Supporting Information Associated with: *Discovery of Low-Energy Pathways to B=N Bond Reduction via η^6-Coordination Guided by Computation and Experiment*

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1. Additional Computational Information

Table S-1. Experimental and calculated carbonyl stretching frequencies for M-$Me_3B_3N_3Me_3$ complexes (Et_2O solution). Calculations were undertaken at the B3LYP/6-31G(d,p)//B3LYP/6-311++G(d,p) level of theory in Et_2O.

Compound	V_{co} Experimental			V_{co} Calculated		
1	1951	1844		1957	1860	1857
2	2072	1997		2069	2002	2001
3	1806	1773	1713	1898	1784	1783
4	2023	1935	1906	2016	1929	1929
5	2011	1944	1930	2046	1926	1902

Table S-2. Experimental and calculated redox potentials for reduced and oxidized $Me_3B_3N_3Me_3$ complexes (Et_2O solution).

Complex	$E_{1/2}$ Experimental	$E_{1/2}$ Calculated
4	0.6	0.12
5	-1.38	-1.49

Table S-3. Calculated pK_a values of $Me_3B_3N_3Me_3$ complexes (Et_2O solution).

Complex	**pK_a (of conjugate acid)**
$H_3B_3N_3H_3$	-15.4
$Me_3B_3N_3Me_3$	-4.3
1	-17
2	-47.7
3 (at N1)	20.8
3 (at H^-)	24.7
4 (at N1)	-1
4 (at H^-)	-5.3

Table S-4. Calculated BDFE values for **4**, hydroquinone species, and reaction solvents.

Compound	BDFE (kcal/mol)
4	52.8
5	39
9,10-H_2-AQ	52.9
CH_2Cl_2	86.4
2-Me-THF	81.7

Table S-5. Calculated thermodynamic hydricity of $Me_3B_3N_3Me_3$ and metal- $Me_3B_3N_3Me_3$ hydride adducts (Et_2O solution).

Complex	ΔG_{H-}
$(H_4B_3N_3H_3)^-$	9.2
$(HMe_3B_3N_3Me_3)^-$	4.0
3	41.1
4	68.7
6	37.2
4-hydroxyphenolate	56.7

Table S-6. NICS(0) values for the M-borazine complexes using the B3LYP/6-31G(d,p) level of theory in Et_2O.

Complex	NICS(0)
$H_3B_3N_3H_3$	-2.678
$[H_4B_3N_3H_3]^-$	0.7981
$[H_3B_3N_3H_4]^+$	0.8697
$[H_4B_3N_3H_4]$	-0.1066
$[H_5B_3N_3H_5]$	-1.8779
$[H_6B_3N_3H_6]$	-1.444
$Me_3B_3N_3Me_3$	-2.8162
$[HMe_3B_3N_3Me_3]^-$	-0.2325
$[Me_3B_3N_3Me_3H]^+$	-0.1514
$[HMe_3B_3N_3Me_3H]$	-1.1816
$[H_2Me_3B_3N_3Me_3H_2]$	-1.5802

Complex	NICS(0)
$[H_3Me_3B_3N_3Me_3H_3]$	-0.9452
$[(Me_3B_3N_3Me_3)Mn(CO)_3]^+$	-13.1629
$[(Me_3B_3N_3Me_3)MnH(CO)_3]$	-3.6748
$[(Me_3B_3N_3Me_3)MnH(CO)_3]^{2+}$	-3.481
$[(Me_3B_3N_3Me_3)Mn(CO)_3]$	-6.3918
$[(Me_3B_3N_3Me_3)Cr(CO)_3]$	-14.5557
$[(Me_3B_3N_3Me_3)CrH(CO)_3]^-$	-3.512
$[(Me_3B_3N_3Me_3)CrH(CO)_3]^+$	-6.9172
$[(Me_3B_3N_3Me_3)Cr(CO)_3]^+$	6.1817

2. NMR Spectra

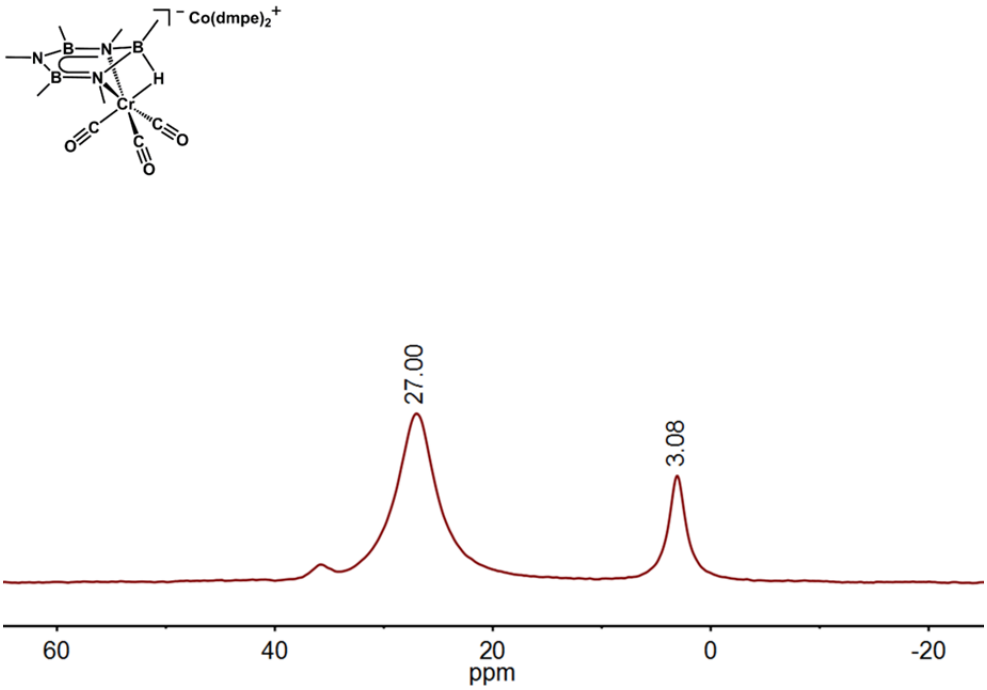


Figure S-1. ^{11}B NMR spectrum of **3** from reaction of **1** with $HCo(dmpe)_2$, 160.4 MHz, 2-Me-THF, -30 ºC.

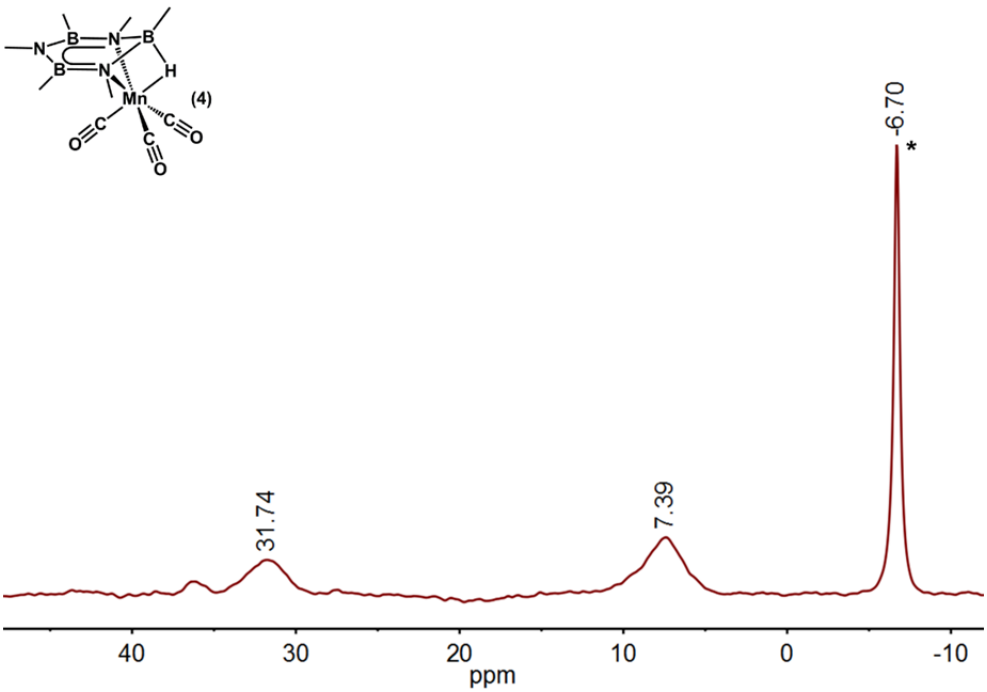


Figure S-2. ^{11}B NMR spectrum of **4** synthesized by reaction of **2** with Cp_2Co and 9,10-anthraquinone, 128.2 MHz, 2-Me-THF. Residual BAr' salt used as internal integration standard.

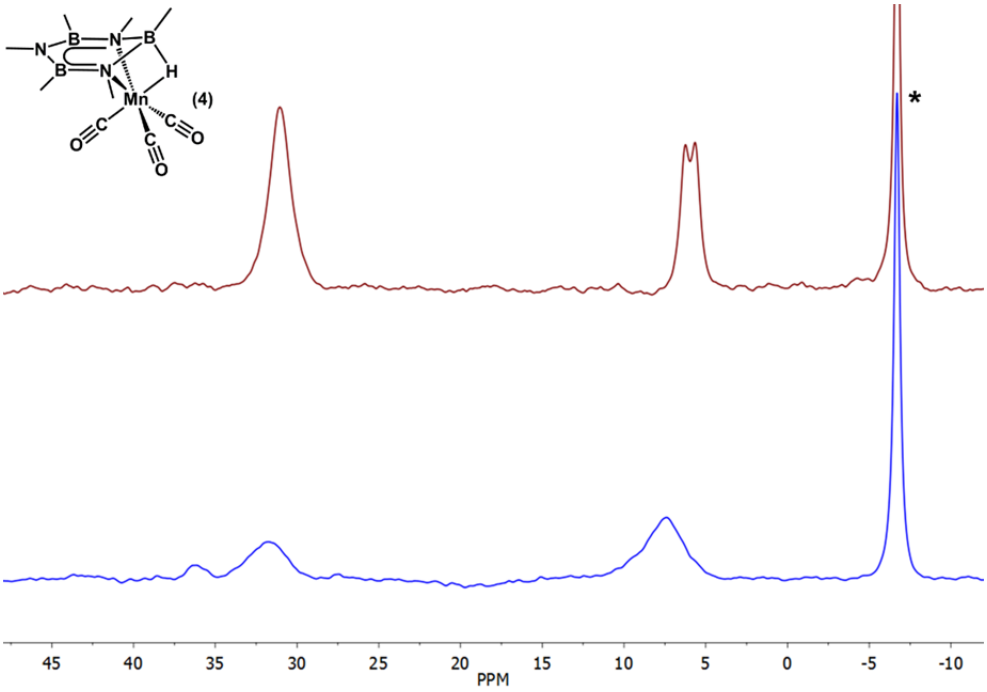


Figure S-3. Overlaid ^{11}B NMR spectra of **4** synthesized by $NaEt_3BH$ addition (Top) and addition of Cp_2Co and 9,10-anthraquinone (Bottom). .*Residual BAr' salt used as internal integration standard. CH_2Cl_2

