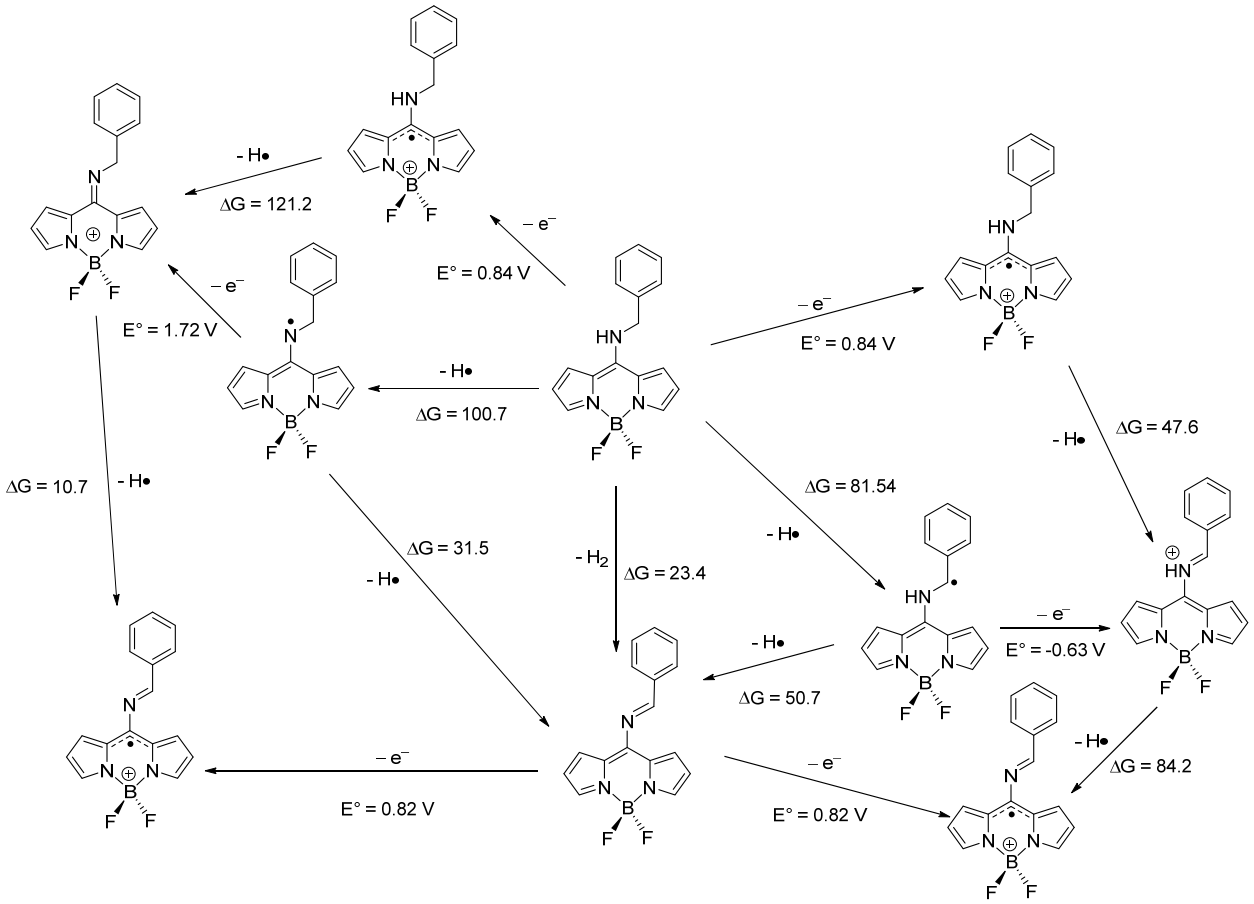


Figure S67. Summary of the influence of an oxidation on H-atom loss from **BoNHCH$_2$Ph** in MeCN.

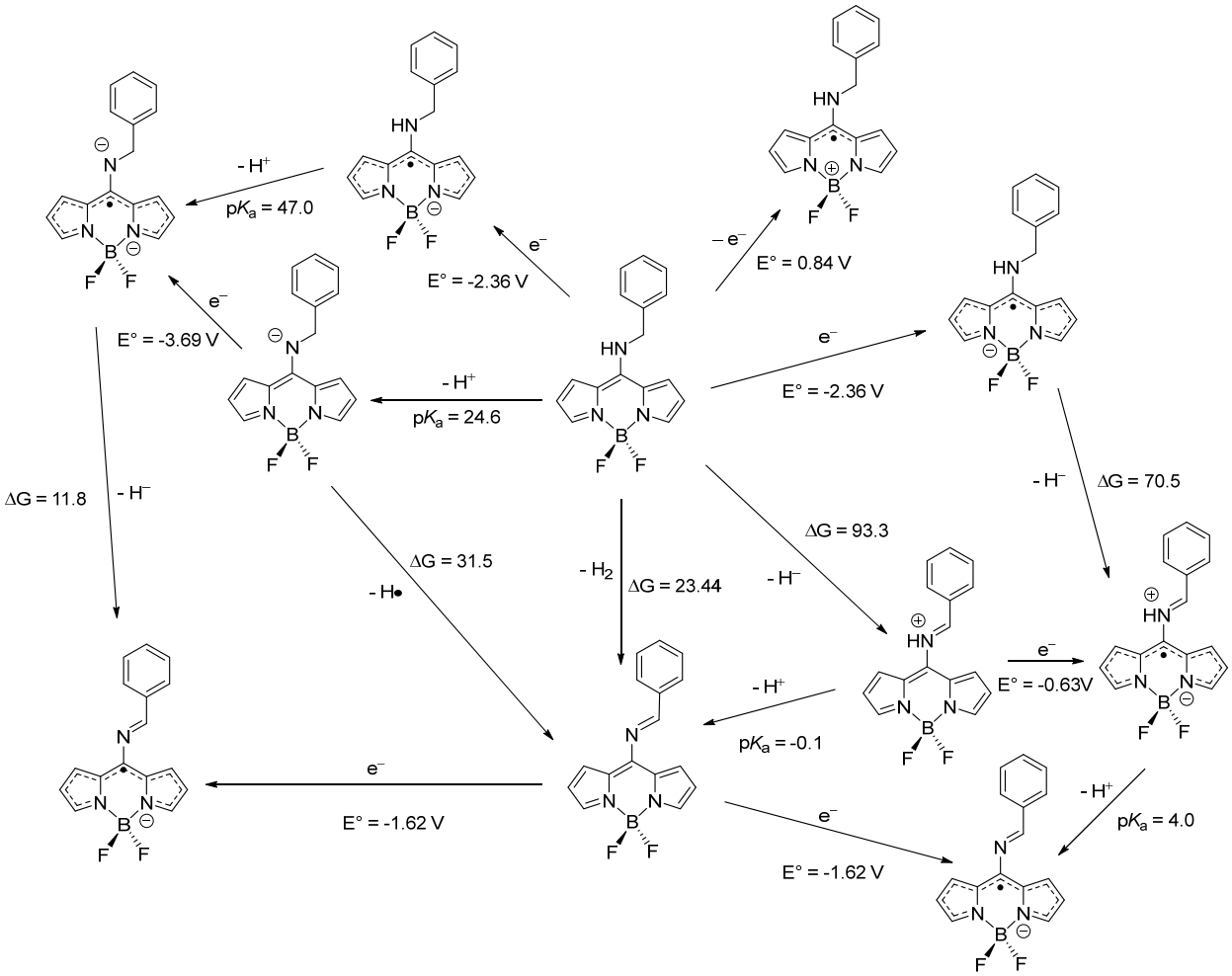


Figure S68. Summary of the influence of a reduction on proton and hydride loss from **BoNHCH$_2$Ph** in MeCN.

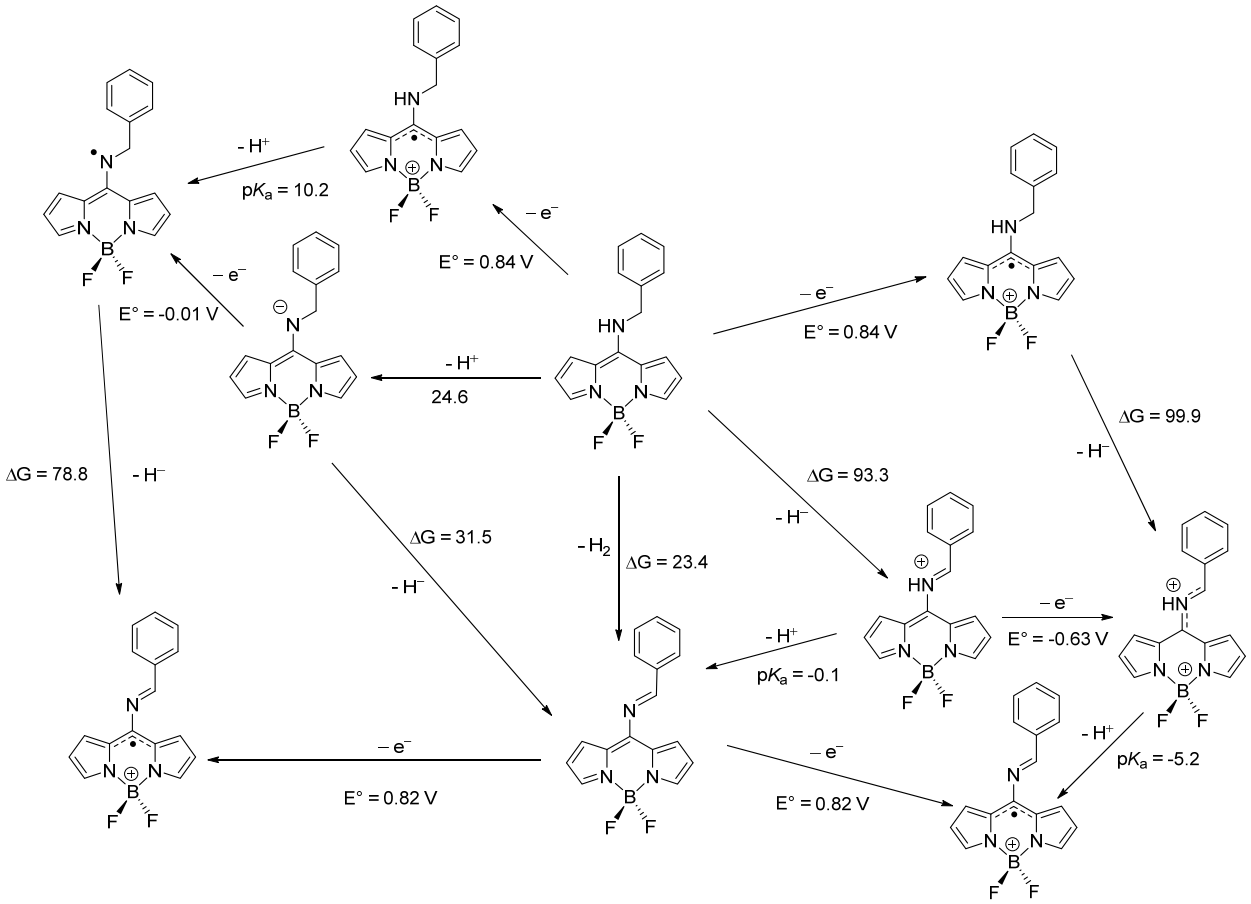


Figure S69. Summary of the influence of an oxidation on proton and hydride loss from **BoNHCH$_2$Ph** in MeCN.

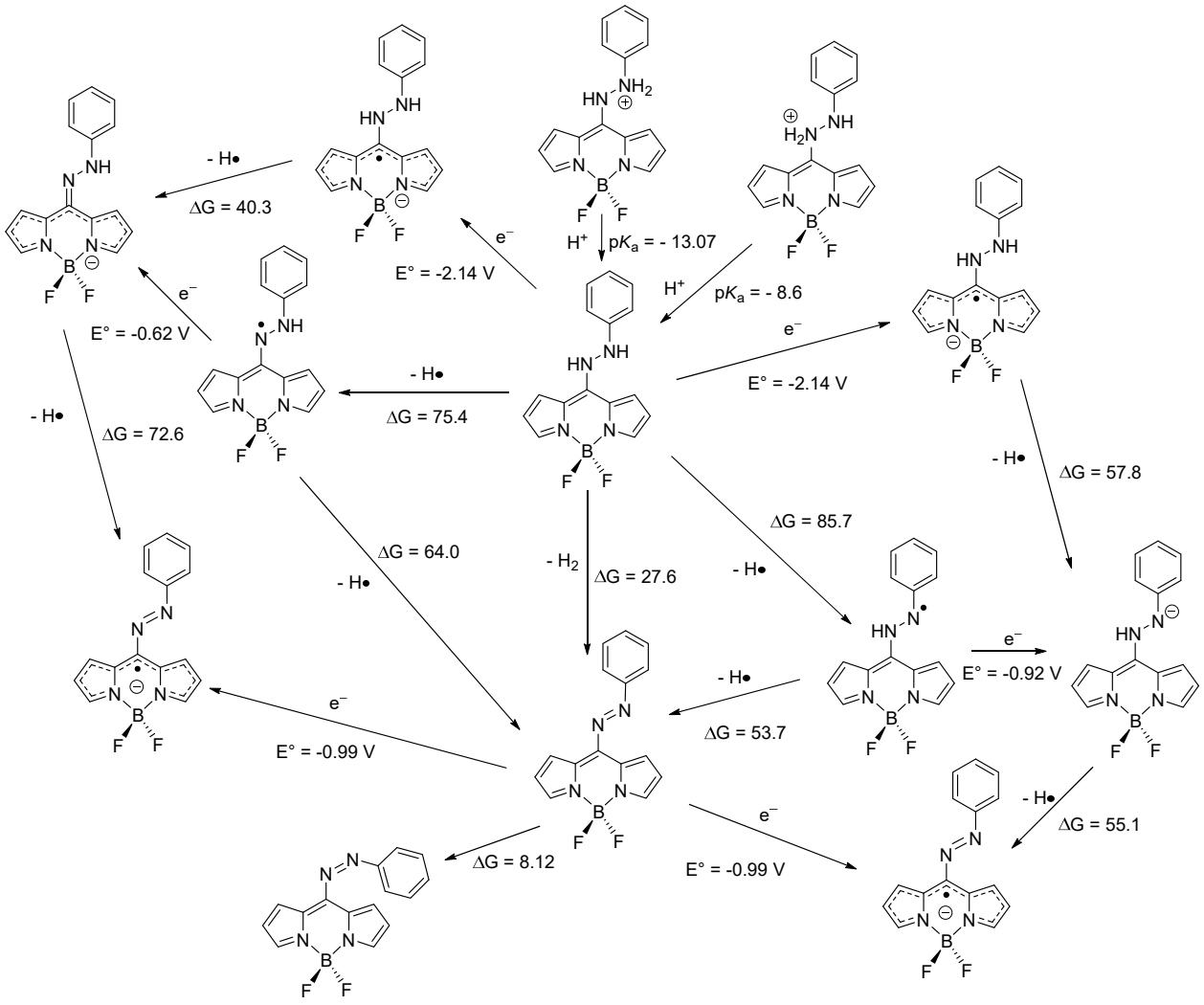


Figure S70. Summary of the influence of a reduction on H-atom loss from **BoNHNHPh** in MeCN.

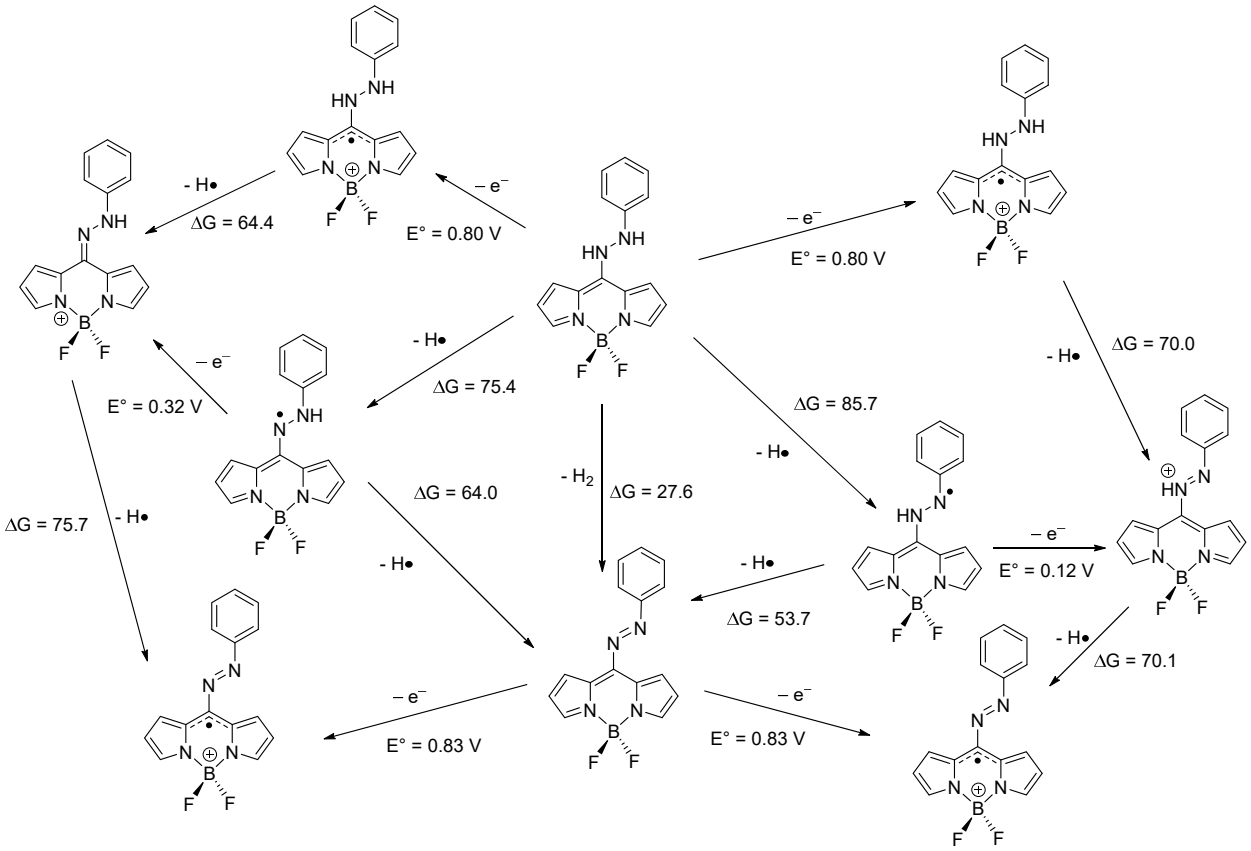


Figure S71. Summary of the influence of an oxidation on H-atom loss from **BoNHNHPh** in MeCN.

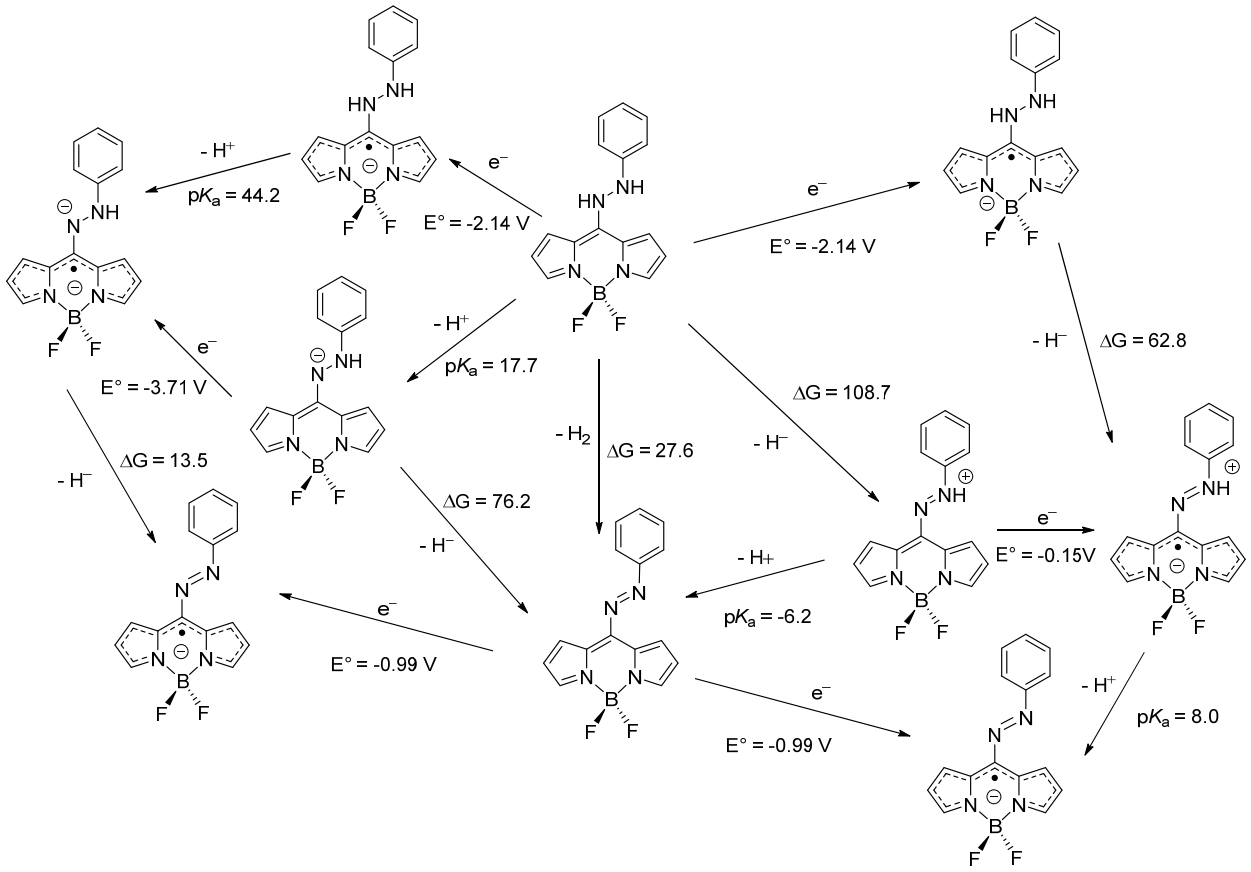


Figure S72. Summary of the influence of a reduction on proton and hydride loss from the proximal hydrogen of **BoNHNHPh** in MeCN.

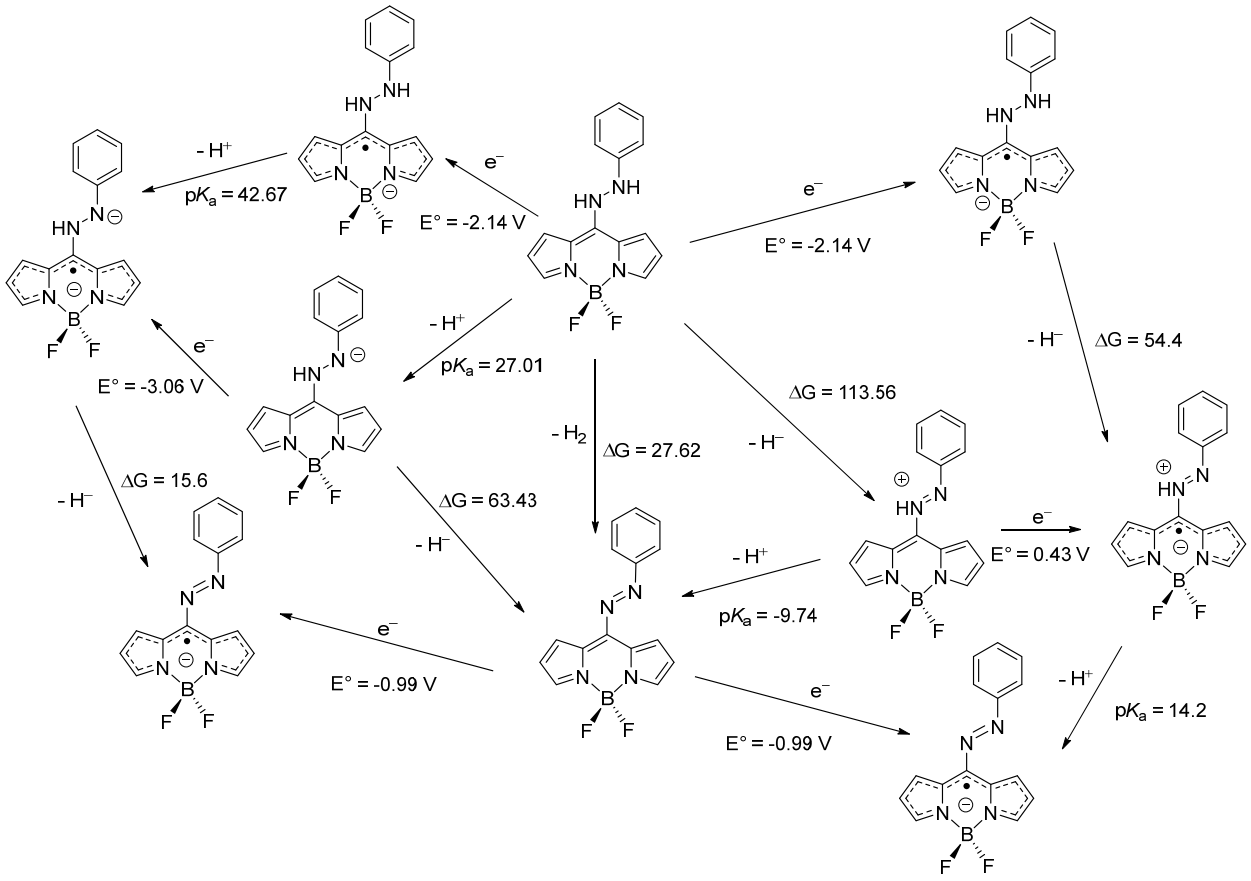


Figure S73. Summary of the influence of a reduction on proton and hydride loss from the distal hydrogen of **BoNHNHPh** in MeCN.

