Supporting information

Thermodynamic Hydricities of Biomimetic Organic Hydride Donors

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Table of Contents

1. ^{1}H NMR Spectra of Me_2N-AcrH and T-AcrH

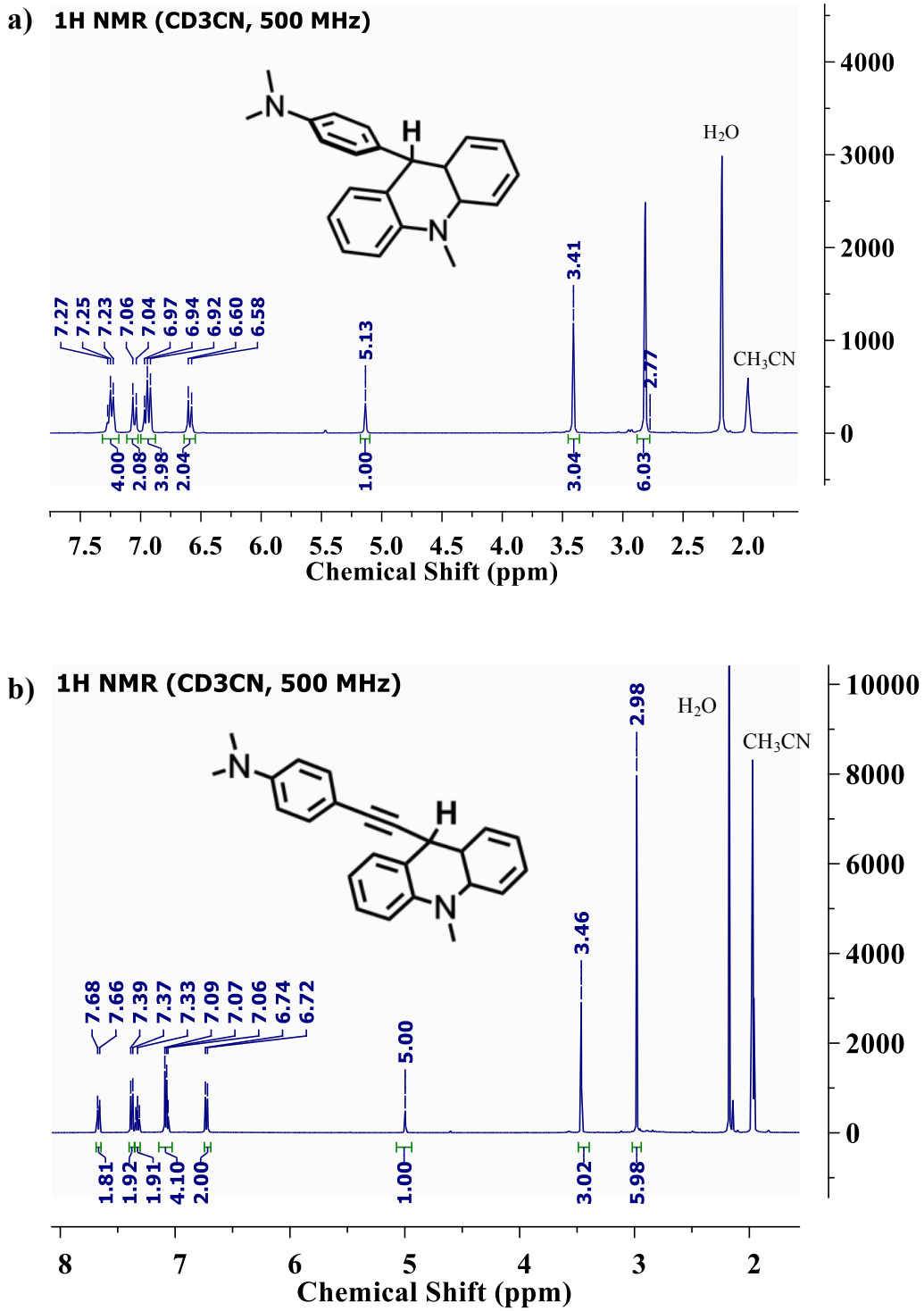

Figure S1. ^{1}H NMR spectra of: a) Me_2N-AcrH and b) T-AcrH, in CD_3CN.