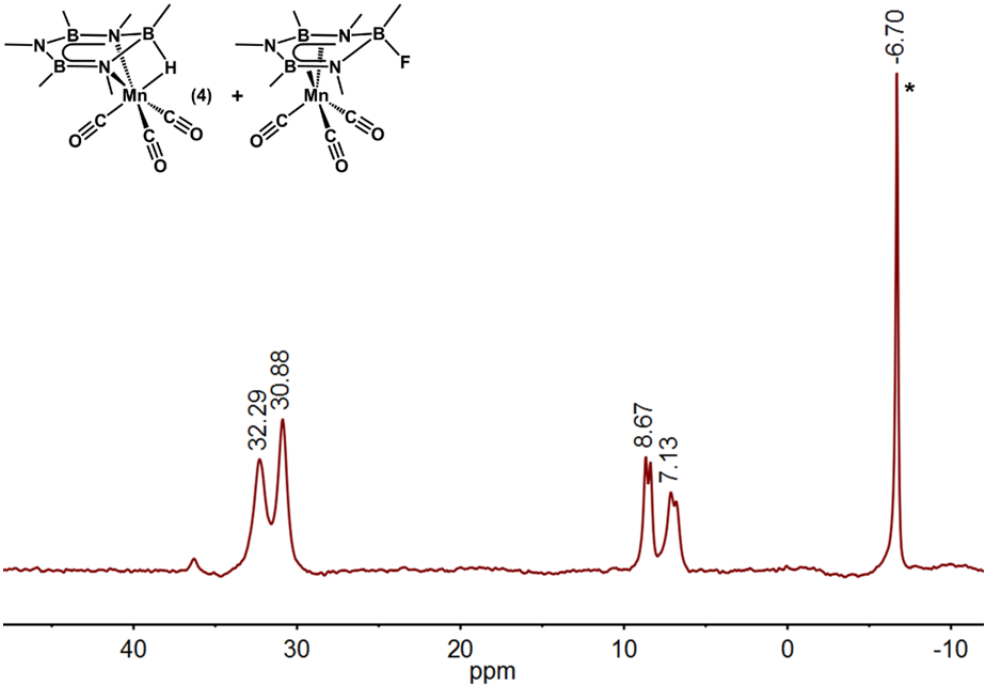


Figure S-4. ^{11}B NMR spectrum of solution containing **4** and $(FMe_3B_3N_3Me_3)Cr(CO)_3$ following controlled potential electrolysis, 128.2 MHz, 0.1 M $TBAPF_6$ in CH_2Cl_2. .*Residual BAr' salt used as internal integration standard.

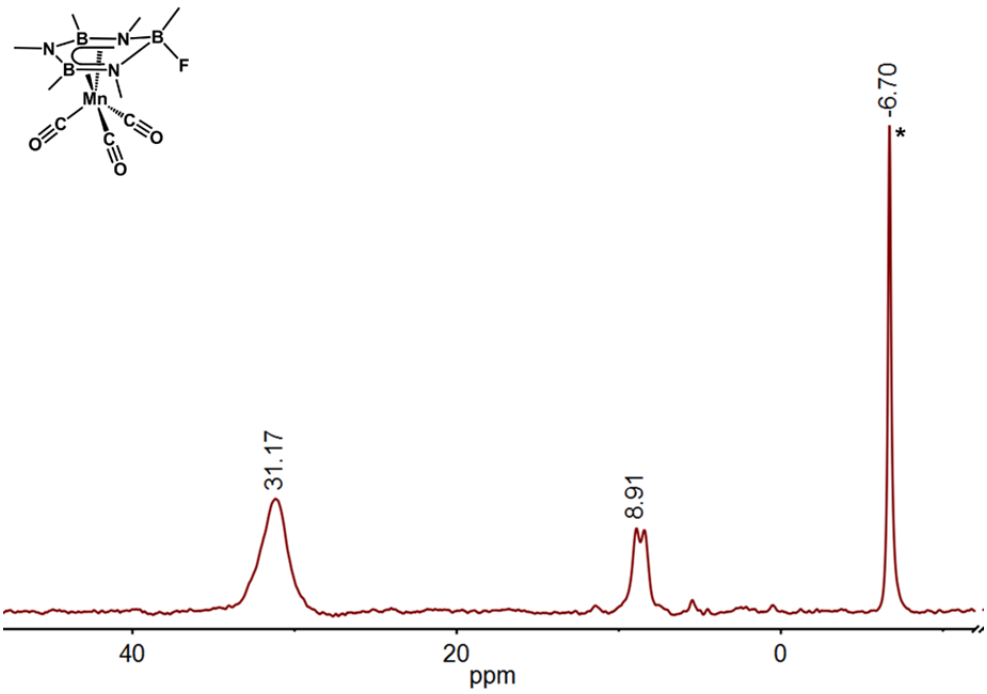


Figure S-5. ^{11}B NMR spectrum of $(FMe_3B_3N_3Me_3)Mn(CO)_3$ synthesized by addition of TBAF to **2**, 128.2 MHz, CH_2Cl_2. . *Residual BAr' salt used as internal integration standard.

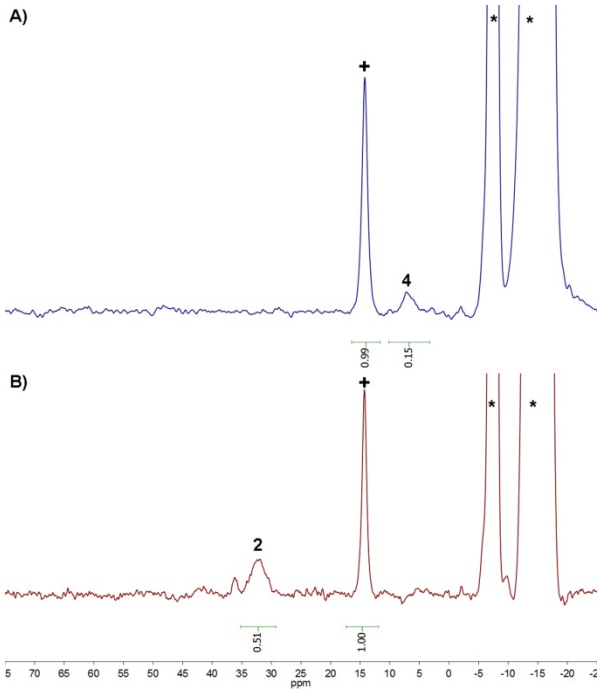


Figure S-6. ^{11}B NMR spectrum of solution following CPE of **2** and 9,10-anthraquinone (A) and solution of **2** (at identical concentration) used as control to determine yield (B) in 0.05 M $TBAB_{11}CH_{12}$ in CH_2Cl_2, 500.1 MHz, 0.1 M $TBAPF_6$ in CH_2Cl_2. $^{+}(TMSO)_3B$ used as external standard, * Electrolyte

3. IR Spectra

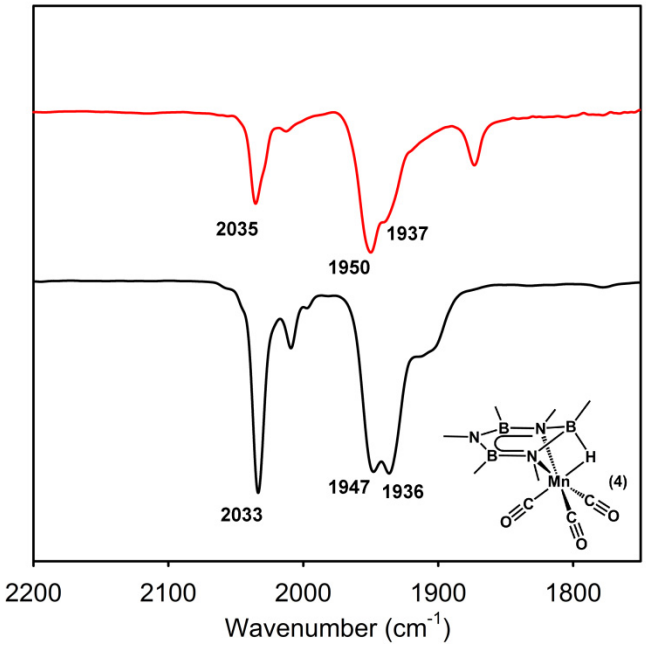


Figure S-7. Overlayed solution-cell IR spectrum of **4** synthesized by $NaEt_3BH$ addition (Top, Et_2O solution) and addition of Cp_2Co and 9,10-anthraquinone (Bottom, 2-Me-THF solution), KBr plate solution cell.

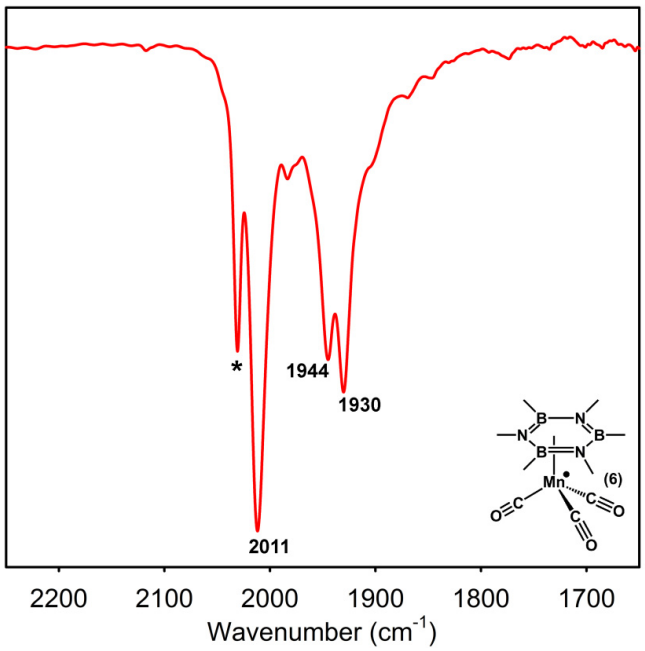


Figure S-8. IR spectrum of solution containing **5**, KBr solution cell, 2-Me-THF solution. *Unidentified by-product.