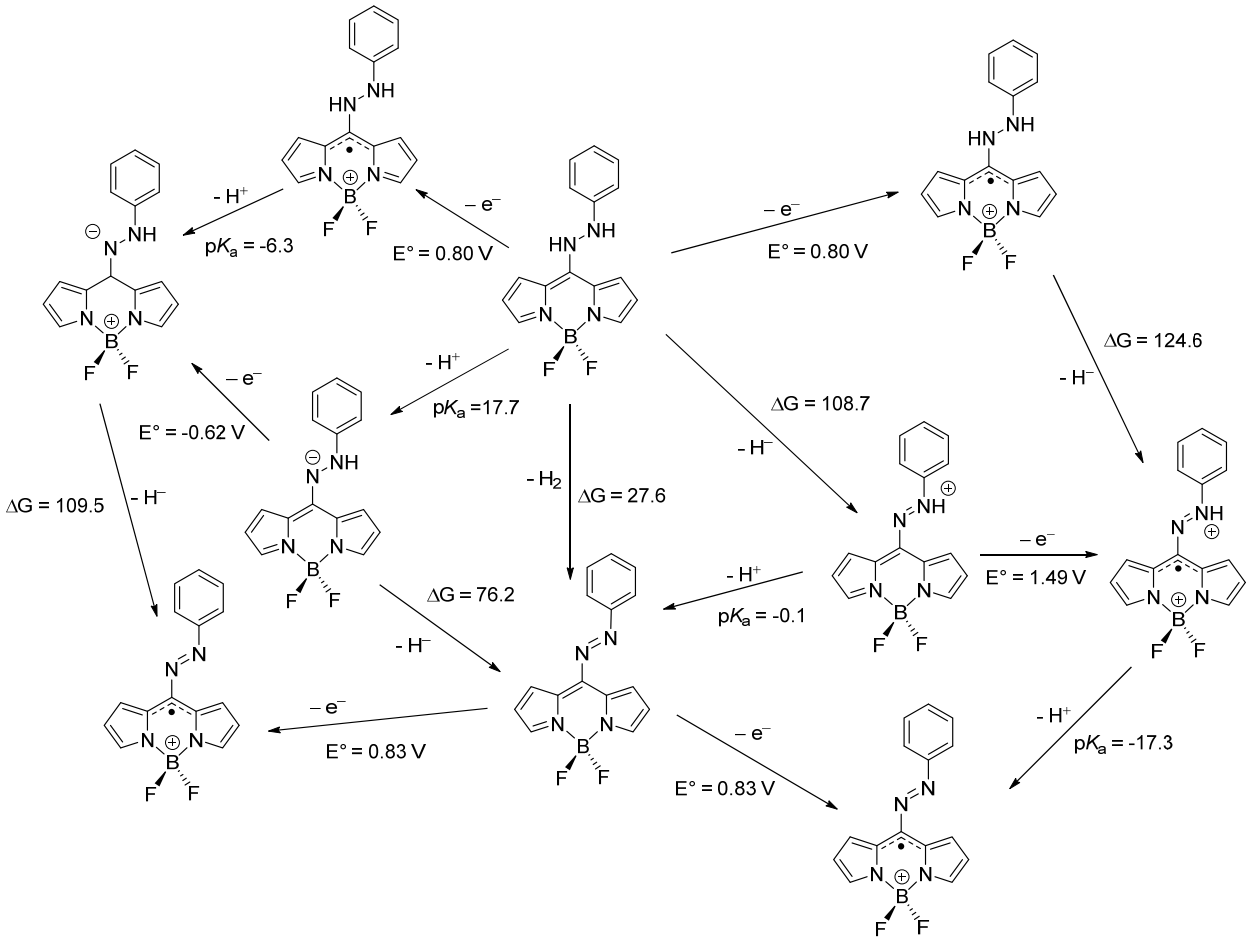


Figure S74. Summary of the influence of an oxidation on proton and hydride loss from the proximal hydrogen of **BoNHNHPh** in MeCN.

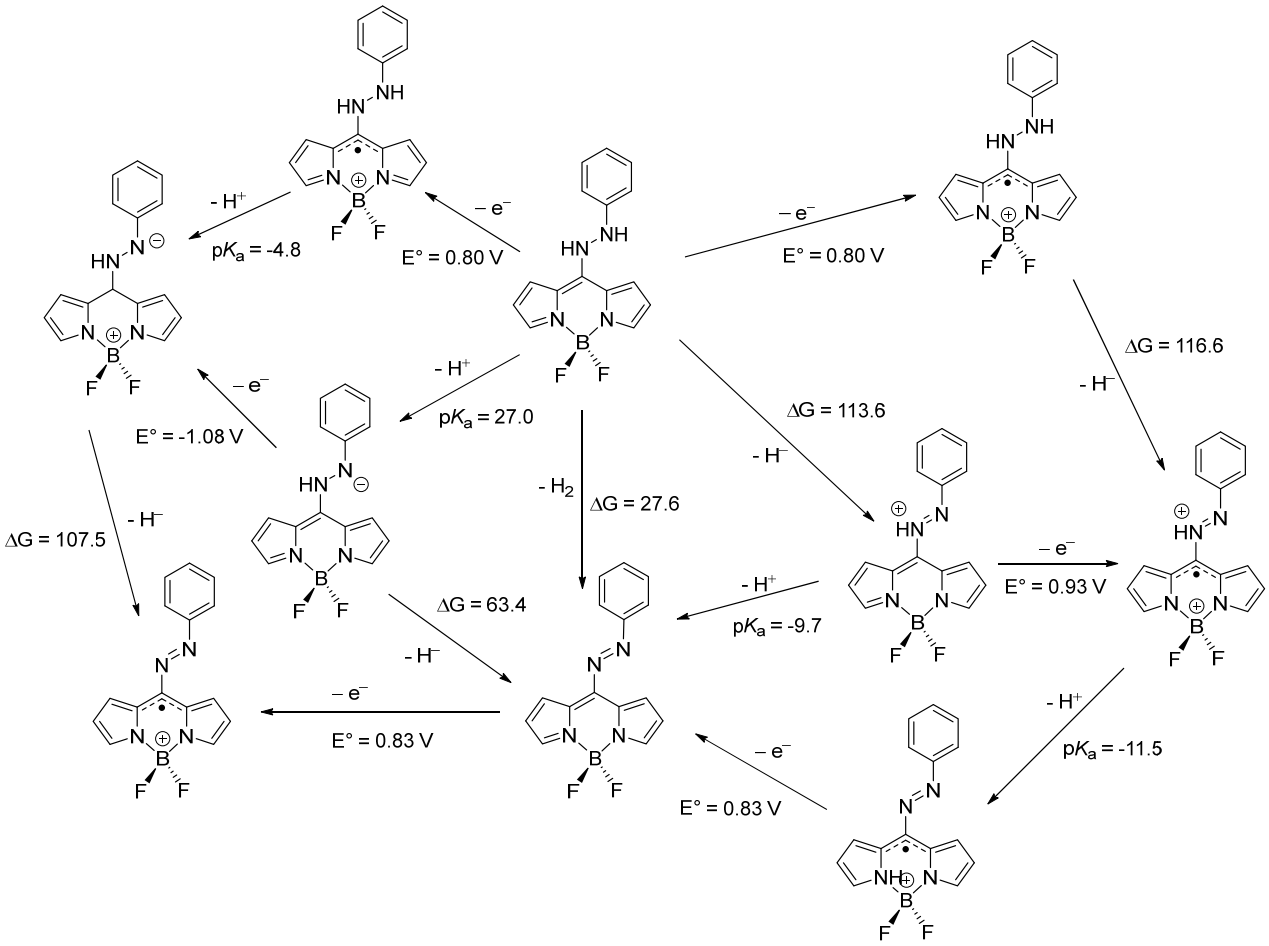


Figure S75. Summary of the influence of a oxidation on proton and hydride loss from the distal hydrogen of **BoNHNHPh** in MeCN.

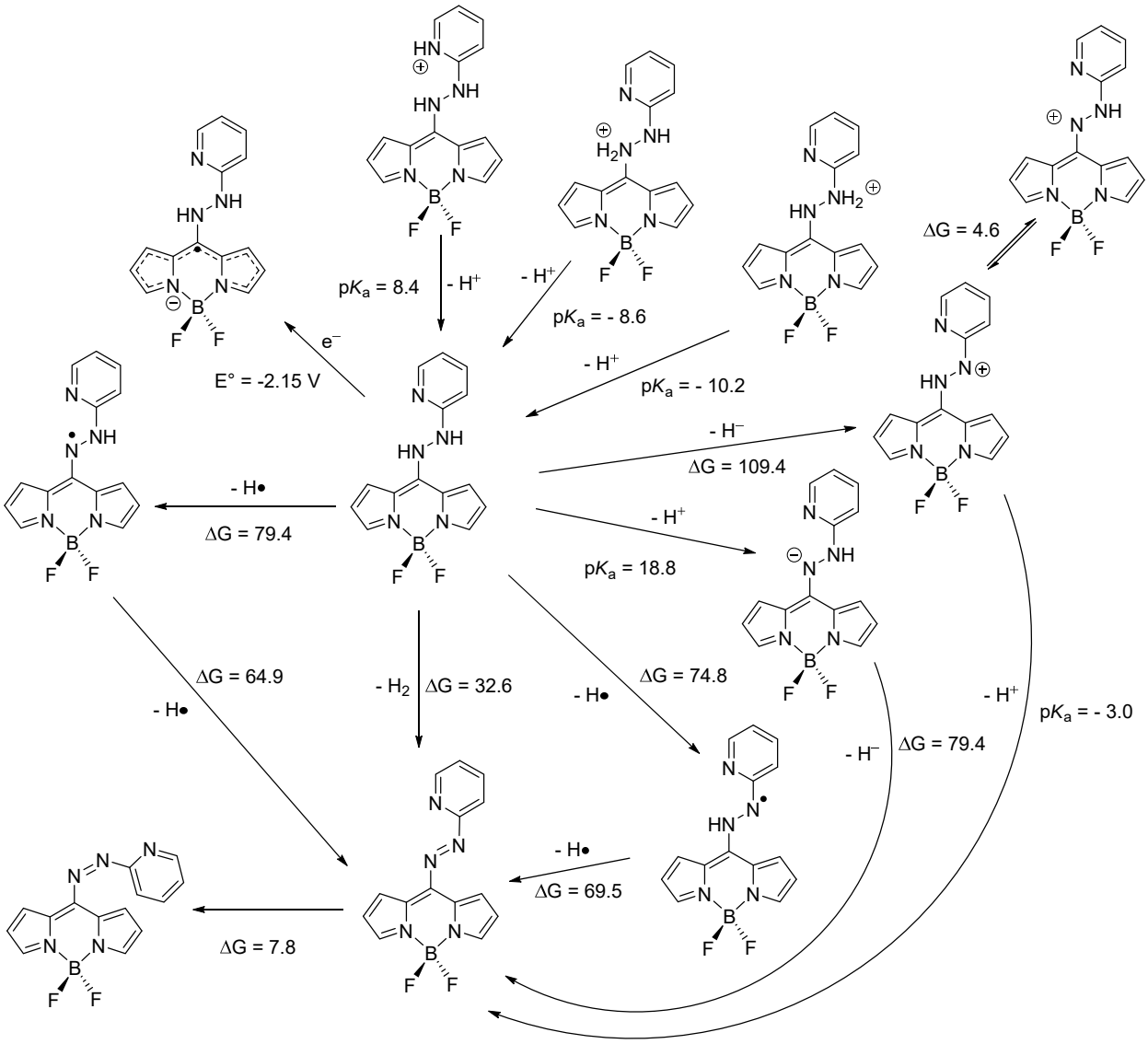


Figure S76. Summary of H_2, proton, hydride, and H-atom loss from **BoNHNHPy** in MeCN.

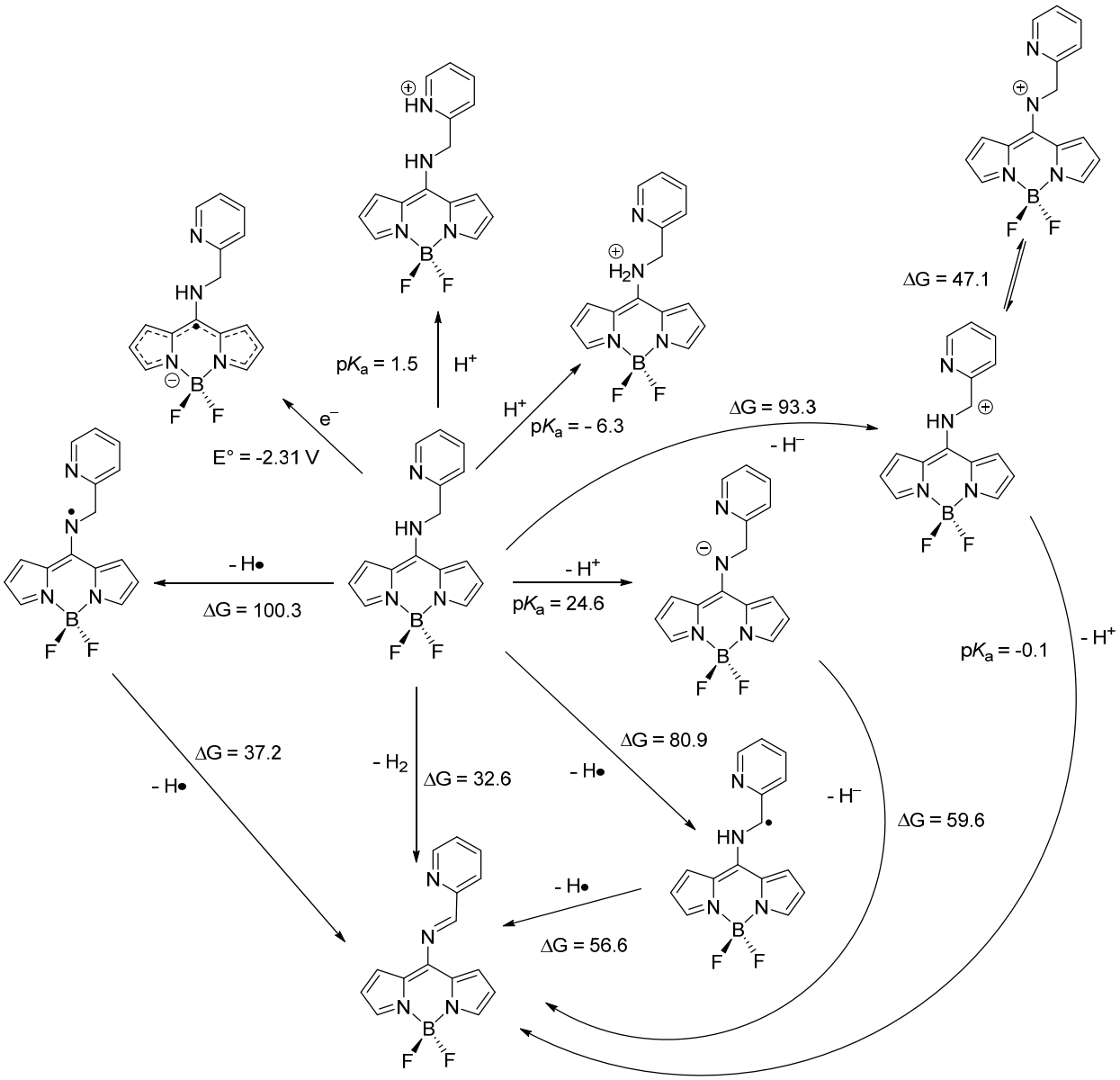


Figure S77. Summary of H_2, proton, hydride, and H-atom loss from **BoNHCH$_2$Py** in MeCN.

15) Gas Phase Energies for the Optimized Hydrazine and Aminomethyl Complexes

Table S5. Gas phase energies for the loss of H_2, protons, hydrides, and H-atoms from hydrazine.

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
NH_2NH_2	-111.8095737	0.031547	0.058316
$[NHNH_2]^+$	-110.8988394	0.0208	0.046583
$[NHNH_2]^-$	-111.119954	0.014154	0.040542
$[NHNH_2]$	-111.1724462	0.017229	0.044142
HN=NH	-110.5909706	0.007239	0.032645
$[HN=N]^+$	-109.6806301	-0.002732	0.020209
$[HN=N]^-$	-109.956392	-0.014615	0.011671
[HN=N]	-109.9820573	-0.008087	0.017381
N_2	-109.4874243	-0.012642	0.009101

Table S6. Gas phase energies for the loss of H_2, protons, hydrides, and H-atoms from phenylhydrazine (**$PhNHNH_2$**).

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
$PhNHNH_2$	-342.7769484	0.105456	0.144059
$[PhNNH_2]^+$	-341.9088263	0.094063	0.132273
$[PhNNH_2]^-$	-342.1682854	0.090398	0.128613
$[PhNH_2NH_2]^+$	-343.1286394	0.118833	0.158451
$[PhNHNH_3]^+$	-343.1249597	0.118561	0.158282
$[PhNNH_2]$	-342.1476054	0.091728	0.130403
$[PhNHNH]^+$	-341.8981985	0.094907	0.132681
$[PhNHNH]^-$	-342.1342436	0.087992	0.126977
[PhNHNH]	-342.1411533	0.091143	0.130189
trans-PhN=NH	-341.5579329	0.080894	0.118868
cis-PhN=NH	-341.5495079	0.080936	0.118439

Table S7. Gas phase energies for the loss of H_2, protons, hydrides, and H-atoms from pyridylhydrazine (**$PyNHNH_2$**).

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
$PyNHNH_2$	-358.8218602	0.093497	0.132281
$[PyHNHNH_2]^+$	-359.2106453	0.107834	0.146304
$[PyNH_2NH_2]^+$	-359.1691281	0.107027	0.146649
$[PyNHNH_3]^+$	-359.1498549	0.106611	0.146222
$[PyNNH_2]^+$	-357.9513756	0.083274	0.120476
$[PyNNH_2]^-$	-358.2213779	0.079004	0.117145
$[PyNNH_2]$	-358.1959916	0.0799	0.118505
$[PyNHNH]^+$	-357.9389278	0.0834	0.120755
$[PyNHNH]^-$	-358.1775731	0.077882	0.116367
[PyNHNH]	-358.1857332	0.080329	0.118789
trans-PyN=NH	-357.5886163	0.068632	0.106738
cis-PyN=NH	-357.5923395	0.069206	0.106748

Table S8. Gas phase energies for the loss of H_2, protons, hydrides, and H-atoms from **$BoNHNH_2$**.

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
$BoNHNH_2$	-791.7720461	0.149553	0.20333
$[BoNHNH_2]^+$	-791.4939492	0.147618	0.201986
$[BoNHNH_2]^-$	-791.8036172	0.144183	0.19998
$[BoNH_2NH_2]^+$	-792.0901866	0.162042	0.216874
$[BoNHNH_3]^+$	-792.0959366	0.163014	0.216889
$[BoNNH_2]^+$	-790.863992	0.138276	0.190493
$[BoNNH_2]^-$	-791.2490937	0.137913	0.189714
$[BoNNH_2]$	-791.143188	0.137025	0.189814
$[BoNHNH]^+$	-790.8503836	0.137529	0.190705
$[BoNHNH]^-$	-791.2100975	0.136206	0.188888
[BoNHNH]	-791.1324124	0.13608	0.189692
trans-BoN=NH	-790.5352602	0.12487	0.177599
cis-BoN=NH	-790.5302768	0.125121	0.177427

Table S9. Gas phase energies for the loss of H_2, protons, hydrides, and H-atoms from hydrazobenzene (**PhNHNHPh**).

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
PhNHNHPh	-573.7261876	0.178216	0.229606
$[PhNNHPh]^+$	-572.8881028	0.167476	0.218272
$[PhNNHPh]^-$	-573.1516463	0.163838	0.214137
[PhNNHPh]	-573.1142529	0.165482	0.216297
trans-PhN=NPh	-572.5255587	0.154967	0.204818
cis-PhN=NPh	-572.5048222	0.154611	0.204153

Table S10. Gas phase energies for the loss of H_2, protons, hydrides, and H-atoms from **BoNHNHBo**.

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
BoNHNHBo	-1471.725684	0.268793	0.348071
$[BoNNHBo]^+$	-1470.808028	0.256235	0.334883
$[BoNNHBo]^-$	-1471.239369	0.256725	0.334907
[BoNNHBo]	-1471.0937	0.255642	0.334673
trans-BoN=NBo	-1470.479837	0.242728	0.322304
cis-BoN=NBo	-1470.469422	0.243971	0.321834

Table S11. Gas phase energies for the loss of H_2, protons, hydrides, and H-atoms from **BoNHCH$_2$Ph**.

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
$BoNHCH_2Ph$	-1006.729514	0.235382	0.301377
$[BoNHCH_2Ph]^+$	-1006.451852	0.232759	0.299909
$[BoNHCH_2Ph]^-$	-1006.761479	0.229478	0.297316
$[BoNCH_2Ph]^{2+}$	-1005.370978	0.214714	0.283043
$[BoNCH_2Ph]^+$	-1005.788719	0.223763	0.287233
$[BoNCH_2Ph]$	-1006.064603	0.219215	0.28615
$[BoNCH_2Ph]^-$	-1006.196344	0.221512	0.286662
$[BoNCH_2Ph]^{2-}$	-1006.055551	0.214313	0.280625
$[BoNHCHPh]^{2+}$	-1005.465188	0.219145	0.287364
$[BoNHCHPh]^+$	-1005.863417	0.224525	0.289642
$[BoNHCHPh]$	-1006.090914	0.222348	0.287769
$[BoNHCHPh]^-$	-1006.164146	0.221681	0.286695
$[BoNHCHPh]^{2-}$	-1006.057907	0.213978	0.281558
trans-BoN=CHPh	-1005.509326	0.211488	0.276149
trans-$[BoN=CHPh]^+$	-1005.233576	0.209468	0.274843
trans-$[BoN=CHPh]^-$	-1005.577261	0.208918	0.273496
cis-BoN=CHPh	-1005.506166	0.211476	0.276399

Table S12. Gas phase energies for the loss of H_2, protons, hydrides, and H-atoms from **BoNHNHPh**.