2. Optimized Structures Used for DFT Calculations

6OH

C	-3.17749	-2.92078	0.07197
C	-3.14625	-2.0108	1.12371
C	-2.08007	-1.121	1.22135
C	-1.03765	-1.10448	0.27273
C	-1.10235	-2.03437	-0.76244
C	-2.16061	-2.94099	-0.86343
C	-0.3133	1.36858	0.22572
C	-1.25398	1.8001	-0.7182
C	-1.54554	3.15771	-0.87795
H	-2.26968	3.48865	-1.61047
C	-0.88765	4.0959	-0.0975
C	0.05063	3.70696	0.84548
C	0.32554	2.34685	1.00147
H	-3.99974	-3.62457	-0.00282
H	-3.94394	-2.01086	1.85486
H	-2.1638	-3.6643	-1.67136
H	-1.1087	5.14991	-0.22923
H	0.55298	4.45515	1.44419
C	0.07174	-0.08387	0.48921
C	1.4455	-0.46303	-0.04623
C	1.96468	-0.02033	-1.26889
C	2.25646	-1.28136	0.75002
C	3.26158	-0.35148	-1.66697
C	3.55272	-1.6292	0.36131
C	4.04112	-1.15247	-0.84524
H	3.66302	-0.00245	-2.60942
H	4.17697	-2.25917	0.9809
H	5.04816	-1.41331	-1.15384
H	0.21737	-0.10628	1.56843
O	1.69423	-1.71241	1.91086
O	1.22492	1.87754	1.90588
C	1.9327	2.79957	2.7083
H	2.54202	3.47358	2.09821
H	1.25809	3.38749	3.3384
H	2.58442	2.20132	3.34181
C	2.47027	-2.49878	2.79158
H	1.83341	-2.70085	3.65038

H	2.76188	-3.44694	2.32949
H	3.36576	-1.96419	3.12344
O	-0.09358	-2.09779	-1.68541
O	1.12992	0.71677	-2.03417
O	-1.9703	-0.20387	2.21778
O	-1.84487	0.84116	-1.46771
C	-0.45066	-1.75163	-3.01464
H	-1.19837	-2.4387	-3.42475
H	-0.8222	-0.72681	-3.05127
H	0.46309	-1.82955	-3.60366
C	1.57599	1.20446	-3.27807
H	2.4304	1.8795	-3.16502
H	1.84449	0.38995	-3.95886
H	0.73593	1.75651	-3.69615
C	-2.98561	-0.13934	3.19793
H	-3.95395	0.1084	2.75224
H	-3.06919	-1.07997	3.75118
H	-2.6902	0.65417	3.8811
C	-2.82756	1.20883	-2.40989
H	-2.41604	1.85504	-3.19206
H	-3.16962	0.27746	-2.85832
H	-3.67625	1.70936	-1.93317

$\underline{6O^{+}}$

C	-0.63017	4.19598	-0.01896
C	0.38667	3.67823	0.76947
C	0.62713	2.30922	0.75706
C	-0.18161	1.43751	-0.03149
C	-1.2129	2.01828	-0.82778
C	-1.42584	3.39185	-0.8209
C	0.01635	0.01375	0.00084
C	1.34004	-0.54937	0.0347
C	1.63264	-1.68566	0.84406
C	2.90253	-2.25143	0.83925
H	3.13884	-3.1015	1.4634
C	3.8827	-1.70585	0.02407
C	3.6458	-0.59911	-0.77787
C	2.38844	-0.00674	-0.76501
H	-0.806	5.26612	-0.0109
H	0.97621	4.34335	1.38415

H	-2.19308	3.84226	-1.43438
H	4.86908	-2.15656	0.01696
H	4.43912	-0.21291	-1.40194
C	-1.13198	-0.86882	-0.00118
C	-1.15933	-2.02351	-0.82739
C	-2.25797	-0.59878	0.8211
C	-2.27188	-2.85858	-0.83685
C	-3.35506	-1.45347	0.81986
C	-3.34678	-2.56374	-0.0116
H	-2.31341	-3.72739	-1.47857
H	-4.20825	-1.2693	1.45744
H	-4.20812	-3.22277	-0.0162
O	-2.16687	0.47208	1.62076
O	-1.90141	1.1828	-1.61009
C	-3.26161	0.81358	2.45676
H	-3.45657	0.02818	3.19125
H	-2.96134	1.72407	2.969
H	-4.16132	1.00583	1.86695
C	-2.97748	1.67902	-2.39271
H	-3.73626	2.14675	-1.76096
H	-2.62307	2.39026	-3.14273
H	-3.39971	0.80798	-2.88694
O	0.64821	-2.11948	1.63662
O	1.56491	1.73206	1.51179
O	2.07339	1.04292	-1.52827
O	-0.09677	-2.21419	-1.62041
C	0.84959	-3.27293	2.43966
H	1.10344	-4.13926	1.82417
H	1.6292	-3.10145	3.18587
H	-0.10032	-3.44611	2.93862
C	2.40983	2.53699	2.32136
H	2.97617	3.24438	1.71114
H	1.83369	3.07208	3.07999
H	3.09269	1.84297	2.80426
C	3.06273	1.62607	-2.36347
H	3.90587	1.99341	-1.77372
H	3.41221	0.91337	-3.11431
H	2.57002	2.46133	-2.85416
C	-0.04932	-3.35584	-2.46204
H	-0.10526	-4.2777	-1.87785