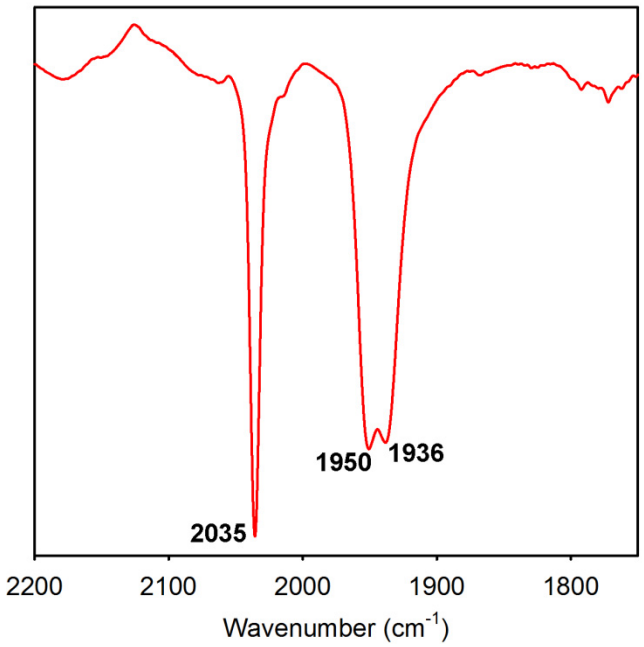


Figure S-9. IR spectrum of solution following controlled potential electrolysis in 0.05 M [$^{n}Bu_4N$][$CB_{11}H_{12}$], KBr plate solution cell, DCM solution.

4. Mass Spectra

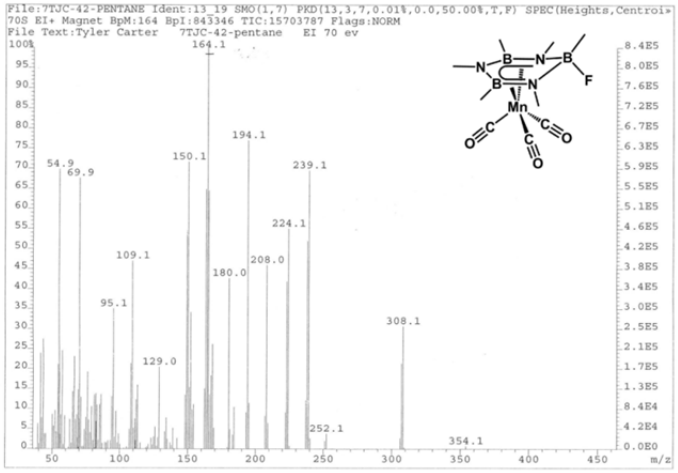


Figure S-10. MS of Mn-F adduct collected by EI ionization.

5. EPR Spectra

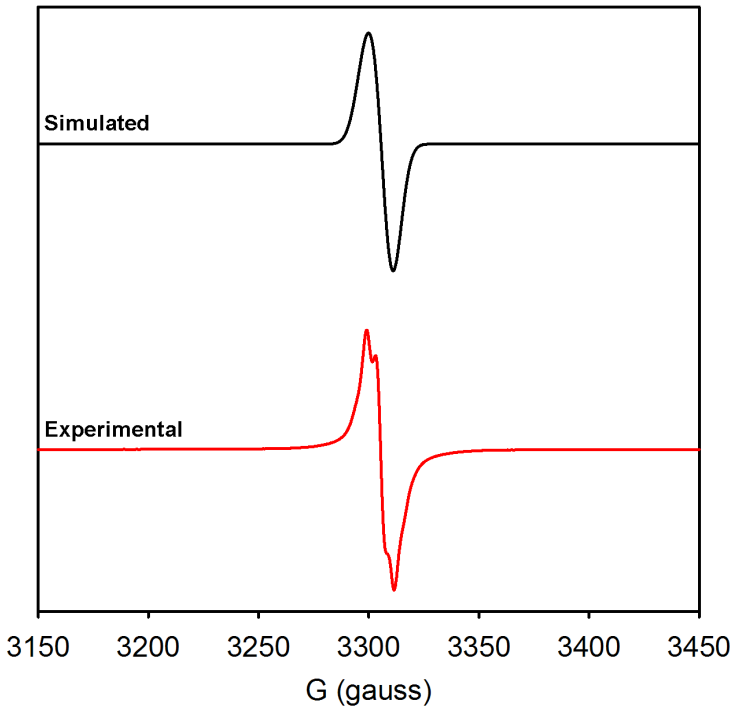


Figure S-11. Experimental (bottom) and simulated (top) X-Band EPR spectrum of DMPO-trapped semiquinone radical, 2-Me-THF, 77 K. (g_x = 1.9949, g_y = 1.9953, g_z = 1.9977)

Note: Further evidence for the intermediacy of a single-electron transfer product was provided by performing the reduction in the presence (excess) of the spin-trapping agent 5,5-Dimethyl-1-Pyrroline-N-Oxide (DMPO), which showed a reduced (30%) yield of **4**. Additionally, a spin-trapped product was observed in the above EPR spectroscopy which suggests an S=½ system that is nearly isotropic (g_x = 1.9949, g_y = 1.9953, g_z = 1.9977). The absence of pronounced ^{55}Mn coupling, and the relatively small shift in g-values as compared to the free electron value, suggests a primarily organic centered radical species consistent with a spin-trapped semiquinone.

6. Electrochemistry

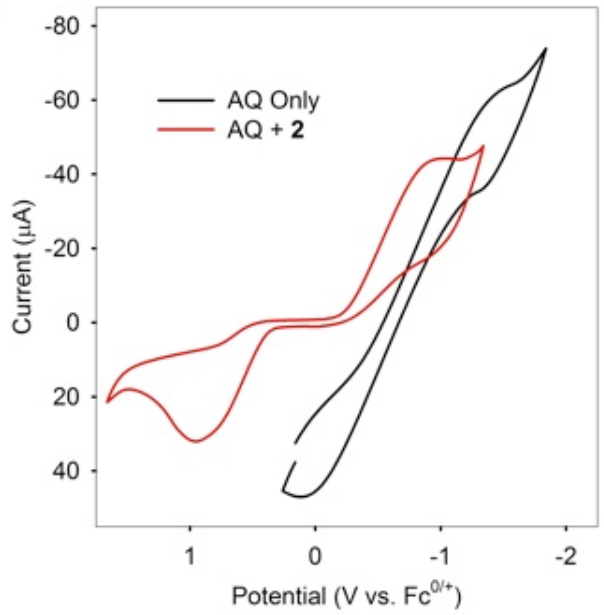


Figure S-12. CV of solution containing AQ with (red) and without (black) added **2**, 0.05 M $^{n}Bu_4NBAr'$/2-Me-THF (100 mV/s).

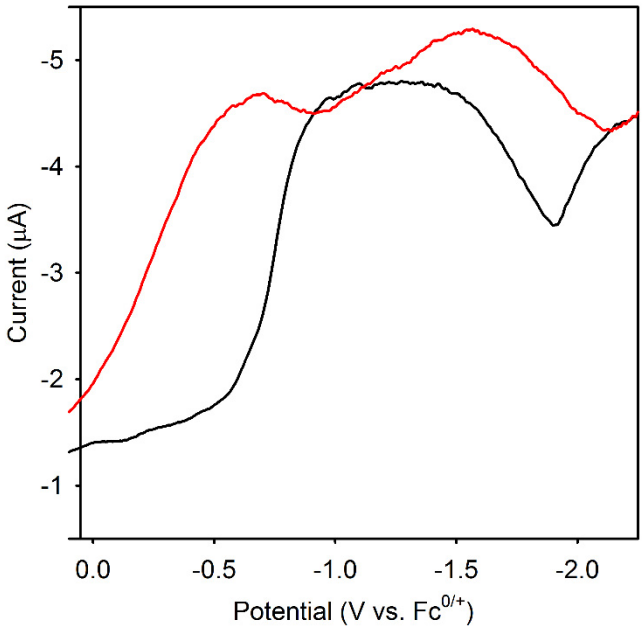


Figure S-13. DPV of AQ solution with (red) and without (black) added **2**, 0.05 M $^{n}Bu_4NBAr'$/2-Me-THF.

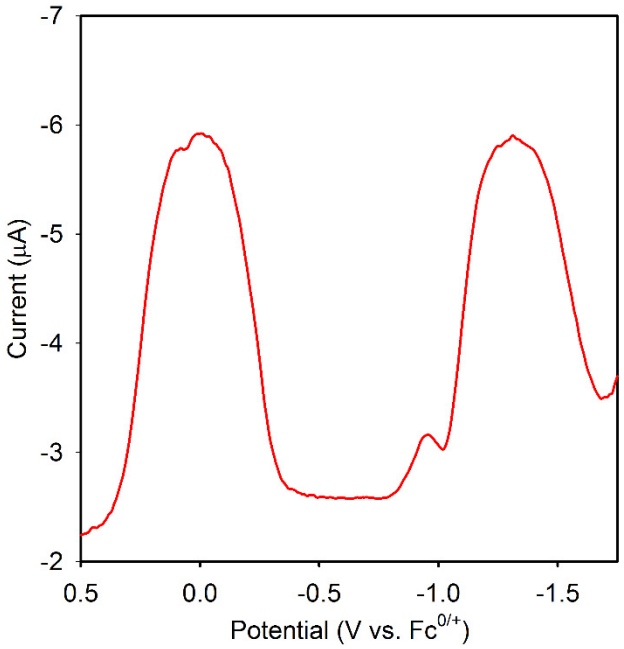


Figure S-14. DPV of solution containing Cp_2Fe and Cp_2Co, 0.05 M $^{n}Bu_4NBAr'$/2-Me-THF.