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
BoNHNHPh	-1022.735243	0.224038	0.289025
$[BoNHNHPh]^+$	-1022.456816	0.220658	0.287493
$[BoNHNHPh]^-$	-1022.779965	0.219697	0.285983
$[BoNNHPh]^+$	-1021.844806	0.212556	0.276894
$[BoNNHPh]^-$	-1022.2193	0.211223	0.275124
[BoNNHPh]	-1022.110938	0.211182	0.275887
$[BoNHNPh]^+$	-1021.847053	0.210605	0.276554
$[BoNHNPh]^-$	-1022.198978	0.210807	0.274862
[BoNHNPh]	-1022.093352	0.210788	0.275302
trans-BoN=NPh	-1021.505092	0.198781	0.263499
trans-$[BoN=NPh]^+$	-1021.228369	0.196736	0.262058
trans-$[BoN=NPh]^-$	-1021.594462	0.195627	0.261454
cis-BoN=NPh	-1021.491136	0.198603	0.263113

Table S13. Gas phase energies for the loss of H_2, protons, hydrides, and H-atoms from **$BoNHCH_2Py$**.

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
$BoNHCH_2Py$	-1022.771016	0.224078	0.289301
$BoNHCH_2Py$ (Orient2)	-1022.764845	0.223497	0.289305
$[BoNHCH_2Py]^+$	-1022.49861	0.221773	0.287803
$[BoNHCH_2Py]^-$	-1022.799762	0.217159	0.285881
$[BoNH_2CH_2Py]^+$	-1023.115756	0.235979	0.302135
$[BoNHCH_2PyH]^+$	-1023.144055	0.240212	0.303034
$[BoNCH_2Py]^+$	-1021.796217	0.210315	0.273744
$[BoNCH_2Py]$	-1022.102407	0.207884	0.27425
$[BoNCH_2Py]^-$	-1022.234969	0.2101	0.274765
$[BoNHCHPy]^+$	-1021.903298	0.21344	0.277699
[BoNHCHPy]	-1022.136134	0.211465	0.276154
$[BoNHCHPy]^-$	-1022.215645	0.21111	0.275134
trans-BoN=CHPy	-1021.543208	0.199333	0.264083
cis-BoN=CHPy	-1021.541066	0.199766	0.264337

Table S14. Gas phase energies for the loss of H_2, protons, hydrides, and H-atoms from **BoNHNHPy**.

Complex	Electronic Energies Gas Phase (Hartrees)	Free Energy Correction Gas Phase (Hartrees)	Enthalpy Correction Gas Phase (Hartrees)
BoNHNHPy	-1038.77661	0.211916	0.276986
BoNHNHPy (Orient2)	-1038.778148	0.210951	0.277088
$[BoNHNHPy]^+$	-1038.503156	0.209347	0.2755
$[BoNHNHPy]^-$	-1038.815922	0.206899	0.274021
$[BoNH_2NHPy]^+$	-1039.11294	0.223381	0.2892
$[BoNHNH_2Py]^+$	-1039.115843	0.226554	0.290976
$[BoNHNHPyH]^+$	-1039.146027	0.225557	0.290741
$[BoNNHPy]^+$	-1037.886922	0.200763	0.264607
$[BoNNHPy]^-$	-1038.253329	0.19921	0.263118
[BoNNHPy]	-1038.143706	0.199233	0.263816
$[BoNHNPy]^+$	-1037.880777	0.200731	0.264603
$[BoNHNPy]^-$	-1038.25503	0.199507	0.263272
[BoNHNPy]	-1038.155542	0.199399	0.264003
trans-BoN=NPy	-1037.535904	0.186161	0.251427
cis-BoN=NPy	-1037.52585	0.187337	0.251161

16) 3D Coordinates of All Computed Structures

The 3D coordinates are organized so that they can be readily visualized in a Mercury. For each complex, the first number is the number of atoms, followed by the complex name, and the 3D coordinates.

6
N_2H_4

N	-0.70553	0.07551	-0.10124
N	0.70553	0.07550	0.10125
H	-1.13600	0.31287	0.78562
H	-1.05358	-0.84140	-0.37252
H	1.13600	0.31293	-0.78560
H	1.05358	-0.84143	0.37245

5
$[NHNH_2]^+$

N	0.53604	0.02955	0.00000
N	-0.67124	-0.15711	-0.00000
H	1.14080	-0.80513	0.00000
H	0.99192	0.95669	-0.00000
H	-1.18636	0.74136	0.00001

5
$[NHNH_2]^-$

N	0.65453	-0.12400	-0.00003
N	-0.80309	-0.11956	-0.00003
H	1.05024	0.40348	0.80288
H	1.05028	0.40388	-0.80267
H	-1.06058	0.89756	0.00021

5
[$NHNH_2$]

N	0.59343	0.02515	-0.07611
N	-0.73762	-0.15126	0.02610
H	1.12354	-0.80129	0.16245
H	1.02434	0.89334	0.22284
H	-1.13859	0.79068	-0.03525

4
HN=NH

N	0.58864	0.18966	-0.00000
N	-0.58864	-0.18966	-0.00000
H	1.16910	-0.66845	0.00000
H	-1.16908	0.66847	0.00000

3
$[HN=N]^+$

N	0.00000	0.00000	-0.65241
N	0.00000	0.00000	0.44072
H	0.00000	0.00000	1.48186

3
$[HN=N]^-$

N	0.13283	0.66609	0.00000
N	0.13283	-0.45389	0.00000
H	-1.85958	-1.48540	0.00000

3
[HN=N]

N	0.06272	0.65772	0.00000
N	0.06272	-0.51550	0.00000
H	-0.87805	-0.99555	0.00000

2
N_2

N	0.00000	0.00000	0.54938
N	0.00000	0.00000	-0.54938

16
$PhNHNH_2$

C	0.02710	1.05675	-0.08053
C	-1.33370	1.34790	-0.01854
C	-2.28028	0.33306	0.04974
C	-1.84763	-0.99366	0.05264
C	-0.49689	-1.29806	-0.00834
C	0.46041	-0.27365	-0.07534
N	1.81116	-0.60792	-0.17732
N	2.80428	0.31983	0.16779
H	0.74985	1.86245	-0.14447
H	-1.65079	2.38624	-0.02470
H	-3.33769	0.56722	0.09991
H	-2.57129	-1.80107	0.10709
H	-0.16715	-2.33369	-0.00639
H	2.04061	-1.52821	0.17102
H	2.94955	0.94652	-0.61813
H	2.50476	0.88313	0.96457

17
$[PhNH_2NH_2]^+$

C	-0.41544	1.28761	-0.02574
C	-1.78182	1.08577	0.15567
C	-2.30158	-0.20573	0.14940
C	-1.46677	-1.30818	-0.03560
C	-0.09995	-1.13054	-0.21916
C	0.38345	0.17067	-0.21133
N	1.83982	0.37467	-0.41354
N	2.61481	-0.39352	0.52676
H	-0.00088	2.29255	-0.02243
H	-2.43336	1.93921	0.30298
H	-3.36588	-0.35631	0.29163
H	-1.87894	-2.31069	-0.03665
H	0.57026	-1.97383	-0.35008
H	2.09955	0.03499	-1.34762
H	2.03352	1.38548	-0.39284
H	2.29023	-0.13902	1.45828
H	3.59581	-0.13803	0.42468

17
$[PhNHNH_3]^+$

C	-0.28011	1.22582	-0.21147
C	-1.63864	1.19893	0.08867
C	-2.29451	-0.02116	0.24249
C	-1.60097	-1.22200	0.09855
C	-0.23964	-1.20665	-0.18695
C	0.40521	0.02054	-0.34064
N	1.82295	0.08638	-0.62533
N	2.55876	0.01480	0.63112
H	0.24370	2.16248	-0.37672
H	-2.18778	2.12880	0.18432
H	-3.35580	-0.03755	0.46475
H	-2.11945	-2.16821	0.20436
H	0.30522	-2.14011	-0.31357
H	2.12597	-0.71998	-1.17178
H	2.29664	0.84571	1.17505
H	3.56794	0.06501	0.44701
H	2.34353	-0.81735	1.20220

15
$[PhNHNH]^+$

C	0.00692	1.14163	-0.00000
C	-1.36310	1.32990	0.00000
C	-2.22770	0.22734	0.00000

C	-1.73484	-1.07856	0.00000
C	-0.36555	-1.29291	-0.00000
C	0.47958	-0.17737	-0.00000
N	1.86296	-0.43554	0.00000
N	2.73582	0.44238	0.00001
H	0.70068	1.97478	-0.00001
H	-1.76675	2.33565	0.00000
H	-3.29997	0.39204	0.00000
H	-2.41496	-1.92190	0.00000
H	0.03743	-2.30283	-0.00000
H	2.11193	-1.43659	0.00001
H	3.66832	0.01069	-0.00000

15

[PhNNH$_2$]$^+$

C	-0.02147	1.12493	0.00000
C	1.33692	1.34273	0.00000
C	2.22747	0.25165	-0.00000
C	1.76808	-1.06393	-0.00000
C	0.40327	-1.30121	0.00000
C	-0.49496	-0.21192	0.00000
N	-1.80584	-0.60111	0.00001
N	-2.73880	0.23635	-0.00001
H	-0.69099	1.98011	0.00001
H	1.72537	2.35446	0.00000
H	3.29553	0.44516	-0.00001
H	2.46842	-1.89053	-0.00001
H	-0.00820	-2.30510	0.00000
H	-3.68644	-0.13416	-0.00000
H	-2.60718	1.24990	-0.00002

15

[PhNHNH]$^-$

C	-0.05998	1.07163	-0.00233
C	1.29468	1.34553	-0.00262
C	2.26104	0.32955	0.00439
C	1.81036	-0.99374	0.00116
C	0.45946	-1.29946	-0.00269
C	-0.52757	-0.27263	0.00538
N	-1.84449	-0.53685	0.03462
N	-2.87136	0.41590	-0.14371
H	-0.83411	1.83048	-0.02849
H	1.61790	2.38643	-0.01110
H	3.32192	0.56066	0.00829
H	2.53322	-1.80922	-0.00138
H	0.13184	-2.33859	-0.00837
H	-2.06776	-1.53022	-0.04703
H	-3.11996	0.66190	0.83197

15

[PhNNH$_2$]$^-$

C	0.08796	1.04199	0.05944
C	-1.26558	1.34486	0.01613
C	-2.25650	0.36375	-0.04140
C	-1.82640	-0.97853	-0.03193
C	-0.49446	-1.31607	0.01510
C	0.55686	-0.32453	0.04549
N	1.81362	-0.73226	0.02964
N	2.73451	0.38371	0.04311
H	0.81193	1.84327	0.16117
H	-1.56029	2.39593	0.03562
H	-3.31060	0.62077	-0.08204
H	-2.56826	-1.77798	-0.06114
H	-0.18228	-2.35805	0.01972
H	3.63014	-0.04603	-0.18163
H	2.53121	0.97312	-0.77787

15

[PhNHNH]

C	0.03129	1.09635	0.00000
C	-1.33771	1.32975	0.00000
C	-2.24771	0.27360	-0.00000
C	-1.77329	-1.03649	-0.00000
C	-0.40832	-1.29004	0.00000
C	0.49716	-0.22313	0.00000
N	1.86372	-0.49144	0.00000
N	2.76367	0.49076	-0.00001
H	0.75155	1.90480	0.00001
H	-1.69857	2.35349	0.00001
H	-3.31436	0.46897	-0.00001
H	-2.46956	-1.86893	-0.00000
H	-0.03942	-2.31278	0.00001
H	2.13481	-1.46802	0.00001
H	3.67532	0.02691	0.00000

15

[PhNNH$_2$]

C	0.06208	1.06418	-0.09146
C	-1.29742	1.34226	-0.02384
C	-2.23195	0.31268	0.06061
C	-1.79529	-1.01513	0.05844
C	-0.44485	-1.30686	-0.01432
C	0.51252	-0.27282	-0.07167
N	1.83106	-0.67099	-0.11373
N	2.71381	0.32167	0.06541
H	0.76766	1.87898	-0.21684
H	-1.63176	2.37479	-0.05104
H	-3.29121	0.54009	0.11350
H	-2.51754	-1.82349	0.11218
H	-0.08281	-2.32951	-0.01560
H	2.45825	1.08360	0.69008
H	3.65281	-0.02504	0.19939

14
trans-PhN=NH

C	0.07102	1.09812	0.00000
C	-1.29760	1.32648	0.00000
C	-2.19202	0.25337	-0.00001
C	-1.71695	-1.05449	-0.00000
C	-0.34503	-1.28988	0.00000
C	0.54231	-0.21741	0.00000
N	1.93298	-0.57257	0.00000
N	2.70553	0.39873	-0.00001
H	0.78606	1.91293	0.00001
H	-1.67476	2.34404	0.00001
H	-3.26086	0.44172	-0.00001
H	-2.41153	-1.88782	-0.00001
H	0.06275	-2.29542	0.00001
H	3.65836	0.00437	-0.00001

14
cis-PhN=NH

C	0.06650	1.09798	-0.14952
C	-1.30333	1.31301	-0.03577
C	-2.17210	0.23316	0.10256
C	-1.67512	-1.06957	0.10217
C	-0.31089	-1.29336	-0.03766
C	0.55801	-0.20802	-0.13231
N	1.95574	-0.50849	-0.26128
N	2.78053	0.23659	0.27914
H	0.74412	1.93483	-0.29345
H	-1.69402	2.32472	-0.06686
H	-3.23934	0.40604	0.19297
H	-2.35378	-1.91038	0.19877
H	0.10459	-2.29522	-0.06183
H	2.30604	1.00415	0.80857

15
$PyNHNH_2$

N	-0.12569	-1.00721	-0.04013
C	1.17115	-1.34020	-0.01255
C	2.21002	-0.42597	0.02148
C	1.87603	0.93336	0.02783
C	0.54951	1.30750	-0.00416
C	-0.42782	0.29093	-0.04133
N	-1.76676	0.62580	-0.10880
N	-2.75536	-0.34789	0.10460
H	1.37871	-2.40804	-0.01498
H	3.24052	-0.75831	0.04413
H	2.65260	1.69149	0.05725
H	0.25214	2.35114	-0.00774
H	-2.02221	1.52812	0.26378
H	-2.84599	-0.87289	-0.76216
H	-2.39443	-1.02017	0.78250

16
$[PyHNHNH_2]^+$

N	-0.06009	-0.94208	-0.00000
C	1.24047	-1.34558	0.00000
C	2.24040	-0.41805	0.00000
C	1.88471	0.94988	-0.00000
C	0.56866	1.34263	-0.00000
C	-0.43482	0.35207	0.00000
N	-1.75428	0.62080	0.00000
N	-2.65062	-0.44499	-0.00000
H	-0.82929	-1.61320	0.00000
H	1.40143	-2.41602	-0.00000
H	3.27503	-0.73317	0.00000
H	2.66315	1.70539	-0.00000
H	0.28385	2.38797	-0.00000
H	-2.06744	1.58332	0.00002
H	-3.23415	-0.41808	0.83181
H	-3.23414	-0.41808	-0.83181

16
$[PyNH_2NH_2]^+$

N	-0.00345	-1.05181	0.25643
C	-1.30020	-1.31271	0.07271
C	-2.23737	-0.30217	-0.14761
C	-1.81206	1.02054	-0.18445
C	-0.45800	1.30834	0.00197
C	0.35097	0.21185	0.21641
N	1.81855	0.36845	0.42536
N	2.53430	-0.25867	-0.65889
H	-1.59061	-2.35746	0.10526
H	-3.28113	-0.55541	-0.29012
H	-2.51718	1.82530	-0.35964
H	-0.07874	2.32417	-0.02790
H	2.04379	-0.02908	1.34926
H	2.06766	1.36280	0.42799
H	3.51331	-0.33427	-0.38668
H	2.13704	-1.19681	-0.73264

16
$[PyNHNH_3]^+$

C	-0.34210	1.24354	-0.18170
C	-1.69412	1.12964	0.11008
C	-2.24447	-0.14807	0.23726
N	-1.54636	-1.27619	0.08587
C	-0.25304	-1.16561	-0.19112
C	0.38794	0.06619	-0.32499

N	1.79887	0.14825	-0.61918
N	2.56289	-0.00774	0.61144
H	0.13800	2.20754	-0.32162
H	-2.31796	2.00807	0.22502
H	-3.29957	-0.26986	0.46471
H	0.29640	-2.09880	-0.33275
H	2.09442	-0.61229	-1.23178
H	3.56733	0.04699	0.40204
H	2.32806	0.78843	1.21654
H	2.36022	-0.87452	1.13371

14
[PyNNH$_2$]$^+$

N	-0.16572	-1.02078	0.00000
C	1.10890	-1.35539	0.00000
C	2.14279	-0.39010	-0.00000
C	1.82734	0.95838	-0.00000
C	0.47779	1.32454	0.00000
C	-0.44941	0.28800	0.00000
N	-1.80034	0.65415	0.00001
N	-2.61076	-0.28602	-0.00001
H	1.34142	-2.41584	0.00000
H	3.17564	-0.72047	-0.00001
H	2.60459	1.71383	-0.00000
H	0.14377	2.35622	0.00000
H	-3.60404	-0.05621	-0.00000
H	-2.26812	-1.26153	-0.00001

14
[PyNHNH]$^+$

N	-0.14207	-1.03403	0.00001
C	1.14880	-1.34372	-0.00001
C	2.15008	-0.35941	-0.00001
C	1.79157	0.98199	-0.00000
C	0.43560	1.32032	0.00000
C	-0.44177	0.25091	-0.00000
N	-1.86748	0.49375	-0.00000
N	-2.74554	-0.36496	0.00000
H	1.39663	-2.40003	0.00002
H	3.19260	-0.65589	-0.00000
H	2.54682	1.75965	0.00001
H	0.10008	2.35265	0.00001
H	-2.19238	1.46949	-0.00001
H	-2.26383	-1.28964	-0.00000

14
[PyNNH$_2$]$^-$

N	-0.17308	-1.02215	0.01807
C	1.11985	-1.32882	0.00001
C	2.18456	-0.43915	-0.01475
C	1.84091	0.93890	-0.01242
C	0.53302	1.32075	0.00226
C	-0.52714	0.32354	0.01483
N	-1.77132	0.73034	0.01313
N	-2.72248	-0.33887	0.09724
H	1.33782	-2.40361	-0.00078
H	3.21244	-0.78426	-0.01917
H	2.62467	1.69704	-0.02303
H	0.23436	2.36507	0.00362
H	-3.40498	-0.14544	-0.63450
H	-2.24336	-1.20539	-0.16480

14
[PyNHNH]$^-$

N	-0.10896	-1.08951	-0.00000
C	1.19784	-1.31437	0.00001
C	2.21322	-0.36154	-0.00001
C	1.79544	0.99588	0.00000
C	0.46594	1.30179	0.00000
C	-0.50942	0.23352	0.00001
N	-1.80851	0.49448	-0.00001
N	-2.91580	-0.32825	0.00001
H	1.47799	-2.37332	-0.00001
H	3.25840	-0.64736	0.00002
H	2.53194	1.79864	-0.00002
H	0.12252	2.33510	0.00001
H	-2.05044	1.47576	0.00002
H	-2.48561	-1.25753	-0.00002

14
[PyNNH$_2$]

N	-0.16856	-1.00669	-0.00489
C	1.12104	-1.33833	-0.00256
C	2.15982	-0.41360	0.00209
C	1.83047	0.94654	0.00236
C	0.50129	1.31693	-0.00062
C	-0.47938	0.30349	-0.00275
N	-1.79818	0.69598	-0.01158
N	-2.63808	-0.32095	0.04287
H	1.33800	-2.40455	-0.00522
H	3.19048	-0.74751	0.00460
H	2.60996	1.70186	0.00499
H	0.18040	2.35188	-0.00005
H	-3.60548	-0.10330	-0.12579
H	-2.27906	-1.26695	-0.05446

14
[PyNHNH]

N	-0.13123	-1.03991	-0.00000
C	1.17242	-1.32546	-0.00000
C	2.17662	-0.36678	0.00000
C	1.79477	0.97785	0.00000
C	0.45216	1.30256	-0.00000
C	-0.47642	0.24698	-0.00000
N	-1.83679	0.51727	0.00000
N	-2.82431	-0.37310	0.00000
H	1.42155	-2.38387	-0.00001
H	3.21909	-0.66004	0.00001
H	2.54285	1.76412	0.00000
H	0.11529	2.33418	-0.00001
H	-2.12929	1.48456	0.00000
H	-2.34037	-1.27964	-0.00001

13
trans-PyN=NH

N	-0.12224	-1.07669	-0.08023
C	1.18708	-1.30624	-0.02427
C	2.14889	-0.29771	0.05450
C	1.72262	1.02508	0.05757
C	0.35855	1.28187	-0.01724
C	-0.51055	0.19450	-0.06638
N	-1.91119	0.53228	-0.13625
N	-2.66605	-0.39662	0.18316
H	1.48969	-2.35054	-0.04693
H	3.20177	-0.55180	0.10148
H	2.43706	1.84008	0.10883
H	-0.04856	2.28608	-0.03422
H	-3.62314	-0.02159	0.07896

13
cis-PyN=NH

N	-0.17713	-1.02917	-0.00001
C	1.12003	-1.32478	-0.00000
C	2.12057	-0.35292	0.00001
C	1.74725	0.98697	0.00001
C	0.39299	1.30329	-0.00000
C	-0.51661	0.25281	-0.00001
N	-1.92826	0.61585	-0.00001
N	-2.75012	-0.30511	0.00001
H	1.37539	-2.38140	-0.00001
H	3.16365	-0.64750	0.00001
H	2.49778	1.77050	0.00002
H	0.02285	2.32181	-0.00001
H	-2.25660	-1.22666	0.00002

25
$BoNHNH_2$

C	-0.968048	2.995333	1.353916
C	-1.775308	1.868407	1.526882
N	-1.251120	0.827146	0.864541
C	-0.100109	1.245508	0.241732
C	0.095992	2.603158	0.540049
N	-0.732138	-1.482771	0.177769
B	-1.898618	-0.581706	0.703141
C	0.412001	-1.059693	-0.483553
C	0.709572	0.324364	-0.496994
C	-0.775350	-2.814806	0.128294
C	0.342759	-3.308633	-0.559891
C	1.091426	-2.206978	-0.951739
N	1.755543	0.857764	-1.152478
N	2.652865	0.099840	-1.893850
F	-2.907570	-0.533629	-0.233787
F	-2.344491	-1.047554	1.917311
H	-1.133705	3.971199	1.784545
H	-2.692389	1.749312	2.085863
H	0.928096	3.227224	0.240944
H	-1.602189	-3.345468	0.579787
H	0.570928	-4.348691	-0.737942
H	2.023360	-2.201216	-1.490477
H	1.835679	1.865816	-1.151738
H	3.595182	0.244976	-1.545694
H	2.605098	0.364509	-2.873030

26
$[BoNH_2NH_2]^+$

C	-3.31209	-0.56674	0.15132
C	-2.28833	-1.55337	0.24800
N	-1.09789	-1.00148	0.07177
C	-1.29013	0.35583	-0.15132
C	-2.69085	0.63193	-0.10084
N	1.37573	-0.61307	0.09146
B	0.29013	-1.76450	-0.06017
C	1.14487	0.73040	-0.14548
C	-0.17081	1.15066	-0.28784
C	2.67980	-0.77648	0.27836
C	3.35155	0.46984	0.17372
C	2.39184	1.42016	-0.09817
N	-0.37635	2.59192	-0.52116
N	-0.79394	3.26541	0.68706
F	0.38424	-2.29138	-1.31258
F	0.42229	-2.66200	0.94969
H	-4.36971	-0.74453	0.27391
H	-2.38049	-2.61612	0.43223
H	-3.15946	1.60342	-0.18577
H	3.08916	-1.75944	0.47187

H	4.41263	0.62704	0.29397
H	2.56659	2.48251	-0.22028
H	-1.13645	2.70165	-1.20401
H	0.48105	2.96994	-0.94896
H	-0.72868	4.27044	0.52900
H	-0.13215	2.99528	1.41450