7. XYZ Coordinates for All Computed Complexes

*(η^6-$Me_3B_3N_3Me_3$)$Cr(CO)_3$ (**1**)*

Cr	-0.00084	0.00354	0.66235
N	-0.38153	-1.37799	-1.06356
N	-0.98873	1.00355	-1.08692
O	0.65654	2.39544	2.34836
N	1.37714	0.33839	-1.07879
O	1.71793	-1.72440	2.41176
O	-2.39321	-0.57901	2.37585
C	0.39894	1.45941	1.70244
B	-1.44508	-0.38167	-1.16975
B	0.40678	1.42607	-1.17952
C	2.14148	-2.20471	-1.36095
C	1.04615	-1.05256	1.73588
C	-1.45750	-0.35468	1.71685
C	2.80694	0.70222	-0.98383
B	1.04582	-1.08218	-1.15978
C	-2.01943	2.05988	-0.99671
C	-0.78155	-2.79650	-0.94601
C	-2.96274	-0.77173	-1.38235
C	0.83225	2.93408	-1.39459
H	2.99740	-1.84172	-1.93798
H	1.74608	-3.07810	-1.88773
H	2.53575	-2.56456	-0.40235
H	3.24820	0.80510	-1.98133
H	3.35673	-0.06213	-0.43549
H	2.92428	1.64517	-0.45063
H	-2.33779	2.37795	-1.99557
H	-1.62941	2.92522	-0.46170
H	-2.88941	1.69477	-0.45170
H	-0.89879	-3.25097	-1.93586
H	-1.72577	-2.88116	-0.40878
H	-0.03064	-3.35709	-0.38996
H	-3.07094	-1.70670	-1.94029
H	-3.51196	-0.00310	-1.93398
H	-3.48473	-0.91037	-0.42732
H	1.77136	3.02213	-1.94878
H	0.97863	3.45365	-0.43935
H	0.07798	3.49974	-1.94945

*[(η^6-$Me_3B_3N_3Me_3$)(μ-H)$Cr(CO)_3$]$^-$ (**3**)*

Cr	-1.09750	0.02384	-0.12551
O	-3.13928	2.16317	-0.54239
O	-3.25181	-2.03095	-0.35658
O	-0.54444	-0.08749	-3.06989
C	-2.32426	1.32273	-0.38827
C	-2.39442	-1.22252	-0.27963
C	-0.75115	-0.05190	-1.90796
N	0.48305	-1.21240	0.92699
N	0.56396	1.25535	0.83123
N	2.24884	-0.08399	-0.40928
C	-0.02961	-2.44911	1.53355
B	1.66719	1.20489	-0.09991
B	0.15045	0.06575	1.71911
C	3.39166	-0.16093	-1.31937
C	0.11687	2.56386	1.33037
C	1.99005	-2.69548	-0.67135
C	0.53453	0.11465	3.28790
C	2.27953	2.53030	-0.73921
B	1.54515	-1.29850	-0.04693
H	0.72620	-2.93475	2.16568
H	-0.35535	-3.16793	0.77786
H	-0.89514	-2.22429	2.16079
H	-1.17810	0.10614	1.68255
H	3.97404	-1.06788	-1.13745
H	4.06440	0.68782	-1.17213
H	3.09675	-0.16695	-2.37863
H	0.89072	3.05819	1.93322
H	-0.76777	2.43861	1.95872
H	-0.15933	3.23459	0.51277
H	2.25582	-2.60418	-1.72971
H	1.22710	-3.47338	-0.59150
H	2.88557	-3.07899	-0.16073
H	1.62558	0.08913	3.42023
H	0.12292	-0.73284	3.84951
H	0.17273	1.02480	3.78171
H	1.62179	3.39954	-0.66924
H	2.53839	2.39906	-1.79516
H	3.21382	2.80014	-0.22557

*(η^6-$Me_3B_3N_3Me_3$)(H_2)$Cr(CO)_3$ (M-H Protonated **3**)*

Cr	1.14586	-0.06053	0.02300
O	3.04984	-2.19900	-0.84729
O	3.04387	2.14814	-0.68138
O	0.35450	0.10942	-2.87404
C	2.30771	-1.36041	-0.51337
C	2.32259	1.27570	-0.39084
C	0.58260	0.04870	-1.73167
N	-0.53966	1.11586	1.12766
N	-0.72540	-1.28444	0.84701
N	-2.15668	0.20801	-0.53535
C	-0.13165	2.30200	1.91214
B	-1.67116	-1.12031	-0.27693
B	-0.55181	-0.18464	1.79026
C	-3.19535	0.41795	-1.55495
C	-0.44909	-2.66450	1.30366
C	-1.57325	2.79449	-0.64537
C	-0.42477	-0.35212	3.35532
C	-2.15177	-2.38763	-1.09113
B	-1.40561	1.34036	-0.04681
H	-0.97510	2.70513	2.48306
H	0.24485	3.08405	1.25396
H	0.66300	2.04470	2.61299
H	-3.72539	1.35385	-1.37073
H	-3.93215	-0.38603	-1.51763
H	-2.78027	0.45450	-2.56953
H	-1.33755	-3.12085	1.75279
H	0.35255	-2.66929	2.04224
H	-0.13009	-3.28279	0.46471
H	-2.00144	2.79570	-1.65019
H	-0.62081	3.33092	-0.69755
H	-2.23457	3.40257	-0.01244
H	-1.33728	0.06183	3.80783
H	0.40698	0.20387	3.79760
H	-0.34647	-1.38838	3.68972
H	-1.31641	-3.04703	-1.34844
H	-2.66430	-2.13620	-2.02155
H	-2.84415	-2.99487	-0.49197
H	2.11816	0.17899	1.49601
H	1.74696	-0.50463	1.67800

*(η^6-$Me_3B_3N_3Me_3H$)(μ-H)$Cr(CO)_3$ (N Protonated **3**)*

Cr	-0.73911	0.01822	-0.47208
O	-1.05265	-2.00137	-2.66830
O	-2.26504	2.08247	-2.01935
O	-3.35199	-0.79473	0.75389
C	-0.94376	-1.21222	-1.81001
C	-1.65832	1.28156	-1.42099
C	-2.32328	-0.49410	0.27953
N	0.30914	1.26555	0.96136
N	2.41614	0.11465	0.15171
N	0.48970	-1.16141	1.08324
C	-0.16735	2.57537	1.44055
B	1.59464	-1.19434	0.17337
B	1.27867	1.21793	-0.22472
C	-0.08122	-2.44405	1.55388
C	3.61869	0.12987	-0.72582
C	-0.67963	0.10122	3.16408
C	1.85993	2.61065	-0.76064
C	2.10354	-2.46259	-0.60100
B	0.00990	0.08595	1.74112
H	2.72749	0.32612	1.10226
H	0.60644	3.07782	2.03254
H	-1.05594	2.45498	2.06125
H	-0.42854	3.21986	0.60127
H	0.51585	-2.84330	2.38007
H	-0.09506	-3.17711	0.74867
H	-1.10491	-2.30023	1.89598
H	4.28122	-0.70076	-0.47845
H	4.15012	1.07151	-0.59219
H	3.30858	0.04467	-1.76744
H	-1.76102	0.26891	3.09938
H	-0.27421	0.90687	3.78646
H	-0.53604	-0.83448	3.71123
H	2.44896	3.14133	-0.00050
H	1.04907	3.27968	-1.06569
H	2.49862	2.48671	-1.64090
H	2.59638	-2.21349	-1.54450
H	1.30624	-3.17307	-0.82675
H	2.84822	-2.99621	0.00797
H	0.72227	0.63850	-1.25114

*[(η^6-$Me_3B_3N_3Me_3$)$Mn(CO)_3$]$^+$ (**2**)*

Mn	0.00476	0.00512	0.66671
N	-0.39202	-1.36865	-0.97853
N	-0.98553	1.00089	-1.00582
O	0.67979	2.38353	2.30932
N	1.36416	0.32905	-1.00992
O	1.71942	-1.72208	2.36669
O	-2.37360	-0.55863	2.35073
C	0.41673	1.45814	1.68314
B	-1.45395	-0.37757	-1.17675
B	0.40502	1.42209	-1.19825
C	2.10361	-2.19890	-1.45799
C	1.05198	-1.05372	1.71458
C	-1.44645	-0.34335	1.70902
C	2.80618	0.68856	-0.94710
B	1.03236	-1.08889	-1.18013
C	-2.01954	2.06915	-0.93806
C	-0.80120	-2.79498	-0.87277
C	-2.94925	-0.75931	-1.45173
C	0.82803	2.90477	-1.48200
H	2.93157	-1.81978	-2.06379
H	1.67945	-3.05805	-1.98449
H	2.54972	-2.58881	-0.53351
H	3.21392	0.78886	-1.95623
H	3.36418	-0.08264	-0.41752
H	2.93756	1.63234	-0.41932
H	-2.31395	2.37202	-1.94599
H	-1.63001	2.93830	-0.40939
H	-2.89977	1.70928	-0.40729
H	-0.93455	-3.22629	-1.86815
H	-1.73954	-2.87797	-0.32541
H	-0.04114	-3.36579	-0.34081
H	-3.03130	-1.68724	-2.02465
H	-3.47624	0.01802	-2.01156
H	-3.51786	-0.91586	-0.52558
H	1.75192	2.96267	-2.06441
H	1.00848	3.46850	-0.55714
H	0.05965	3.45243	-2.03357

*[(η^6-$Me_3B_3N_3Me_3$)(μ-H)$Mn(CO)_3$]$^+$ (**4**)*

Mn	-1.08564	-0.00002	-0.17400
O	-3.10405	2.11577	-0.56353
O	-3.10379	-2.11600	-0.56392
O	-0.25501	0.00026	-3.02454
C	-2.31018	1.28229	-0.43396
C	-2.31004	-1.28244	-0.43415
C	-0.57050	0.00010	-1.91026
N	0.40125	-1.22159	0.80733
N	0.40121	1.22158	0.80734
N	2.26932	0.00003	-0.29445
C	-0.07699	-2.50917	1.35577
B	1.61846	1.25339	-0.00827
B	0.02371	-0.00001	1.64703
C	3.53259	0.00003	-1.04765
C	-0.07709	2.50915	1.35576
C	2.21722	-2.62455	-0.52928
C	0.19575	-0.00001	3.23708
C	2.21715	2.62458	-0.52931
B	1.61849	-1.25335	-0.00830
H	0.68014	-2.96778	2.00048
H	-0.32453	-3.21388	0.55962
H	-0.97743	-2.35051	1.95177
H	-1.36765	-0.00005	1.47461
H	4.12926	-0.87881	-0.79835
H	4.12917	0.87899	-0.79851
H	3.36902	-0.00008	-2.13275
H	0.68003	2.96781	2.00046
H	-0.97751	2.35045	1.95179
H	-0.32468	3.21383	0.55961
H	2.68378	-2.52722	-1.51395
H	1.48457	-3.43238	-0.58873
H	3.00659	-2.96994	0.15398
H	1.26403	-0.00002	3.49275
H	-0.24945	-0.88003	3.71217
H	-0.24941	0.88005	3.71215
H	1.48464	3.43256	-0.58832
H	2.68323	2.52728	-1.51422
H	3.00693	2.96972	0.15360

*[(η^6-$Me_3B_3N_3Me_3$)$Mn(CO)_3$] (**5**)*

Mn	0.70230	-0.00376	-0.51475
O	0.93741	2.12719	-2.54765
O	0.95133	-2.14241	-2.53770
O	3.59462	-0.01110	0.14929
C	0.84333	1.26643	-1.76704
C	0.85722	-1.28585	-1.75274
C	2.44808	0.00388	-0.06100
N	-0.23753	-1.20925	1.06156
N	-0.24246	1.21594	1.04978
N	-2.19568	-0.00166	0.11203
B	0.22005	0.00801	1.73494
B	-1.51380	1.25657	0.30307
C	-2.12973	-2.62718	-0.16846
C	-3.52817	-0.01444	-0.51196
B	-1.50512	-1.25679	0.31069
C	0.37150	2.50169	1.44931
C	0.38822	-2.48667	1.47179
C	1.08529	0.01439	3.05682
C	-2.09753	2.64279	-0.18226
H	-2.88848	-2.96102	0.55401
H	-1.40771	-3.44030	-0.26066
H	-2.64028	-2.53118	-1.13137
H	-4.11827	0.83672	-0.16965
H	-4.06846	-0.92046	-0.23639
H	-3.46992	0.02773	-1.60620
H	0.38607	3.19636	0.61006
H	1.40040	2.34350	1.77186
H	-0.18832	2.96045	2.27063
H	-0.20734	-2.98040	2.24599
H	1.38895	-2.30481	1.86243
H	0.48068	-3.16050	0.62052
H	0.83781	-0.83922	3.69633
H	0.91792	0.92200	3.64463
H	2.16186	-0.04125	2.85904
H	-2.95577	2.54733	-0.84956
H	-1.34336	3.23318	-0.71303
H	-2.41531	3.25217	0.67465

*[(η^6-$Me_3B_3N_3Me_3$)(H_2)$Mn(CO)_3$]$^+$ (M-H Protonated **4**)*

Mn	1.13834	-0.00863	-0.00513
O	3.00073	-2.18717	-0.78845
O	2.92063	2.20296	-0.87621
O	0.19506	-0.07398	-2.83427
C	2.29542	-1.33111	-0.49256
C	2.25566	1.33014	-0.53862
C	0.47878	-0.04440	-1.72294
N	-0.47617	1.19724	0.93608
N	-0.49921	-1.20004	0.93590
N	-2.14412	0.01654	-0.49431
C	-0.12249	2.48717	1.58782
B	-1.55340	-1.24230	-0.12795
B	-0.49499	-0.00138	1.78173
C	-3.28605	0.02570	-1.43238
C	-0.14695	-2.49810	1.57278
C	-1.89414	2.64507	-0.78030
C	-0.41190	0.01965	3.34642
C	-1.99786	-2.60889	-0.76387
B	-1.51951	1.26100	-0.13734
H	-0.98738	2.90910	2.10614
H	0.22250	3.20548	0.84531
H	0.67568	2.33811	2.31596
H	-3.91211	0.89977	-1.25359
H	-3.90379	-0.85913	-1.28058
H	-2.95479	0.04259	-2.47632
H	-1.02715	-2.96048	2.02590
H	0.60311	-2.34593	2.34953
H	0.26489	-3.18373	0.83306
H	-2.46766	2.55209	-1.70378
H	-1.00920	3.25111	-1.00029
H	-2.49918	3.23883	-0.08155
H	-1.13069	0.75093	3.73471
H	0.56629	0.33241	3.72934
H	-0.64295	-0.94732	3.79827
H	-1.22501	-3.38002	-0.74199
H	-2.32755	-2.49602	-1.79993
H	-2.85514	-3.01346	-0.20676
H	1.97302	0.39593	1.49703
H	1.90032	-0.38303	1.54536

*[(η^6-$Me_3B_3N_3Me_3H$)(μ-H)$Mn(CO)_3$]$^+$ (N Protonated **4**)*

Mn	-0.73652	0.02060	-0.46665
O	-0.85581	-1.73460	-2.85511
O	-2.23493	2.20158	-1.80078
O	-3.30633	-1.02261	0.60145
C	-0.83803	-1.05435	-1.92689
C	-1.65834	1.34823	-1.28933
C	-2.29948	-0.63252	0.20186
N	0.15256	1.13453	1.08286
N	2.38378	0.27238	0.22094
N	0.51839	-1.24747	0.88514
C	-0.41154	2.34216	1.72753
B	1.71885	-1.10734	0.09312
B	1.15359	1.29058	-0.06352
C	0.05224	-2.62848	1.19595
C	3.60569	0.50083	-0.61363
C	-0.64497	-0.35893	3.15828
C	1.56529	2.75683	-0.52432
C	2.36895	-2.23909	-0.75984
B	0.00423	-0.14496	1.74539
H	2.65835	0.42149	1.19564
H	0.31391	2.76585	2.42784
H	-1.32157	2.09183	2.27245
H	-0.65296	3.09730	0.98117
H	0.70723	-3.08693	1.94045
H	0.05575	-3.24441	0.29836
H	-0.96225	-2.60400	1.59014
H	4.34911	-0.26733	-0.40238
H	4.01695	1.48130	-0.37988
H	3.33621	0.46748	-1.66891
H	-1.73948	-0.30032	3.13370
H	-0.31237	0.42095	3.85161
H	-0.38647	-1.32564	3.59728
H	2.09909	3.29824	0.26663
H	0.68760	3.35383	-0.78971
H	2.20929	2.75121	-1.40799
H	2.88746	-1.86427	-1.64541
H	1.66618	-3.00981	-1.08037
H	3.13278	-2.74194	-0.14780
H	0.63967	0.70981	-1.14622

$[(Me_6B_3N_3)Mn(CO)_3]^+$ adduct with Anthraquinone
(9.0 kcal/mol higher energy than free species)

Mn	-3.244628	0.000425	0.269584
O	-5.156934	2.134340	-0.499177
O	-5.158856	-2.132856	-0.496148
C	-4.427376	1.300532	-0.193990
C	-4.428558	-1.299244	-0.192188
C	-3.848790	0.001667	1.983708
O	-4.205707	0.002448	3.076026
N	-1.463084	-1.219837	0.527194
N	-1.993539	-0.001068	-1.517497
N	-1.462131	1.219640	0.525836
B	-1.617162	-1.287118	-0.927580
B	-1.616146	1.285348	-0.929015
C	-0.339307	0.000575	2.621069
C	-1.341189	2.501124	1.265278
B	-1.036174	0.000133	1.216788
C	-2.426874	-0.001627	-2.937449
C	-1.343057	-2.500617	1.268049
C	-1.551846	-2.620000	-1.752555
C	-1.550151	2.617402	-1.755287
C	3.140183	3.693272	-0.478586
C	4.447944	3.691316	0.019347
C	5.079272	2.486303	0.319200
C	4.410265	1.274392	0.123617
C	3.086855	1.272762	-0.363764
C	2.463059	2.491108	-0.664299
C	5.122965	-0.000392	0.430541
C	4.409871	-1.274902	0.123431
C	3.086424	-1.272790	-0.363824
C	2.344320	0.000137	-0.553496
C	5.078511	-2.487054	0.318816
C	4.446752	-3.691823	0.018911
O	1.141085	0.000334	-0.849075
C	3.138917	-3.693298	-0.478840
C	2.462170	-2.490894	-0.664373
O	6.253230	-0.000596	0.898038
H	0.291843	0.882225	2.761963
H	0.291051	-0.881487	2.762918
H	-1.065100	0.001338	3.444981
H	-2.015021	3.246347	0.843198
H	-1.602078	2.358456	2.313613
H	-0.315455	2.874991	1.204710
H	-3.028441	-0.884978	-3.149659
H	-1.554535	-0.002211	-3.596486

H	-3.027906	0.881873	-3.150523
H	-0.317530	-2.875153	1.208174
H	-2.017208	-3.245892	0.846575
H	-1.604151	-2.356676	2.316163
H	-1.137996	-2.449206	-2.750908
H	-0.939637	-3.384675	-1.268451
H	-2.544971	-3.063855	-1.901085
H	-1.136637	2.445483	-2.753583
H	-2.543020	3.061783	-1.903946
H	-0.937325	3.382104	-1.272013
H	2.656476	4.633248	-0.725812
H	4.974362	4.629167	0.165611
H	6.094112	2.457454	0.700606
H	1.454328	2.473902	-1.060842
H	6.093396	-2.458574	0.700128
H	4.972877	-4.629866	0.165001
H	2.654861	-4.633096	-0.726058
H	1.453385	-2.473329	-1.060768

$[(Me_6B_3N_3)Mn(CO)_3]^+$ adduct with **6**
(21.3 kcal/mol lower energy than free species with hydride donor ability of 68 kcal/mol)

Mn	-3.039132	0.005048	0.366122
O	-5.107977	2.102964	0.056035
O	-5.073555	-2.132629	0.102210
C	-4.302424	1.282501	0.181173
C	-4.281216	-1.296923	0.208831
C	-3.190296	0.022787	2.163256
O	-3.263568	0.034886	3.314964
N	-1.295885	-1.190734	0.288932
N	-2.185145	-0.008662	-1.635138
N	-1.318047	1.227757	0.264570
B	-1.755505	-1.308526	-1.075323
B	-1.773924	1.308650	-1.104047
C	0.292433	0.050204	2.072824
C	-1.190328	2.472073	1.042234
B	-0.299891	0.031565	0.581558
C	-2.890261	-0.027526	-2.932731
C	-1.145643	-2.415592	1.094048
C	-1.937286	-2.659021	-1.875053
C	-1.970417	2.639471	-1.932439
C	2.906781	3.656615	-0.383889
C	4.301753	3.635509	-0.106544
C	4.946274	2.441717	0.086404
C	4.245205	1.196055	0.036195

C	2.822706	1.219254	-0.224411
C	2.199059	2.484275	-0.443964
C	4.889599	-0.040762	0.218770
C	4.193833	-1.249089	0.043240
C	2.781376	-1.218919	-0.249668
C	2.091520	0.013235	-0.297109
C	4.852494	-2.512673	0.147696
C	4.172905	-3.681729	-0.074708
O	0.744289	0.040427	-0.490501
C	2.794045	-3.653483	-0.425840
C	2.123452	-2.460136	-0.504513
O	6.226009	-0.131430	0.525080
H	0.920502	0.932518	2.237912
H	0.938106	-0.816394	2.252276
H	-0.472025	0.048921	2.857670
H	-1.989970	3.174326	0.793482
H	-1.251918	2.253421	2.109659
H	-0.228586	2.960144	0.857928
H	-3.517095	-0.915419	-3.017988
H	-2.169698	-0.032207	-3.757382
H	-3.528314	0.850257	-3.037542
H	-0.174147	-2.887694	0.920233
H	-1.931641	-3.137918	0.859743
H	-1.213722	-2.174911	2.156303
H	-1.616031	-2.544875	-2.916451
H	-1.353383	-3.474620	-1.440816
H	-2.980513	-2.997097	-1.906342
H	-1.659499	2.504483	-2.974342
H	-3.015509	2.972303	-1.959552
H	-1.385661	3.466657	-1.521582
H	2.411093	4.604751	-0.570988
H	4.860344	4.566215	-0.076116
H	6.023498	2.448651	0.234526
H	1.147753	2.485473	-0.701848
H	5.907597	-2.520841	0.395307
H	4.689074	-4.634294	0.001110
H	2.276430	-4.583957	-0.641927
H	1.082812	-2.427310	-0.801213
H	6.513985	0.695446	0.930292

BH_3

B	0.00000	0.00000	0.00000
H	0.00000	1.18963	0.00000
H	1.03025	-0.59481	0.00000
H	-1.03025	-0.59481	0.00000

$[BH_4]^-$

B	-0.00010	0.00009	0.00020
H	-0.12938	0.51018	-1.11377
H	-0.64671	-1.04788	0.04923
H	1.19129	-0.24214	0.20473
H	-0.41469	0.77941	0.85884