26

[BoNHNH$_3$]$^+$

C	-3.28857	0.97633	-0.38205
C	-2.81264	-0.35957	-0.25087
N	-1.49266	-0.37152	-0.16679
C	-1.04710	0.94455	-0.21365
C	-2.18733	1.79684	-0.34268
N	0.86766	-1.15914	-0.08407
B	-0.59179	-1.58376	0.33276
C	1.27148	0.14745	-0.24993
C	0.31747	1.17780	-0.22456
C	1.93110	-1.94719	-0.24293
C	3.07372	-1.16764	-0.52255
C	2.66378	0.15601	-0.53374
N	0.82537	2.51040	-0.23672
N	1.66277	2.72986	0.91979
F	-0.95476	-2.73036	-0.29595
F	-0.67172	-1.62486	1.69799
H	-4.32120	1.26898	-0.49709
H	-3.37572	-1.28251	-0.19597
H	-2.19184	2.87440	-0.44539
H	1.83517	-3.02133	-0.16023
H	4.06257	-1.54732	-0.73021
H	3.25690	1.01202	-0.83470
H	0.08934	3.21317	-0.23384
H	1.14754	2.76906	1.81333
H	2.20830	3.58981	0.79017
H	2.31279	1.92491	0.96413

25

[BoNHNH$_2$]$^+$

C	3.03451	1.55329	-0.42974
C	2.82315	0.14015	-0.27298
N	1.54102	-0.10332	-0.06356
C	0.86311	1.10385	-0.06310
C	1.81085	2.15126	-0.29601
N	-0.61779	-1.25829	-0.11029
B	0.89019	-1.49435	0.29629
C	-1.29837	-0.04209	-0.07299
C	-0.55463	1.16575	0.07369
C	-1.49635	-2.21503	-0.34490
C	-2.81349	-1.65435	-0.48520
C	-2.69192	-0.30531	-0.30716
N	-1.11518	2.37062	0.25259
N	-2.49442	2.53916	0.31365
F	0.96934	-1.69684	1.63825
F	1.42848	-2.47484	-0.47207
H	3.98402	2.02603	-0.63277
H	3.54218	-0.66861	-0.30680
H	1.59716	3.20600	-0.39731
H	-1.18229	-3.25027	-0.39767
H	-3.71227	-2.21521	-0.69465
H	-3.46141	0.44629	-0.34488
H	-0.50485	3.16209	0.41835
H	-2.79220	3.19224	-0.40601
H	-2.75817	2.89596	1.22838

25

[BoNHNH$_2$]$^-$

C	-0.973426	3.021591	0.903876
C	-1.803049	1.938737	1.139487
N	-1.172028	0.789203	0.773539
C	0.076574	1.113784	0.292827
C	0.227072	2.508262	0.363527
N	-0.755192	-1.578509	0.168841
B	-1.744968	-0.647739	0.912149
C	0.508857	-1.239686	-0.274512
C	0.956795	0.101155	-0.183798
C	-0.936625	-2.908735	-0.050632
C	0.200264	-3.444191	-0.637852
C	1.125028	-2.389788	-0.782509
N	2.252584	0.456573	-0.648748
N	2.229217	0.747520	-2.062803
F	-3.014134	-0.717782	0.337481
F	-1.840547	-1.004242	2.259243
H	-1.212949	4.059587	1.091685
H	-2.806347	1.900792	1.539466
H	1.091452	3.074382	0.038461
H	-1.866293	-3.381630	0.233205
H	0.335386	-4.476571	-0.931926
H	2.114763	-2.416398	-1.214420
H	2.533112	1.288813	-0.129093
H	3.194303	0.899192	-2.344341
H	1.717618	1.619093	-2.219553

24

[BoNHNH]$^+$

C	-3.30720	0.86772	-0.25077
C	-2.77482	-0.45042	-0.21725
N	-1.45243	-0.40661	-0.08562
C	-1.07068	0.91418	-0.02601
C	-2.24351	1.72989	-0.12693
N	0.95559	-1.05681	-0.09820
B	-0.49059	-1.64291	0.17546
C	1.33067	0.28323	-0.02605

C	0.30087	1.21452	0.02804
C	2.05430	-1.78013	-0.24132
C	3.20295	-0.93544	-0.27042
C	2.75781	0.35414	-0.13045
N	0.55548	2.60580	0.11781
N	1.68058	3.10711	0.19030
F	-0.76501	-2.63698	-0.70671
F	-0.58518	-1.99619	1.48698
H	-4.34948	1.12546	-0.36137
H	-3.29075	-1.40000	-0.27787
H	-2.31483	2.81083	-0.13471
H	1.99583	-2.85897	-0.31200
H	4.22363	-1.26651	-0.38847
H	3.35513	1.25155	-0.11946
H	-0.29639	3.18632	0.13518
H	1.60464	4.13193	0.25589

24

[BoNNH$_2$]$^+$

C	-3.33135	0.79571	-0.39275
C	-2.76171	-0.51846	-0.25309
N	-1.44759	-0.44172	-0.12072
C	-1.10092	0.89494	-0.16734
C	-2.29884	1.68517	-0.32205
N	0.97520	-1.02911	-0.08127
B	-0.43605	-1.60898	0.30893
C	1.30431	0.31062	-0.11838
C	0.24668	1.24543	-0.08731
C	2.08686	-1.73797	-0.29242
C	3.18131	-0.87153	-0.49686
C	2.69606	0.41991	-0.39841
N	0.40804	2.61273	0.08164
N	1.46670	2.99943	0.61184
F	-0.70601	-2.72868	-0.40590
F	-0.52428	-1.74361	1.66142
H	-4.37963	1.00808	-0.54003
H	-3.26115	-1.48011	-0.24732
H	-2.33256	2.76108	-0.40960
H	2.05602	-2.81933	-0.29016
H	4.19389	-1.17189	-0.71902
H	3.25920	1.32166	-0.60269
H	1.58460	4.00444	0.74546
H	2.18166	2.33949	0.95015

24

[BoNHNH]$^-$

C	3.24047	1.11710	-0.28451
C	2.83461	-0.19665	-0.15634
N	1.48100	-0.24103	-0.02142
C	1.00024	1.03824	-0.06444
C	2.06907	1.91262	-0.23621
N	-0.83252	-1.11839	-0.10021
B	0.63253	-1.52658	0.18818
C	-1.34675	0.16108	-0.07678
C	-0.43511	1.27033	0.04293
C	-1.86930	-1.98245	-0.24140
C	-3.05762	-1.27639	-0.31315
C	-2.73180	0.09526	-0.20585
N	-0.85071	2.50901	0.21158
N	-2.11075	2.94934	0.22015
F	0.76933	-1.98723	1.49633
F	1.04679	-2.51738	-0.69732
H	4.25527	1.46377	-0.42316
H	3.40540	-1.11368	-0.16123
H	2.01556	2.98660	-0.36552
H	-1.68033	-3.04620	-0.27628
H	-4.04398	-1.70229	-0.43778
H	-3.38016	0.95552	-0.22909
H	-0.08281	3.16736	0.33391
H	-2.02864	3.93600	0.47085

24

[BoNNH$_2$]$^-$

C	3.21772	1.18363	-0.43554
C	2.84482	-0.13645	-0.25686
N	1.49892	-0.20170	-0.07263
C	0.99446	1.07171	-0.12733
C	2.03554	1.95765	-0.35153
N	-0.78830	-1.11305	-0.04442
B	0.68718	-1.45951	0.30397
C	-1.32919	0.14792	-0.12142
C	-0.44720	1.31514	0.02894
C	-1.76359	-2.02020	-0.29063
C	-2.95530	-1.36352	-0.53873
C	-2.68550	0.01932	-0.43098
N	-0.81161	2.52799	0.27231
N	-2.17951	2.77275	0.39693
F	0.81071	-1.74572	1.66207
F	1.09973	-2.55608	-0.44665
H	4.22111	1.54295	-0.62081
H	3.43472	-1.04178	-0.24996
H	1.92570	3.02732	-0.45504
H	-1.52974	-3.07509	-0.27796
H	-3.90314	-1.82409	-0.78083
H	-3.36750	0.83071	-0.63595
H	-2.26541	3.60308	0.97292
H	-2.65282	1.99739	0.86810

24

[BoNHNH]

C	3.22778	1.12954	-0.21728
C	2.81591	-0.20735	-0.16941

N	1.48198	-0.26986	-0.05557
C	0.99079	1.01310	-0.02283
C	2.07506	1.90611	-0.12536
N	-0.84187	-1.11731	-0.08299
B	0.63968	-1.57203	0.14538
C	-1.33391	0.17994	-0.02642
C	-0.41389	1.24129	0.03586
C	-1.87731	-1.94708	-0.20434
C	-3.08153	-1.22055	-0.23522
C	-2.74652	0.11876	-0.11946
N	-0.80359	2.54725	0.12596
N	-2.06609	2.93673	0.14800
F	0.79189	-2.03341	1.43270
F	0.99302	-2.51623	-0.78768
H	4.24340	1.48027	-0.31938
H	3.40085	-1.11514	-0.21039
H	2.03785	2.98729	-0.16050
H	-1.71231	-3.01451	-0.25845
H	-4.07127	-1.63915	-0.33716
H	-3.40462	0.97132	-0.11551
H	-0.04648	3.22045	0.19497
H	-2.04136	3.95606	0.23331

24

[$BoNNH_2$]

C	3.25286	1.06450	-0.36122
C	2.80682	-0.27141	-0.25059
N	1.47643	-0.30105	-0.11700
C	1.02049	0.99578	-0.12704
C	2.13082	1.86772	-0.27124
N	-0.86328	-1.09101	-0.03805
B	0.59690	-1.54601	0.26823
C	-1.31900	0.20854	-0.08769
C	-0.36260	1.28052	-0.02405
C	-1.90281	-1.91662	-0.25069
C	-3.06291	-1.17327	-0.45746
C	-2.70029	0.17359	-0.36097
N	-0.64778	2.58765	0.12457
N	-1.88224	2.88641	0.45335
F	0.75367	-1.80678	1.61076
F	0.93500	-2.62159	-0.51598
H	4.27667	1.37745	-0.49994
H	3.37424	-1.19190	-0.25571
H	2.06643	2.94381	-0.32778
H	-1.75270	-2.98672	-0.24850
H	-4.04440	-1.56783	-0.67230
H	-3.34354	1.01896	-0.55833
H	-2.03774	3.85839	0.67580
H	-2.48358	2.18310	0.87822

23

trans-BoN=NH

C	-3.30032	0.86494	-0.21211
C	-2.76905	-0.43904	-0.11592
N	-1.43899	-0.39164	-0.04168
C	-1.06008	0.93775	-0.08585
C	-2.22459	1.73557	-0.19405
N	0.96608	-1.01153	-0.07903
B	-0.46860	-1.60684	0.17012
C	1.30663	0.33432	-0.08334
C	0.29049	1.29180	-0.05821
C	2.08847	-1.71869	-0.18628
C	3.20350	-0.85765	-0.27704
C	2.71541	0.43422	-0.21606
N	0.54873	2.69172	-0.10699
N	1.52400	3.05293	0.56766
F	-0.73222	-2.59170	-0.74809
F	-0.56349	-2.05865	1.46375
H	-4.34694	1.11419	-0.29880
H	-3.28275	-1.39080	-0.10324
H	-2.23264	2.81252	-0.27371
H	2.05283	-2.79983	-0.19357
H	4.23224	-1.16627	-0.38387
H	3.27345	1.35613	-0.26534
H	1.60669	4.07189	0.42038

23

cis-BoN=NH

C	-1.016707	3.063544	1.015884
C	-1.721290	1.901546	1.403308
N	-1.155054	0.819047	0.873880
C	-0.063044	1.236471	0.130217
C	0.031095	2.646957	0.215588
N	-0.740977	-1.504155	0.087696
B	-1.534591	-0.678017	1.168548
C	0.349351	-1.047872	-0.631418
C	0.702334	0.305989	-0.566181
C	-0.916685	-2.792119	-0.206804
C	0.050497	-3.216188	-1.141015
C	0.848299	-2.118478	-1.416180
N	1.819185	0.791031	-1.298800
N	2.902402	0.203266	-1.191101
F	-2.881595	-0.868803	1.006048
F	-1.097615	-1.025157	2.423194
H	-1.272802	4.075744	1.289444
H	-2.598276	1.808088	2.029637
H	0.771681	3.250390	-0.288932
H	-1.717825	-3.352763	0.255478
H	0.127833	-4.205250	-1.565971
H	1.664024	-2.057439	-2.123274
H	2.835706	-0.584656	-0.509545

26
PhNHNHPh

N	-0.43300	0.57003	-0.03700
N	0.43300	-0.57003	0.03699
C	1.81076	-0.23359	-0.01003
C	-1.81076	0.23359	0.01002
C	-2.72304	1.29659	-0.01260
C	-4.08652	1.04922	-0.00980
C	-4.56751	-0.26129	-0.00634
C	-3.66250	-1.31410	0.00916
C	-2.28767	-1.07777	0.02525
C	2.72304	-1.29659	0.01259
C	4.08652	-1.04922	0.00980
C	4.56751	0.26129	0.00635
C	3.66249	1.31410	-0.00915
C	2.28767	1.07777	-0.02526
H	-0.20937	1.14948	0.76994
H	0.20937	-1.14948	-0.76995
H	-2.34335	2.31372	-0.04716
H	-4.78022	1.88388	-0.02372
H	-5.63471	-0.45382	-0.01619
H	-4.02156	-2.33847	0.02197
H	-1.59728	-1.90994	0.08821
H	2.34335	-2.31372	0.04715
H	4.78022	-1.88388	0.02372
H	5.63471	0.45382	0.01621
H	4.02156	2.33847	-0.02196
H	1.59728	1.90994	-0.08821

25
[PhNNHPh]$^{+}$

N	0.44384	0.48234	-0.00000
N	-0.42301	-0.41954	-0.00000
C	-1.81514	-0.16798	-0.00000
C	1.79085	0.16433	0.00000
C	2.62964	1.29221	-0.00001
C	4.00682	1.12717	-0.00001
C	4.54158	-0.15848	0.00000
C	3.70724	-1.28724	0.00001
C	2.33541	-1.13832	0.00001
C	-2.65449	-1.28283	-0.00001
C	-4.02794	-1.08119	-0.00001
C	-4.53756	0.21594	0.00000
C	-3.67866	1.31916	0.00001
C	-2.30465	1.14022	0.00001
H	-0.15338	-1.41025	-0.00001
H	2.17058	2.27478	-0.00002
H	4.65882	1.99263	-0.00002
H	5.61798	-0.29426	0.00000
H	4.14211	-2.28003	0.00002
H	1.71833	-2.03246	0.00002
H	-2.24421	-2.28943	-0.00002
H	-4.69713	-1.93352	-0.00002
H	-5.61077	0.37135	0.00000
H	-4.08618	2.32356	0.00002
H	-1.62050	1.98015	0.00002

25
[PhNNHPh]$^{-}$

N	0.46651	0.63786	0.38169
N	-0.42272	-0.44279	0.25764
C	-1.75360	-0.20640	0.13005
C	1.72795	0.27308	0.13452
C	2.75567	1.25988	0.31792
C	4.09016	0.97215	0.14219
C	4.52688	-0.31081	-0.23438
C	3.54989	-1.28205	-0.43996
C	2.19547	-1.02181	-0.26968
C	-2.69933	-1.23737	0.34206
C	-4.05281	-1.01077	0.15256
C	-4.52802	0.24187	-0.24214
C	-3.59820	1.26558	-0.43945
C	-2.23858	1.06395	-0.25939
H	-0.17591	-1.28748	0.77006
H	2.43181	2.25386	0.61521
H	4.82270	1.76314	0.30087
H	5.58127	-0.53158	-0.36675
H	3.84912	-2.28213	-0.75469
H	1.47476	-1.80000	-0.49859
H	-2.34701	-2.21818	0.65473
H	-4.75187	-1.82715	0.32161
H	-5.58972	0.41509	-0.38553
H	-3.94446	2.25269	-0.73938
H	-1.51017	1.85249	-0.39858

25
[PhNNHPh]

N	0.44550	0.61647	0.01409
N	-0.41131	-0.39232	0.08021
C	-1.78780	-0.17641	0.04319
C	1.77538	0.24915	-0.01688
C	2.70349	1.27809	0.24272
C	4.06209	1.01746	0.25571
C	4.53792	-0.27096	-0.00273
C	3.63252	-1.28939	-0.28871
C	2.26499	-1.04270	-0.30170
C	-2.64610	-1.25678	0.27396
C	-4.02070	-1.06766	0.22739
C	-4.55067	0.19145	-0.04623
C	-3.68726	1.26167	-0.27488
C	-2.30953	1.09126	-0.23535
H	-0.09117	-1.31542	0.36083

H	2.31346	2.26977	0.44538
H	4.76009	1.82097	0.46802
H	5.60337	-0.47339	0.00481
H	3.99465	-2.28624	-0.52022
H	1.58978	-1.84146	-0.59303
H	-2.23305	-2.23893	0.48921
H	-4.68041	-1.91008	0.40803
H	-5.62470	0.33668	-0.08143
H	-4.09144	2.24592	-0.48920
H	-1.62600	1.91211	-0.41146

24

trans-PhN=NPh

N	0.37519	0.49709	0.00000
N	-0.37519	-0.49709	-0.00001
C	-1.76536	-0.18495	-0.00000
C	1.76536	0.18495	0.00000
C	2.62331	1.28372	-0.00002
C	4.00111	1.09116	-0.00002
C	4.51820	-0.20096	-0.00000
C	3.65656	-1.30048	0.00002
C	2.28177	-1.11553	0.00002
C	-2.62331	-1.28372	-0.00002
C	-4.00111	-1.09116	-0.00002
C	-4.51820	0.20096	0.00000
C	-3.65656	1.30048	0.00002
C	-2.28177	1.11553	0.00002
H	2.18585	2.27666	-0.00003
H	4.66862	1.94640	-0.00003
H	5.59236	-0.35576	-0.00000
H	4.06449	-2.30619	0.00003
H	1.59423	-1.95314	0.00003
H	-2.18585	-2.27666	-0.00003
H	-4.66862	-1.94640	-0.00003
H	-5.59236	0.35576	0.00000
H	-4.06449	2.30619	0.00003
H	-1.59423	1.95314	0.00003

24

cis-PhN=NPh

N	0.61967	1.98994	-0.00697
N	-0.61967	1.98994	0.00696
C	-1.39697	0.78269	0.09419
C	1.39697	0.78269	-0.09419
C	1.18479	-0.17938	-1.08385
C	2.05704	-1.25683	-1.18499
C	3.12582	-1.38502	-0.29958
C	3.34085	-0.41298	0.67470
C	2.49353	0.68621	0.76123
C	-2.49352	0.68620	-0.76125
C	-3.34084	-0.41299	-0.67471
C	-3.12582	-1.38501	0.29959
C	-2.05705	-1.25680	1.18501
C	-1.18481	-0.17936	1.08387
H	0.34641	-0.07766	-1.76506
H	1.89900	-2.00222	-1.95753
H	3.79767	-2.23309	-0.37937
H	4.18128	-0.50027	1.35539
H	2.66171	1.47539	1.48692
H	-2.66169	1.47537	-1.48695
H	-4.18126	-0.50030	-1.35540
H	-3.79767	-2.23308	0.37938
H	-1.89902	-2.00219	1.95757
H	-0.34643	-0.07762	1.76508

44

BoNHNHBo

C	-4.09430	2.72757	1.05274
C	-4.71779	1.73089	0.29172
N	-3.90123	0.67892	0.16088
C	-2.73306	0.95341	0.83265
C	-2.83680	2.23870	1.39853
N	-2.84659	-1.36513	-0.73434
B	-4.24578	-0.69329	-0.50045
C	-1.67777	-1.10106	-0.03547
C	-1.64621	0.03676	0.79871
C	-2.64017	-2.42515	-1.51312
C	-1.32328	-2.88928	-1.35835
C	-0.71275	-2.06405	-0.42753
N	-0.58522	0.34686	1.58636
N	0.58521	-0.34686	1.58637
F	-4.88034	-0.50211	-1.70119
F	-4.98303	-1.46134	0.36988
C	1.32329	2.88929	-1.35834
C	2.64017	2.42514	-1.51312
N	2.84659	1.36513	-0.73434
C	1.67777	1.10106	-0.03547
C	0.71275	2.06405	-0.42753
N	3.90123	-0.67892	0.16089
B	4.24578	0.69329	-0.50045
C	2.73306	-0.95341	0.83265
C	1.64621	-0.03676	0.79871
C	4.71778	-1.73089	0.29173
C	4.09429	-2.72757	1.05274
C	2.83680	-2.23870	1.39853
F	4.88034	0.50210	-1.70120
F	4.98304	1.46134	0.36986
H	-4.51018	3.69131	1.30383
H	-5.69764	1.71796	-0.16409
H	-2.08125	2.77008	1.96316
H	-3.43874	-2.80240	-2.13693
H	-0.87519	-3.72034	-1.88125

H	0.31554	-2.13218	-0.10696
H	-0.62785	1.16678	2.17665
H	0.62784	-1.16677	2.17666
H	0.87519	3.72035	-1.88125
H	3.43874	2.80239	-2.13693
H	-0.31554	2.13219	-0.10695
H	5.69764	-1.71796	-0.16408
H	4.51017	-3.69131	1.30383
H	2.08124	-2.77008	1.96316

43

[BoNNHBo]$^{+}$

C	3.15006	-3.30293	0.76003
C	4.25070	-2.40971	0.66261
N	3.82146	-1.18260	0.38413
C	2.44744	-1.21999	0.29471
C	2.01318	-2.56110	0.53503
N	3.75672	1.20121	-0.33497
B	4.69015	0.14410	0.38088
C	2.36977	1.14854	-0.42004
C	1.75933	-0.05248	-0.06886
C	4.15302	2.37113	-0.81544
C	3.03151	3.13349	-1.24158
C	1.91282	2.37386	-0.99415
N	0.36153	-0.21808	-0.09029
N	-0.46165	0.70926	-0.24764
F	5.82299	-0.04379	-0.34642
F	4.90030	0.53079	1.67108
C	-2.65617	-2.97086	-1.53246
C	-3.82857	-2.45537	-0.94432
N	-3.58209	-1.25930	-0.40404
C	-2.25047	-0.96094	-0.60310
C	-1.65882	-2.03168	-1.33164
N	-3.99450	1.08266	0.34270
B	-4.59478	-0.39522	0.43883
C	-2.65450	1.35960	0.14085
C	-1.80168	0.33355	-0.25545
C	-4.59108	2.21454	0.68093
C	-3.64320	3.29182	0.71054
C	-2.42648	2.75820	0.38865
F	-5.82839	-0.42698	-0.12614
F	-4.54874	-0.77496	1.74735
H	3.21214	-4.36070	0.96528
H	5.30755	-2.60788	0.78477
H	1.00035	-2.94613	0.52662
H	5.20473	2.62556	-0.84017
H	3.07120	4.11620	-1.68630
H	0.88913	2.62958	-1.21638
H	0.00684	-1.17271	0.08207
H	-2.57305	-3.90582	-2.06520
H	-4.81944	-2.88598	-0.89170
H	-0.65737	-2.07425	-1.74236
H	-5.65339	2.23581	0.89185
H	-3.87561	4.32171	0.93586
H	-1.47671	3.26458	0.29720

43

[BoNNHBo]$^{-}$

C	3.42550	-3.27822	0.49578
C	4.44628	-2.34581	0.34586
N	3.92030	-1.11028	0.22548
C	2.55490	-1.21751	0.29742
C	2.21792	-2.56369	0.46661
N	3.68795	1.30416	-0.24533
B	4.73099	0.21554	0.14386
C	2.30943	1.20923	-0.17491
C	1.72049	-0.05023	0.14239
C	3.99890	2.55696	-0.61263
C	2.83474	3.30451	-0.79375
C	1.76044	2.45481	-0.51743
N	0.41452	-0.23574	0.25292
N	-0.51786	0.75748	0.21913
F	5.70807	0.12009	-0.83040
F	5.29533	0.50803	1.37339
C	-2.40930	-3.08877	-1.18987
C	-3.63351	-2.59683	-0.76254
N	-3.47693	-1.35073	-0.26999
C	-2.14994	-1.00595	-0.35507
C	-1.46092	-2.08128	-0.93949
N	-4.11049	0.99260	0.13924
B	-4.62911	-0.45855	0.28893
C	-2.78550	1.35235	0.12537
C	-1.74261	0.34931	0.00956
C	-4.85117	2.12010	0.23637
C	-4.01166	3.22580	0.27732
C	-2.69326	2.73725	0.21472
F	-5.77239	-0.65424	-0.46825
F	-4.86703	-0.75928	1.62128
H	3.54543	-4.34589	0.60542
H	5.51783	-2.48148	0.31799
H	1.22221	-2.98270	0.54135
H	5.03529	2.84338	-0.72475
H	2.78361	4.33964	-1.09771
H	0.70603	2.67232	-0.56054
H	0.08447	-1.17258	0.47927
H	-2.22689	-4.05061	-1.64628
H	-4.61634	-3.04480	-0.78613
H	-0.42037	-2.10557	-1.23376
H	-5.92910	2.05599	0.27577
H	-4.32175	4.25934	0.33625
H	-1.77223	3.30198	0.22053