BH_2CN

C	-0.18738	-0.00003	-0.00072
B	1.34298	0.00001	-0.00003
N	-1.34475	0.00001	0.00040
H	1.91132	-1.03788	0.00082
H	1.91131	1.03791	0.00082

$[BH_3CN]^-$

C	0.27189	0.00019	0.00007
B	-1.31230	-0.00016	-0.00009
N	1.43494	-0.00006	-0.00001
H	-1.70485	0.76726	-0.86350
H	-1.70445	-1.13168	-0.23242
H	-1.70514	0.36450	1.09604

BEt_3

C	1.32676	-0.85908	-0.00019
B	-0.00006	0.00001	-0.00012
C	1.23520	-2.39222	0.00034
C	0.08068	1.57862	-0.00022
C	1.45434	2.26561	0.00025
C	-1.40754	-0.71946	-0.00046
C	-2.68941	0.12654	0.00043
H	1.92615	-0.52427	-0.86163
H	1.92705	-0.52368	0.86036
H	2.22645	-2.85606	-0.00003
H	0.70274	-2.76391	0.88108
H	0.70179	-2.76452	-0.87955
H	-0.50897	1.93041	-0.86161
H	-0.50982	1.93089	0.86037
H	1.36065	3.35600	-0.00005
H	2.04246	1.99009	0.88091
H	2.04329	1.98967	-0.87971
H	-1.41746	-1.40749	0.85972
H	-1.41741	-1.40550	-0.86228
H	-3.58681	-0.49988	-0.00016
H	-2.74504	0.77497	-0.87922
H	-2.74495	0.77318	0.88140

$[HBEt_3]^-$

C	-0.96186	-1.24350	-0.32625
B	0.00067	0.00023	0.18772
C	-0.63542	-2.63493	0.24584
C	-0.59638	1.45579	-0.32379
C	-1.96704	1.86540	0.24430
C	1.55865	-0.20837	-0.33032
C	2.60148	0.76552	0.24732
H	-2.01779	-1.02831	-0.09640
H	-0.92051	-1.30563	-1.42968
H	0.00407	-0.00068	1.44537
H	-1.29706	-3.42926	-0.12934
H	0.39164	-2.93646	0.00924
H	-0.71802	-2.63412	1.33980
H	0.11621	2.26284	-0.08926
H	-0.66745	1.45299	-1.42743
H	-2.31887	2.84116	-0.12134
H	-2.74220	1.13219	-0.00697
H	-1.93258	1.92284	1.33922
H	1.59026	-0.13196	-1.43320
H	1.90012	-1.23240	-0.10909
H	3.62112	0.58654	-0.12385
H	2.63709	0.69275	1.34134
H	2.35399	1.80688	0.01039

NH_3BH_3

B	-0.91691	0.00007	0.00006
N	0.72161	0.00005	0.00005
H	-1.25471	0.27132	-1.13164
H	-1.25483	-1.11576	0.33062
H	-1.25507	0.84427	0.80085
H	1.09962	-0.22131	0.91910
H	1.09960	0.90650	-0.26839
H	1.09869	-0.68575	-0.65113

$[NH_3BH_2]^+$

B	-0.90942	0.00000	-0.00863
N	0.62507	0.00000	-0.00801
H	-1.42801	-1.05557	0.00585
H	-1.42801	1.05557	0.00585
H	1.03611	0.83266	-0.44052
H	1.03611	-0.83267	-0.44050
H	0.95541	0.00001	0.96851

$[SiEt_3]^+$

Si	-0.13111	-0.12513	-0.23403

C	1.30292	-1.22740	-0.62621
H	0.94090	-2.08921	-1.19291
H	1.99774	-0.67748	-1.26879
C	0.12077	1.66342	0.16373
H	-0.63243	2.21577	-0.41497
H	-0.21310	1.77547	1.20694
C	-1.82367	-0.86403	-0.14325
H	-1.99994	-1.31970	-1.12886
H	-1.72700	-1.72633	0.53302
C	2.03905	-1.70215	0.66016
H	1.38436	-2.28250	1.31313
H	2.87284	-2.34380	0.37113
H	2.44701	-0.86689	1.23253
C	-2.99453	0.04309	0.27126
H	-3.91898	-0.53664	0.29192
H	-2.84758	0.46605	1.26678
H	-3.13731	0.86654	-0.43104
C	1.52638	2.25612	-0.03497
H	1.52447	3.30900	0.25239
H	2.27327	1.74840	0.57807
H	1.84578	2.19886	-1.07709

$HSiEt_3$

Si	0.14643	0.00954	0.52542
H	0.40773	0.50646	1.91440
C	-1.18428	-1.33954	0.64080
H	-0.80826	-2.12122	1.31224
H	-2.05821	-0.91332	1.14777
C	-0.44287	1.47986	-0.52020
H	0.37416	2.20950	-0.56777
H	-0.59136	1.13520	-1.55117
C	1.76590	-0.70314	-0.16122
H	2.01926	-1.58623	0.43833
H	1.58089	-1.07653	-1.17585
C	-1.61392	-1.96547	-0.69888
H	-0.77248	-2.44272	-1.20990
H	-2.38255	-2.73106	-0.55439
H	-2.02691	-1.21569	-1.38044
C	2.95746	0.27171	-0.17636
H	3.86506	-0.21044	-0.55275
H	2.76188	1.13837	-0.81452
H	3.17909	0.64814	0.82700
C	-1.72138	2.16934	-0.01038
H	-1.99589	3.02189	-0.63943
H	-2.57389	1.48376	-0.00195
H	-1.59387	2.54367	1.01004

$CHCl_2CHCl_2$

C	-0.676143	-0.369159	-0.010702
C	0.676146	0.369153	0.010691
Cl	-0.526032	-1.932762	-0.882697
Cl	-1.259542	-0.662786	1.662998
Cl	0.525829	1.932893	0.882450
Cl	1.259796	0.662564	-1.662935
H	-1.430032	0.224764	-0.524221
H	1.429978	-0.224666	0.524415

$CHCl_2$_Radical

C	0.048030	-0.108168	-0.088247
Cl	1.401303	0.955643	-0.132092
Cl	-0.269879	-0.997042	1.351823
H	-0.233618	-0.576970	-1.022335

CH_2Cl_2

C	-0.108341	0.009998	-0.108858
Cl	1.431767	0.929262	-0.154566
Cl	-0.251842	-1.037942	1.340383
H	-0.925786	0.725006	-0.088583
H	-0.145798	-0.626323	-0.988377

Me-THF Dimer

C	-2.813836	1.389915	0.058644
C	-3.363131	-0.028828	-0.091794
O	-2.412393	-0.878348	0.552966
C	-1.111184	-0.240202	0.604585
C	-1.303446	1.143186	-0.068602
C	-0.151930	-1.132024	-0.207824
O	1.153475	-0.530902	-0.224676
C	2.179778	-1.532908	-0.074719
C	1.462267	-2.878169	-0.255382
C	0.056575	-2.572867	0.277874
C	-0.701298	-0.103053	2.072753
C	3.303538	-1.251958	-1.061014
H	-3.204079	2.082309	-0.692968
H	-3.062048	1.789585	1.047994
H	-4.336079	-0.180308	0.387382
H	-3.462418	-0.298751	-1.155540
H	-0.692584	1.917107	0.401600
H	-1.015040	1.094015	-1.124232
H	-0.542769	-1.158536	-1.238376
H	2.575548	-1.465372	0.951726
H	1.963908	-3.694529	0.272413

H	1.422069	-3.140143	-1.320106
H	-0.717715	-3.246746	-0.094229
H	0.047197	-2.624539	1.371232
H	-0.827590	-1.049417	2.604870
H	0.343375	0.211717	2.146506
H	-1.328160	0.641351	2.572981
H	4.113548	-1.979536	-0.939922
H	3.716228	-0.251573	-0.901784
H	2.933083	-1.309659	-2.089505

Me-THF Radical

C	-0.438701	0.550436	0.191725
C	-0.457515	-0.945023	0.072931
C	1.032208	-1.287131	0.261814
C	1.716689	-0.061226	-0.357230
O	0.809045	1.037978	-0.166719
C	-1.577527	1.467432	-0.081922
H	-1.107903	-1.424720	0.812227
H	-0.807688	-1.277851	-0.922620
H	1.334205	-2.222087	-0.217501
H	1.270153	-1.355799	1.328080
H	2.673369	0.194834	0.107509
H	1.880315	-0.193949	-1.435734
H	-1.347378	2.484459	0.252261
H	-2.477000	1.130022	0.442802
H	-1.826110	1.527678	-1.157075

Me-THF

C	-0.417654	0.599677	0.464330
C	-0.465259	-0.900733	0.152552
C	1.017179	-1.288644	0.224180
C	1.699150	-0.043785	-0.361778
O	0.820880	1.063831	-0.109580
C	-1.564200	1.425950	-0.097679
H	-0.371984	0.740772	1.557506
H	-1.096583	-1.455372	0.852343
H	-0.857276	-1.058889	-0.859806
H	1.259222	-2.199786	-0.329546
H	1.320480	-1.437710	1.266315
H	2.676625	0.157768	0.092816
H	1.846318	-0.142408	-1.446713
H	-1.412549	2.489558	0.109064
H	-2.513732	1.123022	0.355967
H	-1.636438	1.292575	-1.181917

Anthraquinone

C	-1.239806	0.702912	-0.329960
C	-1.239172	-0.705023	-0.327832
C	0.015214	-1.476315	-0.095100
C	1.268889	-0.703193	0.135379
C	1.268255	0.704742	0.133252
C	0.013884	1.476034	-0.099562
C	2.464267	-1.393762	0.357181
C	3.647154	-0.696140	0.574711
C	3.646525	0.701160	0.572599
C	2.463009	1.397055	0.352963
C	-2.435198	1.393481	-0.551684
C	-3.618107	0.695859	-0.769101
C	-3.617477	-0.701440	-0.766990
C	-2.433941	-1.397336	-0.547466
O	0.013388	2.699427	-0.101711
O	0.015821	-2.699709	-0.093552
H	2.448017	-2.476376	0.355733
H	4.570457	-1.237396	0.746063
H	4.569339	1.243763	0.742313
H	2.445784	2.479645	0.348243
H	-2.418951	2.476095	-0.550222
H	-4.541429	1.237115	-0.940349
H	-4.540311	-1.244043	-0.936600
H	-2.416718	-2.479926	-0.542733