43
[BoNNHBo]

C	3.34397	-3.29410	0.59171
C	4.39497	-2.36967	0.47978
N	3.90434	-1.14063	0.28586
C	2.53146	-1.22420	0.27092
C	2.16271	-2.57449	0.46357
N	3.72124	1.26416	-0.27540
B	4.73117	0.19043	0.26287
C	2.33685	1.16882	-0.29618
C	1.75076	-0.06893	0.01633
C	4.05792	2.48574	-0.68435
C	2.90326	3.23130	-0.99197
C	1.81777	2.40783	-0.74872
N	0.39602	-0.26389	0.03784
N	-0.48449	0.70638	-0.05667
F	5.79400	0.07545	-0.59650
F	5.12007	0.51593	1.53937
C	-2.58661	-3.08633	-1.26644
C	-3.77996	-2.54848	-0.78478
N	-3.56291	-1.31447	-0.30070
C	-2.22452	-1.01866	-0.44152
C	-1.59829	-2.12182	-1.06051
N	-4.05187	1.05478	0.21928
B	-4.64989	-0.39970	0.34675
C	-2.70897	1.33497	0.12225
C	-1.77239	0.30736	-0.12877
C	-4.69504	2.20311	0.44016
C	-3.77258	3.27848	0.48504
C	-2.51927	2.73409	0.29936
F	-5.82362	-0.48524	-0.35618
F	-4.80514	-0.69546	1.67914
H	3.44627	-4.35790	0.74197
H	5.46311	-2.52716	0.53257
H	1.16117	-2.98578	0.49014
H	5.09951	2.77127	-0.74019
H	2.88426	4.24650	-1.35808
H	0.77363	2.63103	-0.89263
H	0.06057	-1.20305	0.25574
H	-2.46331	-4.05250	-1.73137
H	-4.77471	-2.97025	-0.76570
H	-0.57385	-2.18485	-1.40289
H	-5.76964	2.21174	0.56290
H	-4.02459	4.31779	0.63135
H	-1.56519	3.23890	0.26888

42
trans-BoN=NBo

C	3.40129	-3.14351	-1.23443
C	4.43817	-2.21487	-0.98469
N	3.93397	-1.07394	-0.51743
C	2.56125	-1.21556	-0.44713
C	2.21659	-2.51710	-0.89841
N	3.68318	1.15702	0.54224
B	4.71921	0.25364	-0.22090
C	2.30372	0.99388	0.57194
C	1.75824	-0.18465	0.04672
C	3.97830	2.29245	1.17125
C	2.80060	2.90940	1.64434
C	1.74653	2.09592	1.27250
N	0.37568	-0.49667	0.02481
N	-0.37571	0.49675	0.02496
F	5.07555	0.85282	-1.40362
F	5.79871	-0.00342	0.58469
C	-3.40141	3.14350	-1.23442
C	-4.43824	2.21481	-0.98471
N	-3.93400	1.07391	-0.51743
C	-2.56129	1.21560	-0.44708
C	-2.21668	2.51715	-0.89835
N	-3.68315	-1.15703	0.54227
B	-4.71919	-0.25370	-0.22092
C	-2.30370	-0.99382	0.57200
C	-1.75825	0.18472	0.04679
C	-3.97823	-2.29247	1.17130
C	-2.80050	-2.90935	1.64442
C	-1.74646	-2.09582	1.27259
F	-5.79873	0.00332	0.58464
F	-5.07547	-0.85292	-1.40363
H	3.53253	-4.14866	-1.60513
H	5.50593	-2.32600	-1.11806
H	1.21201	-2.91203	-0.93736
H	5.00702	2.61535	1.25817
H	2.75082	3.83359	2.19967
H	0.69749	2.24207	1.47583
H	-3.53268	4.14864	-1.60513
H	-5.50601	2.32589	-1.11812
H	-1.21212	2.91214	-0.93726
H	-5.00693	-2.61541	1.25820
H	-2.75068	-3.83353	2.19977
H	-0.69742	-2.24191	1.47595

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cis-BoN=NBo

C	4.35030	-1.60631	1.37652
C	4.41187	-0.90416	0.15562
N	3.33155	-0.13499	0.01144
C	2.53362	-0.31428	1.12437
C	3.16429	-1.23608	1.99110
N	1.77751	1.64488	-0.74737
B	2.93653	0.70578	-1.25455
C	0.98294	1.41559	0.36688

C	1.33554	0.39845	1.25241
C	1.28552	2.70016	-1.38848
C	0.16075	3.21237	-0.70174
C	-0.03161	2.40806	0.40352
N	0.59885	0.15438	2.44651
N	-0.59885	-0.15442	2.44651
F	2.45981	-0.12842	-2.23339
F	3.99922	1.46352	-1.67283
C	-0.16076	-3.21237	-0.70178
C	-1.28552	-2.70014	-1.38852
N	-1.77751	-1.64487	-0.74740
C	-0.98294	-1.41560	0.36686
C	0.03161	-2.40807	0.40349
N	-3.33155	0.13499	0.01143
B	-2.93651	-0.70575	-1.25457
C	-2.53362	0.31426	1.12437
C	-1.33555	-0.39847	1.25241
C	-4.41188	0.90415	0.15563
C	-4.35032	1.60627	1.37655
C	-3.16430	1.23604	1.99112
F	-2.45978	0.12848	-2.23338
F	-3.99920	-1.46347	-1.67289
H	5.10324	-2.28041	1.75564
H	5.17753	-0.91749	-0.60797
H	2.79063	-1.53852	2.95936
H	1.74466	3.04410	-2.30548
H	-0.42115	4.07220	-0.99582
H	-0.78813	2.51026	1.16832
H	0.42113	-4.07220	-0.99587
H	-1.74466	-3.04406	-2.30553
H	0.78812	-2.51028	1.16828
H	-5.17754	0.91749	-0.60796
H	-5.10327	2.28035	1.75568
H	-2.79064	1.53847	2.95939

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BoNHCH$_2$Ph

C	-1.80656	3.35311	-0.67866
C	-2.87476	2.53519	-0.30254
N	-2.44512	1.27615	-0.13121
C	-1.09357	1.24426	-0.37848
C	-0.67436	2.53727	-0.72503
N	-2.43057	-1.17775	0.07198
B	-3.26824	0.08951	0.45350
C	-1.07160	-1.21814	-0.17777
C	-0.36641	0.01210	-0.31768
C	-2.90313	-2.42743	0.05877
C	-1.86735	-3.32758	-0.21310
C	-0.70907	-2.57099	-0.36212
N	0.96389	0.07847	-0.42798
C	1.91992	-1.01231	-0.30638
F	-4.50777	0.02230	-0.13649
F	-3.34939	0.19984	1.82418
C	3.29513	-0.45729	-0.02670
C	4.34971	-0.68244	-0.90936
C	5.61420	-0.16260	-0.64220
C	5.82795	0.59254	0.50651
C	4.77623	0.82517	1.39129
C	3.51601	0.30080	1.12690
H	-1.85923	4.40740	-0.90434
H	-3.91559	2.77917	-0.14489
H	0.32105	2.84544	-1.01758
H	-3.95253	-2.60998	0.24250
H	-1.95947	-4.39931	-0.30264
H	0.26375	-2.95690	-0.62031
H	1.36387	1.00123	-0.53039
H	1.59034	-1.66012	0.51442
H	1.93399	-1.61357	-1.22355
H	4.18079	-1.26686	-1.80960
H	6.42962	-0.34449	-1.33439
H	6.81204	0.99956	0.71407
H	4.93998	1.41036	2.29012
H	2.69574	0.47322	1.81958

36

[BoNHCH$_2$Ph]$^+$

C	-1.81870	3.33965	-0.78031
C	-2.88602	2.51659	-0.26595
N	-2.44241	1.28653	-0.05768
C	-1.10857	1.24543	-0.40197
C	-0.71091	2.54181	-0.86176
N	-2.45331	-1.15839	0.04884
B	-3.22235	0.08574	0.62523
C	-1.09830	-1.19519	-0.27279
C	-0.35786	0.01411	-0.34196
C	-2.93934	-2.38463	-0.04875
C	-1.91337	-3.28794	-0.46066
C	-0.76504	-2.55032	-0.59488
N	0.96523	0.08003	-0.44060
C	1.92010	-1.03272	-0.35666
F	-4.51200	0.08263	0.20219
F	-3.04893	0.15934	1.97177
C	3.28614	-0.48916	-0.02907
C	4.27365	-0.41878	-1.01114
C	5.52355	0.11375	-0.70562
C	5.78511	0.58121	0.57913
C	4.79939	0.51529	1.56283
C	3.55221	-0.01923	1.26018
H	-1.90874	4.38025	-1.05541
H	-3.91422	2.77973	-0.05208
H	0.26237	2.82068	-1.24017
H	-3.97955	-2.58330	0.17601

H	-2.04036	-4.34525	-0.63848
H	0.19317	-2.91519	-0.92776
H	1.39152	0.99823	-0.47664
H	1.56510	-1.71594	0.42454
H	1.93703	-1.57199	-1.31042
H	4.06999	-0.78826	-2.01262
H	6.29198	0.16012	-1.46946
H	6.76013	0.99236	0.81738
H	5.00656	0.87106	2.56619
H	2.78634	-0.08538	2.02940

36

$[BoNHCH_2Ph]^-$

C	-1.72232	3.37590	-0.47655
C	-2.81241	2.57849	-0.17534
N	-2.41961	1.27661	-0.09944
C	-1.06595	1.21905	-0.34589
C	-0.60257	2.51931	-0.58305
N	-2.44430	-1.18421	0.13046
B	-3.28805	0.09246	0.38276
C	-1.10377	-1.24417	-0.20270
C	-0.37677	-0.02925	-0.37731
C	-2.93166	-2.45260	0.19735
C	-1.92186	-3.35447	-0.08348
C	-0.75625	-2.60030	-0.33969
N	0.99479	0.03462	-0.69038
C	1.93185	-0.98805	-0.31156
F	-4.48124	0.02968	-0.33770
F	-3.58799	0.22235	1.74065
C	3.31323	-0.41541	-0.04513
C	4.45533	-1.18674	-0.26548
C	5.72298	-0.68251	0.01315
C	5.86364	0.60982	0.51176
C	4.72879	1.38891	0.72847
C	3.46273	0.88144	0.45151
H	-1.73644	4.45000	-0.60494
H	-3.84559	2.84151	0.00201
H	0.42113	2.79192	-0.80093
H	-3.97321	-2.61666	0.43389
H	-2.01674	-4.43168	-0.10879
H	0.21175	-2.99024	-0.61651
H	1.19967	0.47891	-1.57938
H	1.54824	-1.44967	0.60559
H	2.03223	-1.80576	-1.04618
H	4.34646	-2.19305	-0.66400
H	6.60130	-1.29590	-0.16667
H	6.85086	1.00895	0.72503
H	4.83057	2.39901	1.11464
H	2.56702	1.47646	0.60504

35

$[BoNCH_2Ph]^{2+}$

C	-1.82784	3.32298	-0.85023
C	-2.91642	2.49671	-0.37413
N	-2.47074	1.26048	-0.13094
C	-1.13351	1.23470	-0.41594
C	-0.71483	2.53698	-0.86474
N	-2.43987	-1.19724	0.09132
B	-3.24756	0.08869	0.59811
C	-1.09227	-1.24671	-0.20813
C	-0.34779	0.00792	-0.31724
C	-2.92546	-2.42883	0.03646
C	-1.86650	-3.35666	-0.32120
C	-0.73027	-2.61746	-0.46508
N	0.94026	0.17458	-0.37745
C	1.87590	-0.92119	-0.28600
F	-4.51937	0.01316	0.15651
F	-3.06717	0.20425	1.93473
C	3.28271	-0.41158	-0.06048
C	4.38013	-1.10733	-0.50092
C	5.67681	-0.61174	-0.22240
C	5.87662	0.61005	0.50932
C	4.78789	1.31453	0.94959
C	3.49248	0.81466	0.67559
H	-1.91891	4.36003	-1.14056
H	-3.95460	2.75884	-0.20663
H	0.28616	2.79088	-1.17894
H	-3.97093	-2.62862	0.24307
H	-1.99079	-4.42222	-0.45497
H	0.23747	-2.98950	-0.76007
H	1.62410	-1.61610	0.53123
H	1.86136	-1.50045	-1.22007
H	4.27628	-2.03017	-1.06286
H	6.54488	-1.16315	-0.57196
H	6.88812	0.95328	0.69986
H	4.90101	2.23978	1.50321
H	2.61900	1.36043	1.01968

35

$[BoNCH_2Ph]^+$

C	0.13356	3.06096	-1.08746
C	-1.16414	2.84747	-0.57188
N	-1.35113	1.55212	-0.32905
C	-0.18889	0.87973	-0.66193
C	0.75496	1.82498	-1.13470
N	-2.46704	-0.62737	0.04598
B	-2.50943	0.88769	0.49838
C	-1.28934	-1.27898	-0.28194
C	-0.15782	-0.51685	-0.57214
C	-3.42291	-1.53820	0.17093
C	-2.90570	-2.83262	-0.10017
C	-1.56643	-2.67592	-0.37990

N	1.04682	-1.19669	-0.86711
C	1.48132	-2.22158	-0.03307
F	-3.71324	1.44158	0.20026
F	-2.16726	0.93521	1.82891
C	2.26167	-0.80188	-0.10064
C	3.50946	-0.81531	-0.81163
C	4.60278	-0.19311	-0.26764
C	4.46933	0.48977	0.95878
C	3.25467	0.55232	1.65257
C	2.14300	-0.07205	1.12893
H	0.53985	4.01087	-1.39991
H	-1.94809	3.56286	-0.36314
H	1.74251	1.60522	-1.51889
H	-4.42577	-1.24562	0.45336
H	-3.47379	-3.75035	-0.10308
H	-0.87526	-3.44870	-0.68854
H	0.96224	-2.41221	0.90572
H	2.04639	-3.03400	-0.47930
H	3.54984	-1.33035	-1.76723
H	5.55711	-0.20456	-0.78068
H	5.33770	0.99290	1.37440
H	3.18645	1.09746	2.58636
H	1.17873	-0.02180	1.62902

35
[BoNCH$_2$Ph]

C	-1.78419	3.38601	-0.46339
C	-2.90014	2.51511	-0.24810
N	-2.47403	1.25046	-0.10470
C	-1.12364	1.24814	-0.21686
C	-0.66675	2.59915	-0.43950
N	-2.42763	-1.21632	0.03086
B	-3.36394	-0.01474	0.26913
C	-1.04575	-1.22432	-0.06787
C	-0.33145	0.03377	-0.14413
C	-2.86317	-2.49422	0.01282
C	-1.78429	-3.35707	-0.10108
C	-0.63155	-2.56007	-0.15273
N	0.94676	0.28402	-0.18592
C	1.88396	-0.80396	-0.11177
F	-4.45122	-0.03809	-0.56912
F	-3.72928	0.10863	1.58844
C	3.31464	-0.32559	-0.01051
C	4.35235	-1.16619	-0.41500
C	5.67876	-0.76514	-0.29124
C	5.98107	0.48697	0.23790
C	4.94995	1.33080	0.64127
C	3.62333	0.92662	0.51889
H	-1.84573	4.45256	-0.61821
H	-3.95566	2.74554	-0.19373
H	0.37026	2.86703	-0.57064
H	-3.92052	-2.70585	0.08458
H	-1.82964	-4.43452	-0.14791
H	0.37720	-2.92236	-0.26030
H	1.64107	-1.44950	0.74960
H	1.76987	-1.44447	-1.00150
H	4.11929	-2.14216	-0.83440
H	6.47571	-1.42766	-0.61346
H	7.01463	0.80369	0.33286
H	5.17899	2.30838	1.05387
H	2.81417	1.58109	0.82579

35
[BoNCH$_2$Ph]$^-$

C	-2.03472	3.35992	-0.46327
C	-3.04941	2.46393	-0.16708
N	-2.52795	1.21738	-0.04720
C	-1.17515	1.29305	-0.25874
C	-0.83795	2.61303	-0.52063
N	-2.35404	-1.23562	0.03130
B	-3.28668	-0.04665	0.40097
C	-0.99400	-1.19526	-0.18629
C	-0.30894	0.10556	-0.22704
C	-2.77096	-2.51828	-0.04195
C	-1.69281	-3.34322	-0.31432
C	-0.56161	-2.50865	-0.40552
N	0.96143	0.32487	-0.27306
C	1.89253	-0.76711	-0.25242
F	-4.49265	-0.16926	-0.28107
F	-3.52317	-0.02884	1.77247
C	3.31851	-0.29025	-0.04547
C	4.36820	-1.21234	-0.08692
C	5.68429	-0.80905	0.11033
C	5.97204	0.53305	0.35325
C	4.93231	1.45738	0.39561
C	3.61411	1.05023	0.19779
H	-2.15145	4.42208	-0.63008
H	-4.11038	2.62061	-0.03351
H	0.16046	2.96023	-0.74304
H	-3.81624	-2.75134	0.10303
H	-1.72016	-4.41646	-0.44050
H	0.43917	-2.83251	-0.63828
H	1.65241	-1.49800	0.53872
H	1.86176	-1.33629	-1.19757
H	4.14502	-2.26065	-0.27690
H	6.48672	-1.54063	0.07398
H	6.99838	0.85326	0.50755
H	5.14779	2.50544	0.58465
H	2.78762	1.75198	0.22318

35
[BoNCH$_2$Ph]$^{2-}$

C	-1.95312	3.39337	-0.20566
C	-3.00780	2.51030	-0.09048
N	-2.51665	1.23211	-0.02952
C	-1.13955	1.28059	-0.10624
C	-0.76258	2.62072	-0.21537
N	-2.39342	-1.21697	-0.00863
B	-3.35046	-0.03108	0.18332
C	-1.00477	-1.18843	-0.09040
C	-0.30360	0.08673	-0.08985
C	-2.82394	-2.51553	-0.06248
C	-1.73489	-3.35099	-0.17648
C	-0.58054	-2.52942	-0.19547
N	1.02195	0.31620	-0.10545
C	1.91403	-0.78029	-0.09128
F	-4.41432	-0.10010	-0.74231
F	-3.93360	-0.05280	1.47003
C	3.35626	-0.31582	-0.01007
C	4.39567	-1.25182	0.01302
C	5.73255	-0.83843	0.09262
C	6.03365	0.52051	0.14588
C	5.00148	1.46021	0.12017
C	3.66503	1.04167	0.04314
H	-2.03403	4.47254	-0.28259
H	-4.07500	2.68138	-0.04661
H	0.25915	2.95942	-0.30602
H	-3.88257	-2.73178	-0.01767
H	-1.76165	-4.43283	-0.24723
H	0.43636	-2.87391	-0.29158
H	1.76158	-1.48836	0.75772
H	1.85657	-1.44201	-0.99087
H	4.14913	-2.31172	-0.03154
H	6.53301	-1.57565	0.11397
H	7.07068	0.84698	0.20794
H	5.23676	2.52176	0.16104
H	2.82322	1.72606	0.02610

35
[BoNHCHPh]$^{2+}$

C	-2.12145	3.35640	-0.30959
C	-3.16470	2.33831	-0.32682
N	-2.64398	1.14788	-0.11903
C	-1.26755	1.30758	0.03233
C	-0.94679	2.70979	-0.08629
N	-2.31034	-1.32538	-0.01821
B	-3.47214	-0.21697	-0.01030
C	-0.94740	-1.10962	0.19556
C	-0.43941	0.19006	0.20451
C	-2.51738	-2.62345	-0.01001
C	-1.26669	-3.33596	0.21478
C	-0.29879	-2.39334	0.35550
N	0.95413	0.40355	0.38854
C	1.90308	-0.16358	-0.34151
F	-4.24745	-0.36068	-1.10092
F	-4.09157	-0.26391	1.18675
C	3.29329	-0.02701	-0.15183
C	4.12657	-0.62388	-1.13319
C	5.50094	-0.51560	-1.03096
C	6.05408	0.17597	0.04957
C	5.24266	0.76316	1.03721
C	3.87271	0.66751	0.94369
H	-2.28484	4.41425	-0.46285
H	-4.23059	2.46581	-0.48641
H	0.04125	3.14547	-0.03577
H	-3.51409	-3.03388	-0.13771
H	-1.16705	-4.41108	0.27257
H	0.74826	-2.55851	0.56864
H	1.22163	1.04670	1.13105
H	1.54262	-0.77189	-1.17112
H	3.68089	-1.15679	-1.96863
H	6.14321	-0.96418	-1.77979
H	7.13335	0.25860	0.13421
H	5.69882	1.28337	1.87154
H	3.26075	1.10797	1.72641

35
[BoNHCHPh]$^{+}$

C	-2.27189	3.34568	0.06434
C	-3.24437	2.31640	-0.03157
N	-2.65899	1.12593	0.00081
C	-1.29189	1.32529	0.10784
C	-1.04354	2.72704	0.13922
N	-2.27485	-1.33049	0.12343
B	-3.33503	-0.26055	-0.35763
C	-0.92077	-1.09777	0.28738
C	-0.45905	0.21759	0.22151
C	-2.50625	-2.61529	0.36877
C	-1.29878	-3.27385	0.70943
C	-0.30088	-2.32367	0.66776
N	0.94101	0.45694	0.31996
C	1.85848	-0.25508	-0.27705
F	-3.47160	-0.34042	-1.71404
F	-4.49491	-0.41589	0.33591
C	3.26986	-0.06129	-0.16150
C	4.08556	-0.82124	-1.02272
C	5.46271	-0.66768	-0.98597
C	6.02916	0.23266	-0.08499
C	5.22805	0.98273	0.78625
C	3.85483	0.84071	0.75296
H	-2.47454	4.40573	0.07515
H	-4.31875	2.39750	-0.13222
H	-0.08115	3.21573	0.21400
H	-3.51018	-3.01336	0.30338

H	-1.20167	-4.31516	0.97616
H	0.73759	-2.46879	0.93341
H	1.21880	1.27063	0.86417
H	1.48004	-1.04585	-0.92273
H	3.63012	-1.51893	-1.71963
H	6.09308	-1.24615	-1.65101
H	7.10726	0.35068	-0.05123
H	5.68662	1.66764	1.48997
H	3.24896	1.40990	1.45270

35
[BoNHCHPh]

C	-2.18798	3.35171	0.11537
C	-3.18191	2.36864	0.06478
N	-2.61851	1.15246	0.02172
C	-1.25233	1.30992	0.03157
C	-0.96349	2.68537	0.08517
N	-2.31356	-1.29463	0.10897
B	-3.35567	-0.19314	-0.27872
C	-0.94221	-1.13758	0.16319
C	-0.40013	0.16889	0.04317
C	-2.60515	-2.56737	0.39848
C	-1.42891	-3.28007	0.66078
C	-0.37547	-2.38277	0.51579
N	0.93669	0.38897	-0.02098
C	1.92369	-0.50318	-0.32857
F	-3.64957	-0.27083	-1.62142
F	-4.47579	-0.31490	0.50767
C	3.30142	-0.18833	-0.16494
C	4.27009	-1.02940	-0.75934
C	5.61950	-0.74732	-0.64378
C	6.04812	0.37704	0.06599
C	5.10639	1.20903	0.67183
C	3.75204	0.93334	0.56846
H	-2.34804	4.41772	0.17158
H	-4.25774	2.46950	0.04710
H	0.01336	3.15077	0.11724
H	-3.63441	-2.89699	0.41066
H	-1.36330	-4.32101	0.93877
H	0.66766	-2.58527	0.70545
H	1.22001	1.35836	0.06800
H	1.60498	-1.42505	-0.79644
H	3.93947	-1.89813	-1.32124
H	6.34630	-1.40334	-1.11133
H	7.10636	0.59649	0.15426
H	5.43364	2.07209	1.24229
H	3.04386	1.56704	1.09534