Anthrasemiquinone radical

C	-1.258513	0.742352	-0.144724
C	-1.244027	-0.681993	-0.217551
C	-0.014298	-1.450331	-0.031259
C	1.199772	-0.680222	0.233782
C	1.185293	0.744123	0.306610
C	-0.044414	1.512482	0.120183
C	2.425089	-1.359055	0.424138
C	3.594865	-0.671500	0.676628
C	3.580531	0.738820	0.748738
C	2.396795	1.424692	0.566498
C	-2.483877	1.421154	-0.334888
C	-3.653656	0.733577	-0.587307
C	-3.639311	-0.676743	-0.659415
C	-2.455553	-1.362592	-0.477242
O	-0.057216	2.772562	0.184553
O	-0.001477	-2.710384	-0.095738
H	2.415649	-2.440867	0.365086
H	4.524867	-1.212021	0.819675
H	4.499509	1.280671	0.947248
H	2.365380	2.506471	0.618074

H	-2.474473	2.502964	-0.275774
H	-4.583676	1.274088	-0.730279
H	-4.558300	-1.218604	-0.857848
H	-2.424127	-2.444374	-0.528748

Anthrasemiquinone

C	-1.263861	0.731863	-0.131149
C	-1.256395	-0.688174	-0.221669
C	-0.009953	-1.453523	-0.048190
C	1.214637	-0.679213	0.230325
C	1.186948	0.744276	0.324278
C	-0.049581	1.429242	0.134768
C	2.427122	-1.360088	0.408549
C	3.600390	-0.675137	0.676970
C	3.581117	0.726422	0.776231
C	2.400767	1.422268	0.605370
C	-2.487444	1.424054	-0.309628
C	-3.653307	0.729366	-0.565150
C	-3.642605	-0.674166	-0.653109
C	-2.455618	-1.367244	-0.483191
O	-0.146038	2.777425	0.199834
O	0.011647	-2.689574	-0.130484
H	2.417283	-2.440014	0.330514
H	4.529852	-1.215361	0.811928
H	4.495659	1.267098	0.990067
H	2.432300	2.503113	0.696553
H	-2.497306	2.503707	-0.242969
H	-4.582782	1.271001	-0.698916
H	-4.562237	-1.211208	-0.854055
H	-2.425650	-2.447672	-0.548344
H	0.715075	3.186421	0.342160

Anthrahydroquinone-2H+

C	-1.280370	0.732792	0.001683
C	-1.279722	-0.721460	0.003878
C	-0.066410	-1.495902	0.003309
C	1.146162	-0.720351	0.000428
C	1.145514	0.733901	-0.001768
C	-0.067798	1.508343	-0.001220
C	2.404914	-1.384674	-0.000348
C	3.601257	-0.704523	-0.003066
C	3.600635	0.720173	-0.005215
C	2.403702	1.399299	-0.004547
C	-2.539122	1.397115	0.002483
C	-3.735465	0.716964	0.005219
C	-3.734843	-0.707732	0.007367

C	-2.537910	-1.386858	0.006681
O	-0.068501	2.808813	-0.003177
O	-0.065708	-2.796373	0.005313
H	2.382779	-2.469646	0.001316
H	4.542220	-1.248526	-0.003577
H	4.541135	1.264968	-0.007365
H	2.380635	2.484235	-0.006148
H	-2.516987	2.482087	0.000818
H	-4.676428	1.260968	0.005745
H	-4.675344	-1.252526	0.009531
H	-2.514843	-2.471794	0.008281

Anthrahydroquinone-H+

C	-1.292456	0.717260	-0.013869
C	-1.273240	-0.725521	-0.041341
C	-0.048765	-1.409141	-0.078525
C	1.169127	-0.713733	-0.052202
C	1.175922	0.727306	0.001461
C	-0.061041	1.496106	0.012589
C	2.432442	-1.387360	-0.073429
C	3.614877	-0.688962	-0.041926
C	3.618233	0.728323	0.012859
C	2.417066	1.403892	0.032472
C	-2.537881	1.384004	-0.006017
C	-3.735362	0.700006	-0.017369
C	-3.721713	-0.716995	-0.028213
C	-2.533170	-1.407068	-0.038543
O	-0.067009	2.762427	0.043388
O	-0.015943	-2.814998	-0.088348
H	2.435401	-2.469781	-0.111202
H	4.557448	-1.228250	-0.058102
H	4.557756	1.270079	0.038297
H	2.387178	2.486945	0.070633
H	-2.515946	2.467773	0.012049
H	-4.678560	1.235651	-0.010800
H	-4.659624	-1.264318	-0.021588
H	-2.543476	-2.491200	-0.026359
H	-0.479093	-3.132725	-0.871662

Anthrahydroquinone

C	-1.217629	0.732856	0.060921
C	-1.221784	-0.711870	-0.042053
C	0.000624	-1.399017	-0.123641
C	1.224997	-0.711294	-0.075532
C	1.229346	0.720283	0.065159
C	0.009021	1.414000	0.127817

C	2.475527	-1.396022	-0.155193
C	3.658149	-0.708687	-0.093547
C	3.662498	0.705728	0.054250
C	2.484081	1.398860	0.129918
C	-2.477005	1.409541	0.090828
C	-3.661634	0.726249	0.056896
C	-3.665501	-0.693314	-0.008645
C	-2.484721	-1.382388	-0.056801
O	0.090136	2.779247	0.239104
O	0.073699	-2.764628	-0.235948
H	2.469110	-2.472155	-0.266502
H	4.599366	-1.243075	-0.156306
H	4.607005	1.235490	0.105812
H	2.484270	2.475009	0.241253
H	-2.514173	2.493258	0.129388
H	-4.600790	1.266286	0.078659
H	-4.607482	-1.228749	-0.019074
H	-2.527642	-2.465911	-0.094840
H	-0.767557	3.153628	0.463289
H	-0.788449	-3.134774	-0.449853

Borazine

B	1.44846	0.08141	-0.00001
N	0.63539	1.25897	-0.00001
B	-0.79473	1.21369	0.00002
N	-1.40803	-0.07923	-0.00000
B	-0.65372	-1.29510	-0.00002
N	0.77263	-1.17974	0.00001
H	2.63882	0.14812	0.00000
H	1.09000	2.16025	-0.00001
H	-1.44765	2.21128	0.00000
H	-2.41587	-0.13625	0.00000
H	-1.19110	-2.35935	0.00002
H	1.32589	-2.02407	0.00003

Borazine+H_2

N	-1.23949	0.76085	0.10531
B	-0.04737	1.47324	0.09716
N	1.20272	0.69263	-0.29098
B	1.20700	-0.82248	0.34647
N	-0.14674	-1.42244	-0.05983
B	-1.32914	-0.69745	-0.12275

H	-2.09659	1.27000	0.27087
H	0.04234	2.63336	0.34005
H	1.23456	0.59465	-1.30844
H	2.05193	1.19052	-0.03470
H	2.15064	-1.41351	-0.13026
H	1.33110	-0.65965	1.54883
H	-0.18439	-2.41748	-0.22371
H	-2.39750	-1.18170	-0.34852

Borazine+2H_2

N	1.13334	0.87688	-0.24009
B	-0.23453	1.40888	0.45147
N	-1.36648	0.55229	-0.16393
B	-1.26514	-0.81183	-0.25865
N	0.00904	-1.37636	0.37707
B	1.36493	-0.69834	-0.22662
H	1.14774	1.21117	-1.20064
H	1.91718	1.33553	0.21717
H	-0.10326	1.20916	1.64862
H	-0.37438	2.58610	0.20731
H	-2.16952	1.01925	-0.55934
H	-2.02757	-1.55705	-0.78674
H	-0.00513	-1.17534	1.37871
H	0.07871	-2.38647	0.28811
H	1.50384	-1.12112	-1.34724
H	2.27477	-0.98450	0.51171

Borazine+3H_2

B	-0.80860	1.34659	0.25082
N	0.71830	1.29447	-0.19944
B	1.57014	0.02696	0.25264
N	0.76245	-1.26880	-0.19978
B	-0.76134	-1.37371	0.25122
N	-1.48073	-0.02571	-0.19838
H	-1.36306	2.26949	-0.30710
H	-0.85471	1.42414	1.45291
H	0.79434	1.42941	-1.20772
H	1.17342	2.11569	0.19486
H	2.64797	0.04579	-0.30267
H	1.65738	0.02815	1.45496

H	0.84214	-1.39966	-1.20812
H	1.24600	-2.07426	0.19315
H	-1.28373	-2.31553	-0.30607
H	-0.80414	-1.45195	1.45342
H	-1.63833	-0.02826	-1.20618
H	-2.41844	-0.04194	0.19838

Me_6Borazine

N	-1.13123	-0.87102	-0.02979
N	1.31997	-0.54407	-0.02989
N	-0.18873	1.41526	-0.02985
B	0.19272	-1.44503	0.01064
B	1.15512	0.88952	0.01079
C	-2.81514	1.16053	0.11212
C	-0.38327	2.87375	-0.09214
B	-1.34785	0.55567	0.01079
C	2.68025	-1.10505	-0.09192
C	-2.29704	-1.76878	-0.09179
C	0.40245	-3.01817	0.11194
C	2.41277	1.85759	0.11225
H	-2.83749	2.12048	0.63339
H	-3.50791	0.49478	0.63222
H	-3.24369	1.33797	-0.88380
H	-0.44197	3.32562	0.90495
H	-1.30137	3.11840	-0.62519
H	0.43695	3.35025	-0.62799
H	3.10035	-1.28111	0.90524
H	3.35162	-0.43200	-0.62403
H	2.68282	-2.05322	-0.62853
H	-2.65833	-2.04611	0.90540
H	-2.05020	-2.68590	-0.62553
H	-3.12020	-1.29640	-0.62677
H	-0.41745	-3.51729	0.63385
H	1.32572	-3.28541	0.63136
H	0.46212	-3.47808	-0.88401
H	2.18266	2.79102	0.63126
H	2.78179	2.13875	-0.88361
H	3.25459	1.39703	0.63473

Me_6Borazine+H_2

B	0.57801	-1.55875	0.27277
N	1.43922	-0.30962	-0.01510
B	0.90285	0.97863	-0.08141
N	-0.58219	1.12713	0.12192
B	-1.47418	0.05919	0.00413
N	-0.86265	-1.28175	-0.44120
C	0.33456	-1.85521	1.85200
C	-0.80417	-1.37435	-1.93357
C	2.86469	-0.59568	-0.14342
C	1.73912	2.30510	-0.35195
C	-3.02970	0.04601	0.26137
C	-1.07067	2.47120	0.47265
H	1.03999	-2.53249	-0.30130
H	-1.48333	-2.02698	-0.13064
H	-0.29365	-2.73944	2.02864
H	1.29225	-2.05682	2.34671
H	-0.12287	-1.01363	2.38976
H	-1.77795	-1.15382	-2.37658
H	-0.49359	-2.38040	-2.21407
H	-0.06767	-0.66186	-2.30001
H	3.46426	0.31331	-0.19248
H	3.22037	-1.17731	0.71558
H	3.07218	-1.19385	-1.03962
H	1.23095	2.96632	-1.06238
H	2.73822	2.11609	-0.74779
H	1.86906	2.89265	0.56597
H	-3.22915	-0.41181	1.24036
H	-3.51338	1.02337	0.26277
H	-3.54962	-0.57901	-0.47350
H	-2.11671	2.44118	0.76963
H	-0.50029	2.88316	1.30845
H	-0.97610	3.16333	-0.36870