35
[BoNHCHPh]$^{-}$

C	-1.99089	3.36456	-0.42301
C	-3.02252	2.47943	-0.16824
N	-2.52311	1.22158	-0.05138
C	-1.16679	1.27795	-0.23024
C	-0.80302	2.60101	-0.47721
N	-2.38518	-1.24971	0.00429
B	-3.35403	-0.05548	0.22799
C	-1.00917	-1.21109	-0.09825
C	-0.36281	0.07382	-0.15890
C	-2.76923	-2.54520	0.09466
C	-1.65715	-3.36735	0.05348
C	-0.53238	-2.52647	-0.07234
N	0.95807	0.23028	-0.17345
C	1.98004	-0.65811	-0.37484
F	-4.42787	-0.13307	-0.65129
F	-3.82406	-0.05905	1.53728
C	3.31508	-0.28306	-0.10043
C	4.39804	-1.06235	-0.59657
C	5.71314	-0.69987	-0.38229
C	6.03957	0.45862	0.33444
C	4.99676	1.22529	0.85103
C	3.66975	0.86601	0.66049
H	-2.08564	4.42990	-0.57912
H	-4.08532	2.64838	-0.07350
H	0.18572	2.96614	-0.72374
H	-3.81807	-2.78831	0.18916
H	-1.65675	-4.44738	0.09485
H	0.49770	-2.83806	-0.10905
H	1.25227	1.19802	-0.05370
H	1.74216	-1.56028	-0.91570
H	4.16953	-1.95679	-1.17094
H	6.50599	-1.32525	-0.78629
H	7.07420	0.74057	0.49784
H	5.22009	2.11337	1.43785
H	2.89671	1.45189	1.15149

35
[BoNHCHPh]$^{2-}$

C	-2.29063	3.33681	-0.27239
C	-3.25068	2.36109	-0.11294
N	-2.64380	1.13490	-0.03418
C	-1.27958	1.31023	-0.14546
C	-1.03098	2.68151	-0.30129
N	-2.29972	-1.30459	0.06854
B	-3.37963	-0.21013	0.08838
C	-0.92465	-1.13292	0.02507
C	-0.38268	0.19206	-0.07681
C	-2.56726	-2.64160	0.19807
C	-1.38161	-3.34346	0.23939
C	-0.33010	-2.39843	0.12548
N	0.97180	0.45480	-0.06553
C	2.00709	-0.35589	-0.55632

F	-4.28793	-0.37890	-0.97527
F	-4.12925	-0.26509	1.27952
C	3.32869	-0.14625	-0.22264
C	4.40988	-0.86764	-0.86490
C	5.73222	-0.61750	-0.58639
C	6.13465	0.35763	0.35164
C	5.10874	1.05037	1.01388
C	3.77045	0.82458	0.76160
H	-2.47248	4.40067	-0.36977
H	-4.32804	2.43303	-0.05765
H	-0.06473	3.14114	-0.46275
H	-3.59251	-2.98101	0.25252
H	-1.27998	-4.41853	0.33081
H	0.73278	-2.58544	0.13065
H	1.20691	1.42855	0.08368
H	1.71563	-1.09868	-1.29146
H	4.14753	-1.62729	-1.60052
H	6.49265	-1.19722	-1.11371
H	7.18257	0.54992	0.56083
H	5.37178	1.79194	1.77119
H	3.02119	1.35020	1.34843

34

trans-BoN=CHPh

C	2.20069	3.34783	0.02021
C	3.17894	2.34199	-0.09787
N	2.60927	1.13612	-0.04482
C	1.24628	1.31870	0.10375
C	0.97895	2.70275	0.14490
N	2.26172	-1.31026	0.15949
B	3.32153	-0.23909	-0.28301
C	0.90385	-1.09203	0.29686
C	0.38529	0.21690	0.22511
C	2.49083	-2.61294	0.34087
C	1.28626	-3.28398	0.61704
C	0.28264	-2.32533	0.59592
N	-0.96762	0.45371	0.35664
C	-1.80038	-0.17724	-0.37854
F	4.44555	-0.33930	0.49894
F	3.60272	-0.39225	-1.62129
C	-3.25015	-0.02843	-0.22744
C	-4.09713	-0.73740	-1.08368
C	-5.47700	-0.62085	-0.95541
C	-6.01133	0.20578	0.02911
C	-5.16873	0.91677	0.88628
C	-3.79232	0.80244	0.76120
H	2.38609	4.41126	0.02510
H	4.24998	2.43385	-0.21624
H	0.00038	3.14037	0.27850
H	3.49628	-3.00409	0.26659
H	1.18205	-4.33807	0.82482
H	-0.76671	-2.46753	0.81240
H	-1.45397	-0.85604	-1.16971
H	-3.67009	-1.37940	-1.84965
H	-6.13303	-1.17169	-1.62069
H	-7.08779	0.29885	0.13055
H	-5.59152	1.55965	1.65101
H	-3.11738	1.34550	1.41456

34

trans-[BoN=CHPh]$^{+}$

C	2.22500	3.34593	0.12105
C	3.22256	2.30946	-0.02982
N	2.64371	1.11853	-0.04635
C	1.28119	1.31285	0.08449
C	1.01512	2.71997	0.18722
N	2.27044	-1.31282	0.17734
B	3.34170	-0.27454	-0.35042
C	0.90137	-1.07682	0.28727
C	0.37255	0.21696	0.15672
C	2.48493	-2.59005	0.43111
C	1.24748	-3.25378	0.74198
C	0.26299	-2.31113	0.65656
N	-0.95395	0.50270	0.23870
C	-1.82725	-0.19122	-0.40950
F	4.48831	-0.38271	0.36591
F	3.48246	-0.41313	-1.69519
C	-3.25500	-0.02802	-0.24178
C	-4.11559	-0.78961	-1.04622
C	-5.49038	-0.66458	-0.90145
C	-6.00486	0.21915	0.04581
C	-5.15205	0.98115	0.85073
C	-3.78006	0.86197	0.71057
H	2.43379	4.40414	0.17701
H	4.29742	2.40603	-0.12335
H	0.03264	3.14907	0.31665
H	3.48642	-3.00125	0.39161
H	1.14940	-4.29430	1.01350
H	-0.78874	-2.43123	0.87406
H	-1.49826	-0.93382	-1.15086
H	-3.70222	-1.47331	-1.78293
H	-6.15937	-1.24965	-1.52205
H	-7.07937	0.31823	0.15938
H	-5.56670	1.66478	1.58299
H	-3.09970	1.44426	1.32311

34

trans-[BoN=CHPh]$^{-}$

C	2.15271	3.35709	0.18449
C	3.14713	2.39439	0.05967
N	2.58323	1.16413	0.00889
C	1.21883	1.31119	0.09492

C	0.92407	2.67199	0.20044
N	2.30187	-1.28057	0.07595
B	3.31373	-0.16399	-0.30191
C	0.93390	-1.14519	0.18464
C	0.33463	0.17158	0.08462
C	2.63161	-2.56658	0.33115
C	1.48617	-3.29341	0.61971
C	0.40575	-2.39604	0.53183
N	-0.97546	0.43504	0.04956
C	-1.88209	-0.46604	-0.26698
F	4.46199	-0.28679	0.47197
F	3.64459	-0.23718	-1.65136
C	-3.29290	-0.17274	-0.16749
C	-4.24753	-1.12729	-0.56967
C	-5.60714	-0.86496	-0.47542
C	-6.05670	0.35823	0.02252
C	-5.12019	1.31512	0.42485
C	-3.76148	1.05902	0.33634
H	2.30766	4.42427	0.26370
H	4.22121	2.49954	0.00015
H	-0.07201	3.07850	0.29433
H	3.66737	-2.87297	0.29705
H	1.44168	-4.34252	0.87632
H	-0.62855	-2.60901	0.75524
H	-1.60324	-1.43783	-0.68205
H	-3.90192	-2.08201	-0.95925
H	-6.32356	-1.61811	-0.79234
H	-7.12008	0.56384	0.09734
H	-5.46055	2.27130	0.81354
H	-3.02419	1.79232	0.64564

34

cis-BoN=CHPh

C	-1.52839	-3.35458	0.55559
C	-2.29228	-2.50436	-0.26269
N	-1.91483	-1.23545	-0.08363
C	-0.88614	-1.22470	0.83920
C	-0.63193	-2.54758	1.24654
N	-1.91493	1.23536	-0.08370
B	-2.26965	-0.00008	-0.97525
C	-0.88624	1.22474	0.83913
C	-0.31498	0.00006	1.24175
C	-2.29249	2.50423	-0.26281
C	-1.52867	3.35455	0.55542
C	-0.63214	2.54766	1.24641
N	0.73194	0.00012	2.12039
C	1.96615	0.00013	1.81249
F	-3.59336	-0.00014	-1.32152
F	-1.42194	-0.00008	-2.07253
C	2.62473	0.00008	0.49145
C	1.95724	0.00004	-0.74421
C	2.69172	-0.00001	-1.92353
C	4.08503	-0.00002	-1.89277
C	4.75508	0.00003	-0.67234
C	4.02618	0.00007	0.50952
H	-1.63835	-4.42575	0.63171
H	-3.07652	-2.74458	-0.96724
H	0.09625	-2.84444	1.98771
H	-3.07675	2.74435	-0.96738
H	-1.63872	4.42572	0.63149
H	0.09602	2.84462	1.98757
H	2.65854	0.00017	2.65874
H	0.87682	0.00004	-0.81701
H	2.16487	-0.00004	-2.87147
H	4.64762	-0.00006	-2.82077
H	5.83932	0.00002	-0.64180
H	4.54431	0.00011	1.46490

35

BoNHNHPh

C	-3.225835	3.057896	0.637313
C	-3.646125	1.954414	1.386696
N	-2.890476	0.888350	1.090151
C	-1.970648	1.262937	0.139578
C	-2.164293	2.622517	-0.155616
N	-1.752417	-1.290768	1.266817
B	-3.110622	-0.573730	1.583044
C	-0.827926	-0.920238	0.304147
C	-0.982619	0.342426	-0.322949
C	-1.387013	-2.470085	1.771712
C	-0.201418	-2.906125	1.164679
C	0.155436	-1.936475	0.236690
N	-0.222543	0.753305	-1.357841
N	0.723651	-0.000503	-2.014087
F	-4.123729	-1.167963	0.864774
F	-3.347017	-0.597593	2.935730
C	2.044341	0.003168	-1.507090
C	2.949496	-0.920594	-2.037332
C	4.265122	-0.933682	-1.591987
C	4.693566	-0.025775	-0.625920
C	3.786720	0.892467	-0.106957
C	2.462838	0.912664	-0.537100
H	-3.638074	4.054375	0.684032
H	-4.441630	1.870509	2.113308
H	-1.577155	3.233998	-0.828125
H	-1.989681	-2.940625	2.536020
H	0.336442	-3.813316	1.394421
H	1.055672	-1.937622	-0.357997
H	-0.504761	1.594090	-1.841004
H	0.368677	-0.917616	-2.268595
H	2.618341	-1.619136	-2.801293
H	4.959323	-1.657097	-2.007015

H	5.721304	-0.036927	-0.280961
H	4.105340	1.601394	0.650331
H	1.757712	1.621362	-0.117575

35

[BoNHNHPh]$^{+}$

C	2.62468	-3.12191	0.40137
C	3.39373	-1.91559	0.51959
N	2.65319	-0.87314	0.18556
C	1.39470	-1.33109	-0.17334
C	1.38032	-2.75512	-0.03693
N	1.79444	1.41947	0.12635
B	3.14755	0.61293	-0.00407
C	0.53184	0.95679	-0.22457
C	0.35422	-0.43010	-0.52563
C	1.68703	2.69175	0.46753
C	0.31671	3.11747	0.36278
C	-0.40291	2.04063	-0.07040
N	-0.78303	-0.91951	-1.03833
N	-1.84928	-0.10381	-1.36269
F	3.64895	0.76576	-1.25808
F	3.98612	0.96193	1.00470
C	-2.99591	-0.20035	-0.51666
C	-4.24697	0.09538	-1.05766
C	-5.36736	0.08220	-0.23567
C	-5.24723	-0.22723	1.11779
C	-3.99464	-0.51856	1.64744
C	-2.86143	-0.50179	0.83763
H	2.97831	-4.11601	0.63122
H	4.42571	-1.78753	0.82083
H	0.53985	-3.41354	-0.20667
H	2.56017	3.25567	0.77167
H	-0.05011	4.10542	0.59851
H	-1.46491	1.97928	-0.24219
H	-0.89626	-1.92570	-1.11874
H	-2.06751	-0.18113	-2.35138
H	-4.34321	0.33244	-2.11375
H	-6.33992	0.30783	-0.65917
H	-6.12505	-0.24205	1.75337
H	-3.89145	-0.75947	2.69992
H	-1.88686	-0.72489	1.26135

35

[BoNHNHPh]$^{-}$

C	-3.632582	2.268372	-0.701821
C	-4.091286	1.133292	-0.054090
N	-3.046811	0.482614	0.526518
C	-1.896824	1.190558	0.262162
C	-2.234184	2.315052	-0.507805
N	-1.672496	-1.274139	1.607966
B	-3.134607	-0.803297	1.393280
C	-0.528998	-0.540835	1.352013
C	-0.632536	0.721336	0.721721
C	-1.301088	-2.447489	2.184345
C	0.080572	-2.492010	2.307180
C	0.580273	-1.284367	1.783188
N	0.542101	1.470965	0.404867
N	0.927083	1.321687	-0.963433
F	-3.870031	-1.782836	0.729082
F	-3.745963	-0.524760	2.615834
C	2.068821	0.569445	-1.217889
C	2.244926	-0.015345	-2.481301
C	3.416608	-0.694335	-2.787483
C	4.438324	-0.812615	-1.847539
C	4.260846	-0.237051	-0.590732
C	3.096802	0.450275	-0.271169
H	-4.237718	2.972893	-1.255866
H	-5.092214	0.735428	0.034275
H	-1.539771	3.052281	-0.890935
H	-2.052020	-3.170728	2.469595
H	0.654765	-3.309973	2.720536
H	1.610337	-0.972075	1.690890
H	0.339027	2.459452	0.527326
H	0.132009	1.078153	-1.550483
H	1.449557	0.065236	-3.217758
H	3.526747	-1.143885	-3.770528
H	5.350422	-1.349228	-2.087198
H	5.042321	-0.325438	0.159179
H	2.947589	0.893369	0.706072

34

[BoNNHPh]$^{+}$

C	1.02897	-3.36829	-0.85069
C	1.91810	-2.70064	0.03176
N	1.71874	-1.38863	-0.02344
C	0.69259	-1.15166	-0.92581
C	0.24671	-2.40004	-1.44295
N	2.07529	1.06489	0.17451
B	2.19833	-0.28062	0.98865
C	1.03912	1.27563	-0.72503
C	0.35455	0.16724	-1.20309
C	2.63120	2.24068	0.43811
C	1.98070	3.26715	-0.29814
C	0.96973	2.66807	-1.01659
N	-0.79305	0.39507	-2.04575
N	-2.01060	0.40966	-1.71849
F	3.46550	-0.49759	1.40996
F	1.24783	-0.22212	1.99470
C	-2.50632	0.25006	-0.45400
C	-3.92637	0.26118	-0.47822
C	-4.64995	0.11228	0.68872
C	-3.96336	-0.03464	1.89500

C	-2.56068	-0.03182	1.93788
C	-1.81586	0.10570	0.78569
H	0.99326	-4.43370	-1.02010
H	2.66576	-3.11572	0.69502
H	-0.52643	-2.54378	-2.18538
H	3.45079	2.31623	1.14092
H	2.24710	4.31312	-0.28841
H	0.27897	3.14430	-1.69886
H	-0.63609	0.54622	-3.04277
H	-4.41327	0.38543	-1.43937
H	-5.73312	0.11492	0.66732
H	-4.52179	-0.14848	2.81897
H	-2.04518	-0.13887	2.88543
H	-0.73926	0.10852	0.87839

34
[BoNHNPh]$^{+}$

C	2.09980	-3.35971	0.14774
C	3.11671	-2.37600	0.07129
N	2.57584	-1.16203	0.02097
C	1.20484	-1.29845	0.05703
C	0.89599	-2.68857	0.13366
N	2.28492	1.30482	0.11030
B	3.33936	0.19168	-0.26957
C	0.90200	1.15210	0.14651
C	0.40392	-0.14603	0.08727
C	2.56273	2.58690	0.29375
C	1.36437	3.33099	0.46202
C	0.32285	2.43902	0.36798
N	-0.98254	-0.41713	0.09045
N	-1.86502	0.46475	-0.04791
F	3.61077	0.26620	-1.60506
F	4.43373	0.29485	0.53242
C	-3.19606	0.12256	-0.02855
C	-4.05098	1.18570	-0.38328
C	-5.41954	0.97689	-0.44011
C	-5.93146	-0.27998	-0.12379
C	-5.08539	-1.33702	0.25497
C	-3.72135	-1.14913	0.30483
H	2.25434	-4.42589	0.21162
H	4.19126	-2.49961	0.04681
H	-0.07984	-3.15466	0.19014
H	3.58947	2.92904	0.29835
H	1.30288	4.39375	0.64018
H	-0.72876	2.65395	0.46438
H	-1.23365	-1.40737	0.17303
H	-3.60670	2.14608	-0.62223
H	-6.08399	1.78471	-0.72270
H	-7.00309	-0.44719	-0.15826
H	-5.50965	-2.29882	0.51861
H	-3.09237	-1.97042	0.63695

34
[BoNNHPh]$^{-}$

C	-2.37161	3.30837	-0.37937
C	-3.26568	2.30136	-0.05864
N	-2.60185	1.11880	0.01974
C	-1.27670	1.35162	-0.24401
C	-1.09909	2.70343	-0.49538
N	-2.18809	-1.30748	-0.01464
B	-3.18303	-0.22760	0.50470
C	-0.86210	-1.11107	-0.31318
C	-0.31087	0.24912	-0.24492
C	-2.49676	-2.60642	-0.23631
C	-1.37650	-3.27848	-0.69152
C	-0.33083	-2.33167	-0.74309
N	0.94138	0.57241	-0.20266
N	1.85117	-0.45232	-0.16846
F	-4.43858	-0.45032	-0.04792
F	-3.25949	-0.26728	1.89296
C	3.18384	-0.14245	0.01853
C	4.08970	-1.16676	0.34261
C	5.44240	-0.89179	0.48210
C	5.92976	0.40241	0.30555
C	5.02886	1.41771	-0.01256
C	3.67154	1.16261	-0.15732
H	-2.61312	4.35217	-0.52648
H	-4.33093	2.33477	0.11915
H	-0.15775	3.16974	-0.74750
H	-3.50400	-2.95548	-0.06049
H	-1.32133	-4.32217	-0.96720
H	0.66234	-2.49668	-1.13461
H	1.52623	-1.33091	0.22744
H	3.71762	-2.17858	0.48316
H	6.12308	-1.70007	0.73523
H	6.98799	0.61469	0.41614
H	5.38864	2.43402	-0.14957
H	2.96505	1.94695	-0.39703

34
[BoNHNPh]$^{-}$

C	2.08977	-3.32133	-0.55108
C	3.06441	-2.40448	-0.19343
N	2.50420	-1.17854	-0.05298
C	1.16510	-1.28491	-0.31692
C	0.87482	-2.60880	-0.63901
N	2.28370	1.28098	0.03678
B	3.24495	0.11495	0.38888
C	0.92080	1.19376	-0.16707
C	0.31714	-0.10677	-0.25356
C	2.61891	2.58912	0.05263
C	1.48624	3.36764	-0.14543

C	0.40013	2.48409	-0.28437
N	-0.98523	-0.28923	-0.30993
N	-1.92171	0.66865	-0.46961
F	4.43727	0.24269	-0.31055
F	3.49685	0.08445	1.75495
C	-3.16618	0.24546	-0.11182
C	-4.26050	1.06112	-0.50828
C	-5.56483	0.70473	-0.23438
C	-5.86440	-0.48007	0.45314
C	-4.80761	-1.27652	0.87766
C	-3.48397	-0.92901	0.62084
H	2.24177	-4.37275	-0.74938
H	4.12552	-2.53303	-0.03681
H	-0.08385	-3.00540	-0.94755
H	3.64881	2.87760	0.20949
H	1.45647	4.44702	-0.19391
H	-0.63775	2.70596	-0.46913
H	-1.29286	-1.26331	-0.32440
H	-4.02778	1.97070	-1.05338
H	-6.37146	1.35500	-0.56497
H	-6.89189	-0.75752	0.66375
H	-5.00902	-2.18248	1.44501
H	-2.69549	-1.53806	1.05385

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[BoNNHPh]

C	2.32009	-3.32423	0.20959
C	3.25774	-2.28307	0.05282
N	2.63024	-1.10167	0.02438
C	1.28014	-1.33525	0.14938
C	1.06936	-2.73061	0.25832
N	2.18596	1.32728	0.07243
B	3.25502	0.28070	-0.37700
C	0.84051	1.09158	0.24554
C	0.35654	-0.26161	0.17273
C	2.42950	2.62420	0.32622
C	1.24589	3.26694	0.68511
C	0.23612	2.30158	0.64290
N	-0.93812	-0.62959	0.14242
N	-1.80384	0.31152	-0.13605
F	3.42662	0.32175	-1.74227
F	4.43033	0.48633	0.30366
C	-3.18034	0.07534	-0.12352
C	-4.02677	1.09191	-0.57613
C	-5.40017	0.89142	-0.56325
C	-5.92980	-0.31303	-0.10433
C	-5.07468	-1.31897	0.34495
C	-3.69874	-1.13623	0.34289
H	2.55183	-4.37589	0.28524
H	4.33343	-2.33037	-0.04608
H	0.10678	-3.20308	0.38405
H	3.43497	3.01142	0.24443
H	1.14158	4.30438	0.96435
H	-0.78907	2.44493	0.95523
H	-1.46663	1.20260	-0.50324
H	-3.60742	2.02732	-0.93674
H	-6.05796	1.67873	-0.91505
H	-7.00311	-0.46693	-0.09609
H	-5.48410	-2.25720	0.70403
H	-3.01990	-1.90478	0.69073

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[BoNHNPh]

C	3.43140	-2.51657	0.28046
C	3.71427	-1.15202	0.43487
N	2.63030	-0.42368	0.14150
C	1.61283	-1.28715	-0.20080
C	2.09861	-2.60650	-0.10926
N	1.12003	1.47710	-0.30739
B	2.43238	1.09724	0.45514
C	0.11967	0.60375	-0.70329
C	0.34603	-0.78442	-0.59926
C	0.76386	2.71018	-0.66863
C	-0.48526	2.68251	-1.31288
C	-0.89467	1.35803	-1.33638
N	-0.58159	-1.72477	-0.97416
N	-1.90680	-1.64794	-1.15602
F	3.48490	1.83397	-0.02854
F	2.25537	1.26244	1.81046
C	-2.64091	-0.92956	-0.23323
C	-3.96237	-0.63944	-0.62893
C	-4.81329	0.05167	0.21736
C	-4.37573	0.43876	1.48467
C	-3.08056	0.12224	1.89924
C	-2.21023	-0.54815	1.05528
H	4.12126	-3.33124	0.44007
H	4.62617	-0.66564	0.75178
H	1.54361	-3.51554	-0.29791
H	1.41737	3.54579	-0.46003
H	-1.01026	3.53484	-1.71653
H	-1.79995	0.96421	-1.77293
H	-0.19214	-2.56429	-1.38545
H	-4.28026	-0.96521	-1.61377
H	-5.82327	0.28231	-0.10447
H	-5.04294	0.97393	2.15167
H	-2.74550	0.40355	2.89189
H	-1.21385	-0.80140	1.39982

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trans-BoN=NPh

C	-2.261357	3.439027	0.947889
C	-3.252739	2.495520	1.287763

N	-2.814602	1.258765	1.047210
C	-1.529473	1.354343	0.547358
C	-1.172631	2.721489	0.480913
N	-2.708673	-1.191994	0.675125
B	-3.560654	-0.078497	1.384307
C	-1.409006	-1.061827	0.206366
C	-0.817504	0.207318	0.176373
C	-3.075454	-2.463377	0.524050
C	-2.029777	-3.207454	-0.060424
C	-0.981550	-2.328092	-0.265749
N	0.482866	0.445624	-0.316085
N	1.304063	-0.458345	-0.061129
F	-4.831129	-0.059871	0.863944
F	-3.558113	-0.284507	2.743237
C	2.600205	-0.247582	-0.602782
C	3.547099	-1.210577	-0.253461
C	4.847926	-1.106402	-0.734131
C	5.192802	-0.042818	-1.563221
C	4.240559	0.918766	-1.913287
C	2.942479	0.824043	-1.436459
H	-2.356601	4.511104	1.029866
H	-4.246238	2.654779	1.684469
H	-0.231147	3.097833	0.109396
H	-4.059902	-2.786572	0.834516
H	-2.062790	-4.258045	-0.305899
H	-0.019908	-2.536071	-0.708032
H	3.239551	-2.024175	0.395197
H	5.588596	-1.851144	-0.464109
H	6.206384	0.041107	-1.941690
H	4.518192	1.742808	-2.562012
H	2.186522	1.556547	-1.694801

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cis-BoN=NPh

C	2.84615	-2.79067	0.02775
C	3.22111	-1.53160	0.53523
N	2.31135	-0.61224	0.20649
C	1.31755	-1.24305	-0.51960
C	1.64208	-2.61134	-0.63757
N	1.18174	1.55813	-0.21317
B	2.26080	0.87528	0.70287
C	0.19170	0.89009	-0.91282
C	0.23779	-0.50476	-1.02171
C	0.93686	2.86464	-0.30824
C	-0.21783	3.08926	-1.08600
C	-0.69071	1.84442	-1.46684
N	-0.69399	-1.16747	-1.84894
N	-1.90763	-1.25187	-1.62043
F	3.47936	1.47980	0.53334
F	1.83375	0.90659	2.01086
C	-2.47892	-0.81943	-0.37862
C	-3.74632	-0.24597	-0.48317
C	-4.39659	0.19505	0.66252
C	-3.80600	0.00922	1.91088
C	-2.56550	-0.61775	2.01312
C	-1.89103	-1.03268	0.87097
H	3.40913	-3.70595	0.12991
H	4.09240	-1.25386	1.11246
H	1.06377	-3.34455	-1.18180
H	1.58566	3.57783	0.18176
H	-0.63270	4.05370	-1.33648
H	-1.54842	1.61987	-2.08573
H	-4.19275	-0.14420	-1.46693
H	-5.36989	0.66722	0.58385
H	-4.32005	0.33814	2.80781
H	-2.11692	-0.78352	2.98644
H	-0.93462	-1.53705	0.95340

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BoNHCH$_2$Py

C	-1.79327	3.38301	-0.36205
C	-2.88081	2.53610	-0.13498
N	-2.45671	1.26696	-0.03805
C	-1.09069	1.25730	-0.19022
C	-0.65546	2.57426	-0.39629
N	-2.43176	-1.19802	-0.02298
B	-3.31869	0.03490	0.36300
C	-1.05789	-1.21468	-0.17021
C	-0.35666	0.02812	-0.18626
C	-2.88615	-2.45165	-0.11889
C	-1.82162	-3.32991	-0.34095
C	-0.66471	-2.55569	-0.37174
N	0.97218	0.11559	-0.22934
C	1.92546	-0.96186	-0.19547
F	-4.49097	0.00727	-0.35556
F	-3.54636	0.03445	1.72204
C	3.32541	-0.40299	-0.01907
C	4.40947	-1.27013	0.12545
C	5.67631	-0.72572	0.27527
C	5.81890	0.66027	0.27585
C	4.67904	1.43830	0.12562
N	3.45518	0.92117	-0.01998
H	-1.83670	4.45297	-0.49866
H	-3.93212	2.76563	-0.03585
H	0.35916	2.90124	-0.58292
H	-3.94396	-2.65149	-0.02207
H	-1.89179	-4.39894	-0.47326
H	0.33002	-2.92705	-0.55540
H	1.40287	1.03571	-0.19890
H	1.69128	-1.64775	0.62906
H	1.88802	-1.54468	-1.12603
H	4.25374	-2.34442	0.12172

H	6.54107	-1.37056	0.39218
H	6.78942	1.12820	0.39142
H	4.74209	2.52291	0.12142

35
BoNHCH$_2$Py Orient2

C	-1.89100	3.32132	-0.74881
C	-2.91918	2.48814	-0.30074
N	-2.45388	1.24152	-0.13295
C	-1.11697	1.23376	-0.45207
C	-0.74492	2.52914	-0.84142
N	-2.37785	-1.20603	0.11669
B	-3.20781	0.05276	0.53863
C	-1.03681	-1.22273	-0.21685
C	-0.36304	0.01761	-0.40458
C	-2.83076	-2.46299	0.11764
C	-1.80007	-3.34320	-0.23087
C	-0.66540	-2.56645	-0.44351
N	0.96104	0.10569	-0.57117
C	1.94376	-0.95495	-0.43437
F	-4.48756	-0.04816	0.04894
F	-3.18156	0.19416	1.90862
C	3.29086	-0.37987	-0.05644
N	4.33718	-0.84877	-0.73839
C	5.54535	-0.38239	-0.41629
C	5.76573	0.56660	0.57777
C	4.66849	1.04956	1.28265
C	3.40489	0.56678	0.96442
H	-1.97916	4.36966	-0.99062
H	-3.95436	2.71380	-0.08808
H	0.22602	2.85317	-1.19338
H	-3.86414	-2.66466	0.36211
H	-1.88219	-4.41479	-0.33089
H	0.29357	-2.92824	-0.77944
H	1.32892	1.03009	-0.75081
H	1.59546	-1.63606	0.35030
H	2.06194	-1.52521	-1.36151
H	6.37779	-0.78527	-0.98767
H	6.77055	0.91296	0.79049
H	4.79420	1.78462	2.07095
H	2.52156	0.90332	1.49886

35
[BoNHCH$_2$Py]$^+$

C	-1.68418	3.36741	-0.53398
C	-2.81365	2.54177	-0.17575
N	-2.41826	1.28575	-0.01533
C	-1.06552	1.23099	-0.24645
C	-0.59425	2.54491	-0.57590
N	-2.48095	-1.16770	-0.02134
B	-3.29654	0.06690	0.50083
C	-1.10226	-1.21931	-0.21620
C	-0.34273	-0.02450	-0.21029
C	-2.96852	-2.39122	-0.15879
C	-1.92123	-3.30497	-0.46532
C	-0.75619	-2.57865	-0.49457
N	0.97757	0.04271	-0.25077
C	1.92525	-1.04916	-0.21499
F	-4.52016	0.11540	-0.08662
F	-3.30789	0.08370	1.86093
C	3.31382	-0.46046	-0.00758
C	4.42130	-1.28877	0.14716
C	5.66358	-0.69196	0.32206
C	5.75065	0.69794	0.33515
C	4.58589	1.43647	0.17251
N	3.38721	0.86813	0.00328
H	-1.72585	4.42727	-0.73766
H	-3.85115	2.81892	-0.03819
H	0.41973	2.81418	-0.83666
H	-4.02692	-2.57801	-0.03018
H	-2.04083	-4.36255	-0.64582
H	0.22474	-2.96052	-0.72596
H	1.46259	0.94572	-0.20081
H	1.67128	-1.74022	0.59953
H	1.90003	-1.60913	-1.15882
H	4.31157	-2.36842	0.13273
H	6.55157	-1.30191	0.44807
H	6.70048	1.20131	0.46981
H	4.60705	2.52192	0.17772

35
[BoNHCH$_2$Py]$^-$

C	-1.70918	3.36378	0.19295
C	-2.80620	2.52315	0.28457
N	-2.42120	1.23876	0.05127
C	-1.06421	1.23415	-0.19330
C	-0.59299	2.55287	-0.10961
N	-2.41396	-1.24011	-0.01827
B	-3.34895	-0.00519	0.06193
C	-1.06733	-1.22046	-0.31920
C	-0.37920	0.01394	-0.44471
C	-2.80557	-2.53958	0.08450
C	-1.72253	-3.37358	-0.14415
C	-0.61095	-2.54291	-0.40459
N	1.02865	-0.00292	-0.64504
C	1.76487	-0.11816	0.62226
F	-4.21993	0.02209	-1.02890
F	-4.10035	-0.03844	1.23706
C	3.24578	-0.06497	0.36000
C	4.09267	-1.13634	0.65700
C	5.44829	-1.02722	0.37600
C	5.91930	0.14612	-0.20374

C	4.99870	1.15497	-0.47316
N	3.69810	1.06573	-0.20047
H	-1.71638	4.43576	0.33742
H	-3.84025	2.74553	0.50717
H	0.43675	2.86539	-0.22904
H	-3.83568	-2.77717	0.30978
H	-1.73960	-4.45516	-0.12452
H	0.40284	-2.83248	-0.64467
H	1.32258	0.86483	-1.08838
H	1.49706	0.68985	1.32278
H	1.49053	-1.07109	1.08473
H	3.67886	-2.03782	1.09645
H	6.12594	-1.84592	0.60018
H	6.96811	0.27987	-0.44544
H	5.32675	2.08668	-0.93087

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[BoNH$_2$CH$_2$Py]$^+$

C	-0.49437	3.20464	-0.28561
C	-1.83867	2.76244	-0.40472
N	-1.91870	1.45972	-0.16717
C	-0.64158	1.00267	0.11945
C	0.26172	2.10262	0.04723
N	-2.74701	-0.89683	-0.01727
B	-3.25084	0.60758	-0.04572
C	-1.45199	-1.30987	0.25074
C	-0.45295	-0.35228	0.33391
C	-3.50736	-1.97950	-0.12036
C	-2.72877	-3.14922	0.07837
C	-1.43681	-2.73261	0.31348
N	0.91028	-0.80959	0.58288
C	1.73983	-1.06058	-0.65203
F	-4.03333	0.81148	-1.14010
F	-3.85719	0.89664	1.14075
C	3.14973	-0.59086	-0.33096
C	4.24692	-0.93306	-1.11016
C	5.48340	-0.40663	-0.74774
C	5.57247	0.42373	0.36663
C	4.41717	0.70114	1.08734
N	3.22717	0.20051	0.73868
H	-0.14977	4.21650	-0.43522
H	-2.72650	3.33306	-0.64423
H	1.33148	2.06587	0.21216
H	-4.56582	-1.89065	-0.32717
H	-3.09466	-4.16397	0.04179
H	-0.58026	-3.37050	0.49209
H	1.50389	-0.09450	1.09908
H	1.68704	-2.11710	-0.91805
H	1.29608	-0.46667	-1.45516
H	4.13996	-1.58609	-1.96976
H	6.36851	-0.64632	-1.32695
H	6.52025	0.84615	0.67783
H	4.43596	1.33552	1.96748
H	0.88814	-1.64470	1.17550

36
[BoNHCH$_2$PyH]$^+$

C	-1.16187	3.23441	1.38051
C	-1.88702	2.71334	0.29171
N	-1.67983	1.39832	0.19467
C	-0.78414	1.02650	1.18573
C	-0.44542	2.18079	1.92865
N	-1.95849	-0.95290	-0.44694
B	-1.88631	0.47535	-1.04346
C	-1.09074	-1.32583	0.56518
C	-0.40108	-0.32542	1.29343
C	-2.59496	-2.04305	-0.88232
C	-2.17557	-3.16396	-0.14304
C	-1.22086	-2.71919	0.76157
N	0.68778	-0.68608	2.05884
C	1.73757	-1.47194	1.40968
F	-0.66597	0.52305	-1.78309
F	-2.96577	0.80719	-1.78417
C	2.46287	-0.70030	0.31701
C	3.82762	-0.45949	0.32750
C	4.41609	0.27106	-0.70554
C	3.63307	0.77411	-1.74125
C	2.27398	0.52194	-1.72035
N	1.74787	-0.20213	-0.71878
H	-1.17774	4.25905	1.71938
H	-2.51787	3.22283	-0.42411
H	0.18908	2.22643	2.80409
H	-3.30733	-1.97542	-1.69305
H	-2.55151	-4.16978	-0.25234
H	-0.73396	-3.29934	1.53390
H	1.05987	0.07927	2.60943
H	2.46704	-1.77345	2.16259
H	1.30448	-2.37895	0.98637
H	4.42557	-0.84576	1.14494
H	5.48575	0.45224	-0.69481
H	4.06096	1.35274	-2.55001
H	1.56183	0.86911	-2.46001
H	0.73255	-0.34615	-0.78901

34
[BoNCH$_2$Py]$^+$

C	1.14956	3.31221	-1.15550
C	1.85599	2.66619	-0.09087
N	1.57601	1.36128	-0.07554
C	0.71693	1.11189	-1.11315
C	0.41207	2.34582	-1.78627

N	1.78150	-1.08261	0.29024
B	1.96160	0.29066	1.03250
C	0.84021	-1.33364	-0.68151
C	0.24454	-0.21707	-1.34272
C	2.34628	-2.24698	0.63278
C	1.80584	-3.29658	-0.14949
C	0.86367	-2.72995	-0.98157
N	-0.87866	-0.19541	-2.05401
C	-1.85861	-1.11486	-1.69408
F	1.04934	0.39079	2.05478
F	3.25195	0.46112	1.41683
C	-2.43869	-0.42519	-0.36243
N	-1.58297	-0.17486	0.58404
C	-1.99962	0.26678	1.77070
C	-3.35573	0.49589	2.00040
C	-4.26226	0.26270	0.97018
C	-3.80870	-0.20103	-0.26420
H	1.21776	4.36089	-1.40244
H	2.54471	3.08870	0.63058
H	-0.23617	2.43654	-2.64475
H	3.09291	-2.28478	1.41521
H	2.10175	-4.33350	-0.10324
H	0.30291	-3.22777	-1.75994
H	-2.65755	-1.17070	-2.43092
H	-1.50369	-2.09130	-1.34402
H	-1.23072	0.45482	2.51214
H	-3.68519	0.87400	2.96111
H	-5.32196	0.44293	1.11833
H	-4.48429	-0.40617	-1.08577

34

[BoNHCHPy]$^{+}$

C	1.98227	3.38034	-0.11908
C	3.03372	2.42928	-0.02633
N	2.54116	1.19776	-0.02219
C	1.16095	1.29076	-0.10162
C	0.80409	2.66979	-0.15395
N	2.34385	-1.28147	-0.11729
B	3.32623	-0.13015	0.33900
C	0.97176	-1.15719	-0.24189
C	0.41361	0.12155	-0.17456
C	2.66868	-2.54715	-0.35940
C	1.50803	-3.30016	-0.66164
C	0.43980	-2.43018	-0.59680
N	-0.99910	0.26105	-0.21458
C	-1.85979	-0.50693	0.37056
F	3.48538	-0.18493	1.69423
F	4.48511	-0.20226	-0.36921
C	-3.27794	-0.22685	0.23351
C	-4.22771	-1.02715	0.86212
C	-5.57152	-0.69110	0.68647
C	-5.88082	0.41081	-0.09469
C	-4.84130	1.15525	-0.68287
N	-3.56618	0.84629	-0.52534
H	2.10389	4.45209	-0.15765
H	4.10090	2.59407	0.04547
H	-0.19496	3.07915	-0.22321
H	3.70189	-2.86525	-0.31721
H	1.48497	-4.34769	-0.92057
H	-0.58934	-2.65843	-0.83865
H	-1.41301	1.05430	-0.72137
H	-1.48652	-1.33692	0.96620
H	-3.92974	-1.87863	1.46543
H	-6.35268	-1.28062	1.15277
H	-6.91045	0.70823	-0.25805
H	-5.06160	2.02350	-1.29641

34

[BoNCH$_2$Py]$^{-}$

C	-2.01209	3.35970	-0.46466
C	-3.02805	2.46599	-0.16555
N	-2.50930	1.21830	-0.04729
C	-1.15712	1.29049	-0.26268
C	-0.81742	2.60976	-0.52554
N	-2.34189	-1.23545	0.03039
B	-3.27037	-0.04476	0.40245
C	-0.98200	-1.19773	-0.19018
C	-0.29452	0.10035	-0.23283
C	-2.75992	-2.51784	-0.04115
C	-1.68285	-3.34394	-0.31535
C	-0.55077	-2.51110	-0.40969
N	0.97651	0.31591	-0.28094
C	1.90772	-0.77538	-0.26016
F	-4.47845	-0.16259	-0.27655
F	-3.50333	-0.02500	1.77458
C	3.32501	-0.28792	-0.04405
N	4.28171	-1.22441	-0.10369
C	5.54262	-0.83994	0.09299
C	5.92341	0.47221	0.35535
C	4.92333	1.43854	0.41479
C	3.60384	1.05747	0.21234
H	-2.12685	4.42208	-0.63145
H	-4.08824	2.62522	-0.02897
H	0.18082	2.95477	-0.75236
H	-3.80505	-2.75014	0.10631
H	-1.71146	-4.41719	-0.44077
H	0.44957	-2.83575	-0.64386
H	1.68345	-1.51220	0.52887
H	1.90304	-1.34493	-1.20373
H	6.29453	-1.62618	0.03692
H	6.96821	0.72237	0.50669
H	5.17040	2.47720	0.61690

H	2.77330	1.75249	0.23980

34
[BoNHCHPy]$^-$

C	1.80591	3.37880	-0.35807
C	2.88095	2.53423	-0.14059
N	2.43582	1.25744	-0.02455
C	1.07262	1.26205	-0.16298
C	0.64737	2.57142	-0.37299
N	2.42733	-1.20789	-0.03280
B	3.29005	0.02303	0.36110
C	1.05782	-1.23308	-0.17422
C	0.33179	0.01356	-0.10809
C	2.90191	-2.45899	-0.23099
C	1.85085	-3.31670	-0.51075
C	0.67291	-2.54340	-0.47358
N	-0.98549	0.08100	-0.04284
C	-1.97119	-0.86605	0.07029
F	3.55416	0.01841	1.72581
F	4.48029	0.01412	-0.35435
C	-3.29741	-0.40416	0.08508
C	-4.40510	-1.28638	0.27463
C	-5.68173	-0.78176	0.27302
C	-5.89248	0.59657	0.08708
C	-4.76114	1.38433	-0.08613
N	-3.51056	0.93632	-0.09370
H	1.85255	4.44867	-0.50488
H	3.93713	2.74613	-0.05974
H	-0.36892	2.90061	-0.54816
H	3.96340	-2.64770	-0.16008
H	1.92618	-4.37322	-0.72573
H	-0.32315	-2.87959	-0.71313
H	-1.39808	1.01634	-0.07247
H	-1.69750	-1.88532	0.27951
H	-4.21739	-2.34628	0.41829
H	-6.52724	-1.45055	0.41724
H	-6.88427	1.03217	0.07820
H	-4.87101	2.46011	-0.23074

34
[BoNCH$_2$Py]

C	1.83729	3.39004	-0.38594
C	2.93497	2.49478	-0.17417
N	2.48445	1.23614	-0.06163
C	1.13553	1.25955	-0.19075
C	0.70618	2.62290	-0.39147
N	2.39903	-1.23092	-0.00018
B	3.34546	-0.05316	0.30166
C	1.01793	-1.21434	-0.11257
C	0.32371	0.05603	-0.15370
C	2.81561	-2.51352	-0.06400
C	1.72503	-3.35457	-0.22315
C	0.58459	-2.53939	-0.25459
N	-0.95145	0.32372	-0.18849
C	-1.89622	-0.75510	-0.14193
F	3.67155	0.02848	1.63434
F	4.45673	-0.06727	-0.50456
C	-3.32502	-0.27809	-0.01227
C	-3.65168	1.05286	0.24070
C	-4.99442	1.39328	0.36140
C	-5.95645	0.39921	0.22703
C	-5.52410	-0.90065	-0.02312
N	-4.24181	-1.24239	-0.14219
H	1.91971	4.45806	-0.51946
H	3.99371	2.70470	-0.10240
H	-0.32295	2.91442	-0.53191
H	3.86885	-2.74386	0.01064
H	1.75463	-4.42983	-0.31293
H	-0.42793	-2.88239	-0.38850
H	-1.82065	-1.36485	-1.05607
H	-1.67094	-1.44321	0.68900
H	-2.86105	1.78665	0.33699
H	-5.28493	2.42057	0.55872
H	-7.01462	0.61847	0.31297
H	-6.24483	-1.70759	-0.13496

34
[BoNHCHPy]

C	-1.88356	3.37495	0.25044
C	-2.95353	2.47978	0.12599
N	-2.49154	1.22397	0.05264
C	-1.11759	1.26749	0.11457
C	-0.71815	2.61227	0.23379
N	-2.38845	-1.24116	0.05099
B	-3.32135	-0.04436	-0.33212
C	-1.01272	-1.19877	0.16118
C	-0.36191	0.06351	0.10021
C	-2.79412	-2.49445	0.28559
C	-1.69134	-3.30806	0.56853
C	-0.56379	-2.49458	0.49490
N	0.98689	0.18422	0.06560
C	1.93406	-0.74552	-0.20542
F	-3.56327	-0.04596	-1.68742
F	-4.48014	-0.10335	0.40407
C	3.30232	-0.34236	-0.14028
C	4.34757	-1.23260	-0.45630
C	5.65117	-0.77781	-0.37445
C	5.88840	0.54155	0.01387
C	4.78972	1.35155	0.30277
N	3.53037	0.93855	0.23435
H	-1.95922	4.44739	0.34703
H	-4.01606	2.67113	0.07597

H	0.29352	2.98650	0.32151
H	-3.84625	-2.73861	0.24743
H	-1.72096	-4.35821	0.81653
H	0.44782	-2.78812	0.72994
H	1.38667	1.11003	0.22313
H	1.62422	-1.71748	-0.55745
H	4.11995	-2.25020	-0.75589
H	6.47743	-1.44036	-0.61041
H	6.89399	0.93681	0.09088
H	4.93623	2.38585	0.60472

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trans-BoN=CHPy

C	-2.16640	3.35175	0.05065
C	-3.15016	2.35401	-0.09260
N	-2.59018	1.14359	-0.04503
C	-1.22820	1.31576	0.12520
C	-0.95102	2.69739	0.18633
N	-2.26343	-1.30603	0.15891
B	-3.30691	-0.22592	-0.30158
C	-0.90559	-1.09859	0.31052
C	-0.37829	0.20734	0.25061
C	-2.50247	-2.60892	0.32694
C	-1.30500	-3.28979	0.60918
C	-0.29467	-2.33756	0.60443
N	0.97488	0.43402	0.39815
C	1.80111	-0.16395	-0.36240
F	-3.56039	-0.37433	-1.64622
F	-4.44780	-0.32019	0.45598
C	3.26441	-0.01990	-0.21634
C	4.09283	-0.70641	-1.10512
C	5.47150	-0.57865	-0.96507
C	5.95885	0.22777	0.05322
C	5.04254	0.87369	0.88950
N	3.72578	0.76117	0.76875
H	-2.34503	4.41622	0.06663
H	-4.21892	2.45495	-0.22374
H	0.02885	3.12399	0.34499
H	-3.50930	-2.99329	0.23759
H	-1.20968	-4.34608	0.81003
H	0.75175	-2.48687	0.82988
H	1.45718	-0.81500	-1.17766
H	3.66192	-1.32437	-1.88663
H	6.14637	-1.09731	-1.63769
H	7.02378	0.36217	0.20572
H	5.39525	1.51309	1.69520