Me6Borazine+2H_2

B	0.52325	-1.57136	0.43376
N	1.50298	-0.32509	0.19359
B	0.89422	1.07525	-0.40971
N	-0.63708	1.15859	-0.07113
B	-1.48491	0.07148	-0.03226
N	-0.84257	-1.29844	-0.38210

C	0.18779	-1.74631	2.00533
C	-0.72843	-1.48912	-1.86303
C	2.73996	-0.71677	-0.53883
C	1.75657	2.29542	0.23055
C	-3.02701	-0.00189	0.30930
C	-1.16156	2.51868	0.08417
H	1.01716	-2.56679	-0.05167
H	1.80993	-0.06480	1.12942
H	1.05218	1.01271	-1.62062
H	-1.47851	-2.02424	-0.05617
H	-0.49731	-2.58261	2.19246
H	1.10037	-1.97064	2.57159
H	-0.25850	-0.85366	2.46376
H	-1.70832	-1.38705	-2.33378
H	-0.32734	-2.48214	-2.06646
H	-0.05758	-0.73528	-2.26884
H	3.42088	0.13119	-0.62131
H	3.24260	-1.53570	-0.02124
H	2.47162	-1.04838	-1.54050
H	1.49687	3.26857	-0.19895
H	2.82986	2.16540	0.04782
H	1.62748	2.38457	1.31963
H	-3.48819	0.94737	0.58383
H	-3.59653	-0.40825	-0.53699
H	-3.19541	-0.69531	1.14384
H	-2.24506	2.51935	0.19563
H	-0.72933	3.01687	0.95610
H	-0.91692	3.12648	-0.79391

Me_6Borazine+3H_2

B	0.60101	1.49615	0.14686
N	-0.94576	1.20548	-0.22574
B	-1.59645	-0.22779	0.14604
N	-0.57104	-1.42207	-0.22552
B	0.99496	-1.26879	0.14820
N	1.51769	0.21599	-0.22291
C	0.77010	1.92291	1.69776
C	2.09875	0.29816	-1.59613
C	-1.30562	1.66370	-1.60075
C	-2.05192	-0.29243	1.69652

C	1.27561	-1.62970	1.69963
C	-0.78723	-1.96182	-1.60105
H	0.96531	2.40108	-0.57525
H	-1.44336	1.83978	0.39675
H	-2.56181	-0.36552	-0.57671
H	-0.87197	-2.17054	0.39632
H	1.59810	-2.03673	-0.57265
H	2.31403	0.32970	0.40180
H	1.81539	2.17952	1.91378
H	0.19153	2.83118	1.91097
H	0.46797	1.17298	2.43346
H	2.82612	-0.50100	-1.74169
H	2.57464	1.26825	-1.74229
H	1.31333	0.18627	-2.34181
H	-2.38371	1.59227	-1.74743
H	-0.97503	2.69198	-1.74988
H	-0.81688	1.03553	-2.34370
H	-2.54926	-1.24725	1.91105
H	-2.79717	0.48473	1.91030
H	-1.25217	-0.17761	2.43278
H	0.77610	-0.99295	2.43441
H	0.97316	-2.66303	1.91386
H	2.35090	-1.58441	1.91600
H	-0.18296	-2.85715	-1.74978
H	-1.84232	-2.19362	-1.74920
H	-0.49185	-1.22207	-2.34335

$[Me_6BorazineH]^+$ (Protonated borazine)

N	14.055317	2.157442	17.173573
N	15.517447	0.447244	16.104399
N	16.509833	2.601228	16.866846
B	14.159706	0.832403	16.743602
B	16.769617	1.304352	16.417325
C	14.953537	4.596613	17.594564
C	17.643574	3.525971	17.064098
B	15.172727	3.099812	17.183575
C	15.325419	0.469535	14.601013
C	12.754092	2.641951	17.675061
C	13.053372	-0.275354	16.772511
C	18.162986	0.648579	16.133775
H	15.723345	-0.526968	16.341951
H	15.677441	5.275831	17.140847

H	15.072260	4.698295	18.682475
H	13.953338	4.963863	17.358113
H	17.573486	4.009425	18.039317
H	17.648228	4.297745	16.291202
H	18.586993	2.984545	17.018088
H	14.496122	-0.185351	14.332004
H	16.240069	0.130229	14.113924
H	15.102501	1.493829	14.300590
H	12.883316	3.160712	18.625791
H	12.073076	1.806997	17.831129
H	12.299822	3.331344	16.959953
H	12.712505	-0.452668	17.798406
H	13.379869	-1.237830	16.368865
H	12.167449	0.033474	16.207129
H	18.777856	0.643464	17.040434
H	18.726304	1.219759	15.387923
H	18.102329	-0.383664	15.777852

$[Me_6BorazineH]^-$ (Hydride Addition to $Me_6Borazine$)

N	14.127482	2.372294	16.960724
N	15.512977	0.441166	16.281063
N	16.580837	2.565419	17.194029
B	14.242852	0.991226	16.493971
B	16.846524	1.231433	16.434846
C	15.059797	4.535279	18.118950
C	17.801345	3.232390	17.574403
B	15.308597	3.111440	17.404649
C	15.723674	-0.901114	15.798361
C	12.814782	2.955742	17.138467
C	12.870819	0.180613	16.249197
C	17.531774	1.519148	14.964446
H	17.635216	0.544327	17.111024
H	15.943510	4.954383	18.605010
H	14.268218	4.471766	18.875808
H	14.720131	5.280845	17.387100
H	18.522096	2.496418	17.958030
H	17.650011	3.988751	18.351589
H	18.293533	3.733122	16.724402
H	16.588776	-1.347500	16.308944
H	15.950940	-0.932886	14.720037
H	14.861868	-1.555317	15.966450
H	12.369792	2.753291	18.129184
H	12.105267	2.578537	16.394662
H	12.842244	4.044472	17.025229
H	12.174575	0.307789	17.087361
H	13.004378	-0.892435	16.095628

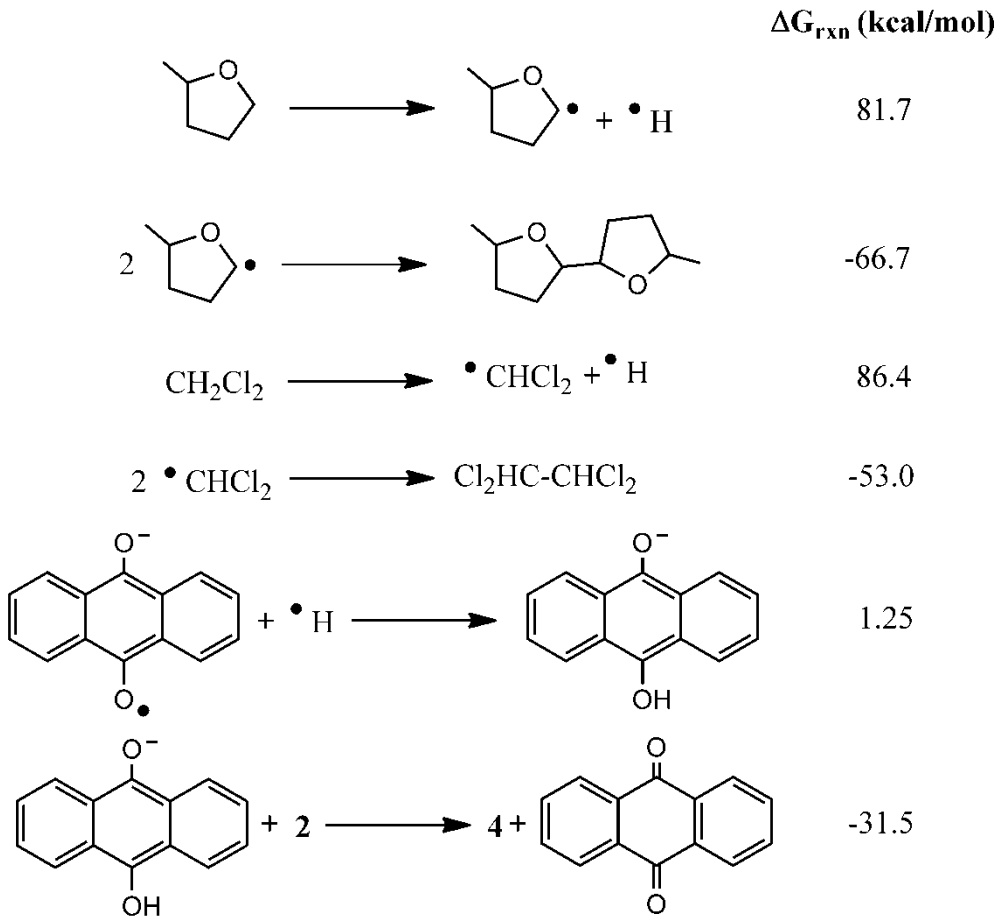
H	12.349046	0.562813	15.361207
H	18.487350	2.057873	15.042752
H	16.869567	2.125593	14.328118
H	17.751418	0.593369	14.412944

$[H_6BorazineH]^-$ (Hydride Addition to Borazine)

B	-1.371994	0.123524	0.457072
N	-0.645300	-1.193225	0.068974
B	0.675530	-1.317973	-0.371698
N	1.497617	-0.134803	-0.499009
B	0.964993	1.170347	-0.174838
N	-0.357185	1.283454	0.264763
H	-2.381776	0.296811	-0.250002
H	-1.773375	0.077216	1.634548
H	-1.184181	-2.043439	0.143388
H	1.143893	-2.392554	-0.648169
H	2.449524	-0.220410	-0.815878
H	1.671285	2.139072	-0.289589
H	-0.689031	2.211978	0.480436

$[H_6BorazineH]^+$ (Proton Addition to Borazine)

B	-1.469517	0.148290	0.324716
N	-1.036259	-1.005672	-0.421814
B	0.259898	-1.226094	-0.868931
N	1.289378	-0.123348	-0.559224
B	0.856549	1.092779	0.280667
N	-0.482196	1.147696	0.645714
H	-1.729514	-1.712608	-0.631102
H	2.125435	-0.547343	-0.137910
H	1.661985	0.224272	-1.453882
H	-0.787514	1.948579	1.183787
H	-2.593931	0.268489	0.665769
H	0.637866	-2.168050	-1.467397
H	1.682234	1.890775	0.544936



Scheme S-1. Free energies of H-atom abstraction, solvent dimerization, and hydride transfer reactions proposed during the AQ mediated reduction of **2** to hydride **4**.