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cis-BoN=CHPy

C	1.51793	3.35430	-0.56051
C	2.27859	2.50387	0.26087
N	1.90130	1.23514	0.08068
C	0.87523	1.22485	-0.84549
C	0.62277	2.54812	-1.25380
N	1.90115	-1.23527	0.08060
B	2.24129	-0.00012	0.97745
C	0.87508	-1.22480	-0.84557
C	0.30540	0.00007	-1.24811
C	2.27828	-2.50406	0.26070
C	1.51752	-3.35435	-0.56072
C	0.62245	-2.54801	-1.25397
N	-0.74670	0.00017	-2.12201
C	-1.97545	0.00018	-1.80017
F	1.36909	-0.00010	2.05784
F	3.55654	-0.00021	1.35105
C	-2.61178	0.00011	-0.45516
C	-1.93152	0.00007	0.76803
C	-2.68804	0.00001	1.93584
C	-4.07358	-0.00001	1.84747
C	-4.65614	0.00004	0.58010
N	-3.95134	0.00010	-0.54596
H	1.62926	4.42528	-0.63716
H	3.05995	2.74410	0.96864
H	-0.10235	2.84555	-1.99784
H	3.05962	-2.74443	0.96846
H	1.62872	-4.42534	-0.63745
H	-0.10269	-2.84530	-1.99802
H	-2.70791	0.00024	-2.60864
H	-0.85180	0.00009	0.84295
H	-2.18753	-0.00002	2.89816
H	-4.69626	-0.00006	2.73506
H	-5.73747	0.00003	0.46845

34

BoNHNHPy

C	-1.513719	3.848277	0.596419
C	-2.199323	3.244806	1.653020
N	-1.885610	1.941230	1.713679
C	-0.987384	1.670179	0.710003
C	-0.739844	2.851230	-0.002520
N	-2.002465	-0.469009	2.223520
B	-2.289301	0.942563	2.840511
C	-1.102728	-0.752658	1.214961
C	-0.522147	0.333633	0.497868
C	-2.495593	-1.622624	2.686308
C	-1.939062	-2.696347	1.983989
C	-1.054275	-2.154062	1.054969
N	0.465505	0.171587	-0.377755
N	1.020599	-1.058651	-0.692588
F	-3.626624	1.059246	3.135067
F	-1.493858	1.134743	3.949253
C	1.935049	-1.016489	-1.757185

C	2.701916	-2.155003	-2.044450
C	3.562933	-2.087959	-3.122378
C	3.632455	-0.913142	-3.878318
C	2.829696	0.149670	-3.502353
N	1.995048	0.109730	-2.454566
H	-1.585523	4.883374	0.298573
H	-2.890450	3.669664	2.366767
H	-0.105999	2.965948	-0.872224
H	-3.215542	-1.617087	3.492466
H	-2.168608	-3.741083	2.129538
H	-0.499891	-2.694957	0.304848
H	0.844141	0.942148	-0.921350
H	1.379939	-1.516832	0.143787
H	2.605071	-3.051425	-1.441586
H	4.174912	-2.945923	-3.380472
H	4.292204	-0.829223	-4.732886
H	2.848458	1.085574	-4.053517

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BoNHNHPy Orient2

C	-2.59112	3.14551	-0.20763
C	-3.32295	1.98165	-0.46295
N	-2.58069	0.90428	-0.17517
C	-1.35468	1.33220	0.27746
C	-1.34323	2.73743	0.26183
N	-1.74697	-1.41706	-0.11195
B	-3.06598	-0.57834	-0.20182
C	-0.51595	-0.98865	0.36352
C	-0.33056	0.39255	0.60406
C	-1.67229	-2.72723	-0.34606
C	-0.38768	-3.20058	-0.03740
C	0.34452	-2.11118	0.41215
N	0.81113	0.90840	1.10830
N	1.93067	0.15709	1.36073
F	-3.71405	-0.84916	-1.38336
F	-3.85835	-0.83520	0.89395
C	2.99731	0.22188	0.45207
N	4.17957	-0.08425	0.97719
C	5.23032	-0.09867	0.15379
C	5.15206	0.19673	-1.20140
C	3.90144	0.51587	-1.72755
C	2.79086	0.52900	-0.89770
H	-2.93085	4.15876	-0.35924
H	-4.33097	1.86265	-0.83392
H	-0.52497	3.39116	0.53422
H	-2.53639	-3.25985	-0.71859
H	-0.04294	-4.21816	-0.14190
H	1.37511	-2.10581	0.72573
H	0.89102	1.91671	1.16523
H	2.22615	0.14607	2.33044
H	6.18287	-0.35484	0.61067
H	6.03951	0.17579	-1.82194
H	3.78922	0.74684	-2.78193
H	1.79939	0.75325	-1.27383

34

[BoNHNHPy]$^{+}$

C	-1.86794	3.37230	-0.38749
C	-2.96252	2.44860	-0.18680
N	-2.48758	1.21964	-0.01895
C	-1.12209	1.27836	-0.09565
C	-0.71904	2.63848	-0.32697
N	-2.37050	-1.23526	-0.11199
B	-3.32147	-0.09058	0.36265
C	-0.97978	-1.17959	-0.13940
C	-0.32891	0.06731	-0.02303
C	-2.74085	-2.48408	-0.37012
C	-1.60058	-3.29630	-0.58913
C	-0.49581	-2.48843	-0.43328
N	0.97700	0.23348	0.11188
N	1.88037	-0.80873	0.12722
F	-4.48087	-0.09053	-0.34420
F	-3.46832	-0.11375	1.71531
C	3.22906	-0.34682	0.11130
C	4.26957	-1.26068	0.27279
C	5.55969	-0.75800	0.21576
C	5.75854	0.60655	-0.00468
C	4.64622	1.41949	-0.15275
N	3.39168	0.95061	-0.09084
H	-1.97086	4.43318	-0.56245
H	-4.02781	2.64000	-0.16130
H	0.29230	2.99677	-0.45953
H	-3.78895	-2.75324	-0.37974
H	-1.61364	-4.34654	-0.83811
H	0.53642	-2.76606	-0.57635
H	1.45247	1.14210	0.08503
H	1.68091	-1.44963	0.89742
H	4.07009	-2.31549	0.42589
H	6.40620	-1.42521	0.33602
H	6.75445	1.02789	-0.06055
H	4.74835	2.48629	-0.32412

34

[BoNHNHPy]$^{-}$

C	-0.822325	3.785497	1.869923
C	-1.462290	2.843027	2.657494
N	-1.576144	1.673016	1.972004
C	-1.010110	1.844621	0.728954
C	-0.527629	3.159588	0.638129
N	-1.884775	-0.735261	1.467382
B	-2.255493	0.372624	2.486583
C	-1.346148	-0.536591	0.210915

C	-0.952306	0.760212	-0.193710
C	-2.131696	-2.064255	1.611694
C	-1.754370	-2.738689	0.458248
C	-1.254816	-1.775530	-0.440235
N	-0.295908	0.929238	-1.447575
N	1.120268	0.873527	-1.301917
F	-3.638581	0.540194	2.553107
F	-1.774191	0.050874	3.754639
C	1.786259	-0.248854	-1.752788
C	3.005593	-0.607576	-1.134738
C	3.716563	-1.676102	-1.639398
C	3.212177	-2.378251	-2.737408
C	2.001949	-1.946823	-3.262308
N	1.298459	-0.909592	-2.806509
H	-0.589726	4.802000	2.156717
H	-1.843530	2.917787	3.665984
H	-0.014351	3.590092	-0.212430
H	-2.563479	-2.437261	2.529824
H	-1.829848	-3.805353	0.295480
H	-0.860220	-1.914321	-1.437149
H	-0.508681	1.845987	-1.828177
H	1.421022	1.189632	-0.382591
H	3.356501	-0.053594	-0.269815
H	4.651991	-1.973207	-1.173497
H	3.731531	-3.229837	-3.161007
H	1.564284	-2.465691	-4.114428

35

[BoNH$_2$NHPy]$^+$

C	-2.93805	3.04425	-0.34581
C	-3.63670	1.82373	-0.16392
N	-2.78164	0.81102	-0.08748
C	-1.50124	1.32194	-0.21365
C	-1.59549	2.73453	-0.37415
N	-1.81169	-1.49375	-0.01789
B	-3.14335	-0.68935	0.28132
C	-0.54597	-0.94210	-0.15670
C	-0.43442	0.43304	-0.23875
C	-1.68337	-2.81295	-0.04673
C	-0.31730	-3.17349	-0.20273
C	0.40075	-2.00167	-0.26738
N	0.90268	1.00343	-0.39784
N	1.71093	0.90169	0.77237
F	-4.14754	-1.13547	-0.52038
F	-3.41645	-0.76057	1.61616
C	3.04637	0.56001	0.42058
C	4.09133	0.62739	1.33656
C	5.33284	0.19959	0.88807
C	5.48229	-0.27241	-0.41904
C	4.37164	-0.29816	-1.24501
N	3.16790	0.11963	-0.82293
H	-3.38739	4.02047	-0.44536
H	-4.70184	1.65128	-0.08271
H	-0.78562	3.44221	-0.50264
H	-2.55220	-3.45170	0.04489
H	0.06361	-4.18172	-0.26055
H	1.47037	-1.89231	-0.38852
H	0.83250	1.96670	-0.74887
H	1.53723	0.46653	-1.09471
H	1.57562	1.68103	1.40793
H	3.93513	0.98596	2.34746
H	6.18504	0.23046	1.55833
H	6.44235	-0.61196	-0.78672
H	4.42477	-0.65207	-2.26880

35

[BoNHNH$_2$Py]$^+$

C	0.32921	2.97892	-1.58701
C	-0.77280	2.88819	-0.69581
N	-1.08742	1.61762	-0.48180
C	-0.19249	0.82815	-1.19400
C	0.71048	1.68895	-1.88361
N	-2.26079	-0.42670	0.29454
B	-1.91658	1.03833	0.73339
C	-1.41230	-1.17685	-0.49583
C	-0.34797	-0.55074	-1.15933
C	-3.22871	-1.22748	0.74112
C	-3.04113	-2.53564	0.24361
C	-1.89506	-2.51100	-0.53428
N	0.62606	-1.41783	-1.73274
N	1.33567	-2.08498	-0.64223
F	-3.03152	1.77083	0.96670
F	-1.04684	0.96084	1.81271
C	2.14364	-1.17291	0.20510
C	1.57429	-0.53190	1.29020
C	2.40645	0.37731	1.94450
C	3.70532	0.56404	1.48419
C	4.14228	-0.14877	0.36640
N	3.35557	-1.01122	-0.28301
H	0.76733	3.89363	-1.95652
H	-1.31608	3.68028	-0.19676
H	1.50582	1.39338	-2.55550
H	-4.00462	-0.84265	1.38918
H	-3.69560	-3.37624	0.41741
H	-1.49964	-3.31389	-1.14379
H	1.34238	-0.90247	-2.24580
H	0.61265	-2.58173	-0.10224
H	1.97158	-2.77135	-1.06909
H	0.54505	-0.68084	1.60167
H	2.02604	0.93141	2.79539
H	4.37608	1.25920	1.97518
H	5.14637	-0.02520	-0.02568

35
[BoNHNHPyH]$^+$

C	-3.13774	2.92388	-0.25309
C	-3.71717	1.64161	-0.37355
N	-2.79589	0.70317	-0.17789
C	-1.59135	1.32691	0.08876
C	-1.80204	2.73015	0.04340
N	-1.61310	-1.47032	-0.13698
B	-3.05270	-0.83670	-0.01182
C	-0.40974	-0.82973	0.11603
C	-0.42656	0.56885	0.26613
C	-1.37266	-2.75819	-0.35690
C	0.00998	-3.01521	-0.26199
C	0.61863	-1.81134	0.03859
N	0.74391	1.30308	0.52627
N	1.77811	0.68164	1.20241
F	-3.84950	-1.30217	-1.01631
F	-3.54207	-1.08260	1.24235
C	2.93704	0.43994	0.54974
C	4.01727	-0.25343	1.12658
C	5.16043	-0.43368	0.38316
C	5.26112	0.06635	-0.93333
C	4.18967	0.72970	-1.45771
N	3.06308	0.89563	-0.71109
H	-3.65036	3.86511	-0.37975
H	-4.74274	1.36723	-0.58047
H	-1.06244	3.50966	0.17309
H	-2.18801	-3.43687	-0.56766
H	0.48903	-3.97163	-0.40597
H	1.68185	-1.66787	0.15414
H	0.54839	2.21704	0.92409
H	1.56828	0.16293	2.05028
H	3.92803	-0.62520	2.14057
H	5.99782	-0.96767	0.81963
H	6.15827	-0.06803	-1.52251
H	4.15928	1.14728	-2.45599
H	2.24618	1.36714	-1.09856

33
[BoNNHPy]$^+$

C	-2.30221	3.33240	-0.20342
C	-3.23985	2.27266	0.01227
N	-2.62167	1.10120	0.00766
C	-1.27554	1.33665	-0.20420
C	-1.06811	2.75178	-0.32531
N	-2.17077	-1.34320	-0.11292
B	-3.21943	-0.30856	0.44749
C	-0.83000	-1.08808	-0.32054
C	-0.40170	0.25578	-0.29053
C	-2.39021	-2.63842	-0.34416
C	-1.19011	-3.27155	-0.73152
C	-0.20501	-2.30140	-0.72841
N	0.93994	0.63833	-0.33749
N	1.76767	-0.18770	0.08727
F	-4.43004	-0.50021	-0.13818
F	-3.22732	-0.35419	1.81089
C	3.17429	0.01453	0.09857
N	3.79206	-1.02461	0.64267
C	5.11749	-0.95473	0.71559
C	5.83638	0.15093	0.24675
C	5.14962	1.22070	-0.32192
C	3.76227	1.16664	-0.40965
H	-2.54853	4.38134	-0.26910
H	-4.31039	2.32914	0.16567
H	-0.12081	3.23266	-0.51864
H	-3.38175	-3.05471	-0.22731
H	-1.08136	-4.31011	-1.00406
H	0.81713	-2.43659	-1.05829
H	1.47109	-1.09283	0.49729
H	5.62217	-1.80570	1.16106
H	6.91705	0.16436	0.32791
H	5.68532	2.08648	-0.69433
H	3.16917	1.96276	-0.84322

33
[BoNHNPy]$^+$

C	-2.02862	3.34750	-0.40409
C	-3.06357	2.38806	-0.27273
N	-2.54369	1.17351	-0.11428
C	-1.17166	1.28659	-0.13218
C	-0.83662	2.66186	-0.31211
N	-2.28972	-1.30146	-0.03280
B	-3.33797	-0.14870	0.23908
C	-0.90207	-1.17210	-0.03779
C	-0.39196	0.11979	-0.06528
C	-2.58006	-2.59055	-0.10637
C	-1.38644	-3.36375	-0.16557
C	-0.33388	-2.48388	-0.11694
N	1.00070	0.37451	-0.05797
N	1.86676	-0.51837	-0.00789
F	-4.40728	-0.28672	-0.58947
F	-3.65013	-0.13343	1.56700
C	3.21838	-0.15279	0.04569
N	4.00384	-1.17867	-0.29456
C	5.30992	-0.96255	-0.30895
C	5.88208	0.26793	0.04921
C	5.05304	1.31209	0.44570
C	3.67841	1.10927	0.44712
H	-2.16423	4.40732	-0.55615
H	-4.13622	2.52928	-0.28261
H	0.14739	3.10652	-0.39580

H	-3.61115	-2.92016	-0.10903
H	-1.33706	-4.43928	-0.24221
H	0.71756	-2.71955	-0.15504
H	1.26370	1.36804	-0.10075
H	5.93436	-1.80073	-0.60220
H	6.95965	0.38718	0.03692
H	5.46737	2.26220	0.76314
H	3.01824	1.89270	0.80882

33

[BoNNHPy]$^-$

C	-2.48361	3.28252	-0.33830
C	-3.34767	2.23631	-0.06213
N	-2.64191	1.07826	0.01376
C	-1.31933	1.36740	-0.20680
C	-1.18583	2.72941	-0.42738
N	-2.13001	-1.32821	-0.04055
B	-3.18057	-0.29515	0.46729
C	-0.80677	-1.07511	-0.30407
C	-0.31028	0.30583	-0.19841
C	-2.38420	-2.63304	-0.29442
C	-1.22936	-3.25329	-0.73633
C	-0.22011	-2.26641	-0.74573
N	0.92607	0.68183	-0.11347
N	1.85381	-0.32100	-0.03784
F	-4.41171	-0.56276	-0.11935
F	-3.28905	-0.35853	1.85267
C	3.18982	-0.05328	0.06890
C	4.05514	-1.11103	0.44656
C	5.40913	-0.86721	0.50878
C	5.89391	0.41011	0.20485
C	4.95780	1.37151	-0.15037
N	3.64214	1.17041	-0.22758
H	-2.76113	4.31903	-0.47312
H	-4.41798	2.22629	0.08603
H	-0.25345	3.23178	-0.63963
H	-3.38154	-3.02249	-0.14998
H	-1.12831	-4.28816	-1.03155
H	0.78660	-2.38697	-1.11951
H	1.53362	-1.22014	0.31065
H	3.64408	-2.08783	0.68325
H	6.08919	-1.66377	0.79797
H	6.95051	0.64698	0.24410
H	5.28561	2.38137	-0.39568

33

[BoNHNPy]$^-$

C	-1.88320	3.37750	-0.25447
C	-2.93271	2.48201	-0.12236
N	-2.44456	1.22236	-0.02751
C	-1.07756	1.28530	-0.09631
C	-0.69633	2.61707	-0.24184
N	-2.32864	-1.24603	-0.05046
B	-3.29329	-0.05732	0.20367
C	-0.94868	-1.20754	-0.08642
C	-0.28542	0.06772	-0.05474
C	-2.71214	-2.53702	-0.13475
C	-1.59372	-3.35554	-0.22916
C	-0.46760	-2.51465	-0.19620
N	1.02034	0.19704	-0.02458
N	1.92196	-0.81244	-0.03791
F	-4.35467	-0.09677	-0.69049
F	-3.77297	-0.09005	1.50743
C	3.18151	-0.33447	0.01346
C	4.25758	-1.27377	0.00582
C	5.54880	-0.81602	0.05445
C	5.80318	0.56873	0.11085
C	4.70195	1.40755	0.11396
N	3.43262	1.00076	0.06854
H	-1.96663	4.44963	-0.36173
H	-3.99951	2.65013	-0.09310
H	0.31311	2.99149	-0.35176
H	-3.76369	-2.78715	-0.11813
H	-1.59881	-4.43278	-0.31752
H	0.57588	-2.77512	-0.25341
H	1.42676	1.13628	0.01591
H	4.01423	-2.32941	-0.03847
H	6.37426	-1.52398	0.04955
H	6.80963	0.96779	0.15066
H	4.84399	2.48816	0.15691

33

[BoNNHPy]

C	-2.29242	3.32819	-0.22247
C	-3.23582	2.29060	-0.05138
N	-2.61530	1.10608	-0.02290
C	-1.26625	1.33314	-0.16237
C	-1.04691	2.72968	-0.28021
N	-2.17886	-1.32570	-0.06825
B	-3.24110	-0.27613	0.38626
C	-0.83426	-1.09539	-0.25346
C	-0.34602	0.25841	-0.18812
C	-2.42813	-2.62470	-0.31262
C	-1.24991	-3.27185	-0.67642
C	-0.23646	-2.30792	-0.64765
N	0.94420	0.63654	-0.16039
N	1.81339	-0.30466	0.10646
F	-4.42247	-0.47670	-0.28501
F	-3.40305	-0.30981	1.75287
C	3.19325	-0.06732	0.11220
C	4.02801	-1.08915	0.58274
C	5.39337	-0.85586	0.57112

C	5.86713	0.36730	0.10117
C	4.93712	1.30452	-0.34062
N	3.61992	1.10257	-0.34424
H	-2.52113	4.38024	-0.30163
H	-4.31045	2.34496	0.05629
H	-0.07966	3.18924	-0.41855
H	-3.43383	-3.00875	-0.22009
H	-1.15019	-4.31119	-0.95030
H	0.78554	-2.45493	-0.96871
H	1.48035	-1.20114	0.46258
H	3.61419	-2.02453	0.94596
H	6.07858	-1.61788	0.92686
H	6.92667	0.59119	0.07564
H	5.26539	2.27030	-0.71610

33

[BoNHNPy]

C	-1.85817	3.37390	-0.22690
C	-2.92685	2.47158	-0.14103
N	-2.46087	1.21917	-0.04843
C	-1.08689	1.26942	-0.06804
C	-0.69108	2.61734	-0.18062
N	-2.33012	-1.25156	-0.05738
B	-3.32219	-0.06460	0.18640
C	-0.94397	-1.19498	-0.06246
C	-0.32330	0.07026	-0.03903
C	-2.69282	-2.53163	-0.15109
C	-1.55530	-3.35355	-0.22313
C	-0.45077	-2.51687	-0.16467
N	1.02669	0.23419	-0.01812
N	1.89365	-0.75492	-0.01628
F	-4.35449	-0.11819	-0.71905
F	-3.77396	-0.09314	1.48613
C	3.20234	-0.30567	0.01653
C	4.21673	-1.27732	0.02419
C	5.53123	-0.84662	0.05732
C	5.79690	0.52332	0.08196
C	4.71935	1.40761	0.07193
N	3.45027	1.01406	0.03985
H	-1.93716	4.44621	-0.32135
H	-3.99174	2.65647	-0.14016
H	0.31998	2.99772	-0.24460
H	-3.74075	-2.79835	-0.15859
H	-1.55552	-4.42923	-0.31380
H	0.59058	-2.78822	-0.20375
H	1.41466	1.18117	0.01068
H	3.94311	-2.32545	0.00490
H	6.34318	-1.56606	0.06447
H	6.81154	0.90197	0.10848
H	4.88743	2.48136	0.09077

32

trans-BoN=NPy

C	-2.314339	3.441549	0.677305
C	-3.294254	2.508105	1.074517
N	-2.827059	1.265516	0.944587
C	-1.534981	1.345752	0.462327
C	-1.203541	2.711152	0.290422
N	-2.666299	-1.203650	0.765438
B	-3.557949	-0.056799	1.363711
C	-1.355449	-1.087949	0.317015
C	-0.794411	0.187496	0.195029
C	-3.003944	-2.489800	0.720505
C	-1.927999	-3.262268	0.232180
C	-0.890951	-2.386019	-0.025103
N	0.515270	0.434553	-0.287510
N	1.321792	-0.486187	-0.064981
F	-4.813523	-0.102572	0.810233
F	-3.589264	-0.157937	2.733825
C	2.631417	-0.240351	-0.587876
N	3.379729	-1.339908	-0.619689
C	4.619203	-1.218612	-1.090965
C	5.161951	-0.009570	-1.522464
C	4.368131	1.132647	-1.466548
C	3.068955	1.023322	-0.992028
H	-2.431894	4.514506	0.669696
H	-4.298989	2.678152	1.436987
H	-0.263758	3.076881	-0.095113
H	-3.989818	-2.804858	1.035246
H	-1.933827	-4.331695	0.086134
H	0.091752	-2.613176	-0.407574
H	5.210811	-2.129848	-1.118685
H	6.182635	0.031632	-1.885284
H	4.756872	2.093725	-1.786654
H	2.400140	1.872186	-0.925963

32

cis-BoN=NPy

C	-2.91540	2.68470	0.02259
C	-3.22928	1.41056	0.53471
N	-2.28034	0.53299	0.20259
C	-1.32168	1.20663	-0.53185
C	-1.70984	2.55868	-0.65186
N	-1.04852	-1.58382	-0.21823
B	-2.17448	-0.95732	0.68350
C	-0.08783	-0.86742	-0.91426
C	-0.21291	0.51795	-1.03741
C	-0.73045	-2.87414	-0.30044
C	0.44636	-3.04116	-1.06232
C	0.85529	-1.77735	-1.44978
N	0.68562	1.23352	-1.87049
N	1.89007	1.35439	-1.62116

F	-3.36211	-1.61115	0.48236	H	-4.08470	1.09452	1.11601
F	-1.77286	-0.98796	1.99916	H	-1.17039	3.31588	-1.20336
C	2.41814	0.88982	-0.35804	H	-1.34408	-3.61903	0.18808
N	3.47778	0.10275	-0.48194	H	0.91851	-3.98326	-1.29580
C	4.03836	-0.33201	0.64718	H	1.71819	-1.50815	-2.04406
C	3.59733	0.03658	1.91609	H	4.88941	-0.99742	0.52952
C	2.51118	0.89957	2.01595	H	4.10154	-0.33784	2.79918
C	1.89451	1.34283	0.85235	H	2.14233	1.21984	2.98442
H	-3.51890	3.57348	0.12721	H	1.04028	2.01032	0.87475

17) Reference

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