H	-0.85265	-3.33335	-3.20268
H	0.91196	-3.30318	-2.96671
6O ·			
C	-2.9945	-3.2096	0.0843
C	-3.2298	-1.9908	0.7564
C	-2.261	-0.9717	0.7465
C	-1.006	-1.094	0.0462
C	-0.8453	-2.3309	-0.663
C	-1.7958	-3.3666	-0.6268
C	-0.366	1.3558	0.083
C	-1.5	1.8468	-0.6451
C	-1.9048	3.195	-0.6097
H	-2.7884	3.5261	-1.1737
C	-1.1541	4.1343	0.1206
C	-0.0079	3.7127	0.8196
C	0.3635	2.3531	0.8118
H	-3.749	-4.0129	0.1093
H	-4.1659	-1.8566	1.3174
H	-1.5754	-4.2854	-1.1936
H	-1.4598	5.1929	0.1436
H	0.5741	4.4453	1.3972
C	0.0162	-0.0542	0.0763
C	1.4281	-0.4269	0.0478
C	2.4106	0.3271	-0.6817
C	1.934	-1.5971	0.7057
C	3.7727	-0.0297	-0.7199
C	3.2861	-1.9868	0.6363
C	4.2136	-1.1948	-0.0644
H	4.491	0.5756	-1.2912
H	3.6267	-2.8932	1.1576
H	5.2752	-1.4878	-0.1082
O	1.0242	-2.303	1.4463
O	1.4331	1.892	1.5348
C	2.3055	2.8241	2.1274
H	2.7313	3.5397	1.3868
H	1.8216	3.4207	2.9371
H	3.1387	2.2487	2.5749
C	1.2943	-3.656	1.7332
H	0.3656	-4.0888	2.1543

H	1.566	-4.2268	0.8166
H	2.1102	-3.7915	2.4826
O	0.2843	-2.5818	-1.4229
O	1.9234	1.3923	-1.3947
O	-2.4324	0.19	1.4519
O	-2.1476	0.9182	-1.4198
C	0.4523	-1.7176	-2.5432
H	-0.2467	-1.9923	-3.3692
H	0.2847	-0.6548	-2.2688
H	1.4932	-1.8362	-2.9032
C	2.8303	2.2473	-2.0499
H	3.5709	2.6983	-1.3505
H	3.3964	1.7364	-2.8643
H	2.2346	3.0638	-2.5011
C	-3.6883	0.4585	2.0306
H	-4.5135	0.4373	1.2819
H	-3.9509	-0.2554	2.8461
H	-3.6329	1.4765	2.4613
C	-3.3987	1.2492	-1.9741
H	-3.3347	2.0539	-2.7447
H	-3.7886	0.3343	-2.4607
H	-4.1304	1.5749	-1.2

$6O^{-}$ with K^{+}

C	-2.9894	-3.2241	0.1589
C	-3.2434	-2.01	0.8297
C	-2.2767	-0.9912	0.8461
C	-1.0047	-1.1027	0.1779
C	-0.8279	-2.3344	-0.5387
C	-1.7744	-3.3737	-0.5253
C	-0.3839	1.3575	0.2135
C	-1.5177	1.8283	-0.5322
C	-1.9243	3.1762	-0.5317
H	-2.8066	3.4917	-1.1062
C	-1.1769	4.1366	0.1741
C	-0.0314	3.7364	0.8834
C	0.34	2.3785	0.9112
H	-3.7422	-4.029	0.1608
H	-4.1909	-1.8782	1.372
H	-1.54	-4.2875	-1.0937

H	-1.4834	5.1949	0.1651
H	0.5526	4.483	1.4408
C	0.0126	-0.053	0.2272
C	1.4315	-0.415	0.1839
C	2.4044	0.3563	-0.5457
C	1.9557	-1.5956	0.8048
C	3.767	0.0075	-0.6031
C	3.3076	-1.9768	0.7168
C	4.2231	-1.167	0.0244
H	4.4747	0.6284	-1.1701
H	3.6518	-2.8941	1.2169
H	5.2855	-1.4525	-0.0379
O	1.0683	-2.3348	1.5579
O	1.4128	1.9478	1.6639
C	2.4038	2.8893	2.0272
H	2.7544	3.4784	1.1512
H	2.0609	3.6038	2.8112
H	3.2596	2.3158	2.4331
C	1.2596	-3.7367	1.6251
H	0.3228	-4.1723	2.0246
H	1.4498	-4.1601	0.6155
H	2.0952	-4.0309	2.3016
O	0.3136	-2.5763	-1.2819
O	1.9069	1.4276	-1.2396
O	-2.4722	0.1624	1.5751
O	-2.1576	0.8816	-1.288
C	0.4923	-1.7149	-2.4035
H	-0.1984	-1.993	-3.2344
H	0.3215	-0.6513	-2.1362
H	1.5366	-1.8354	-2.7515
C	2.7986	2.2614	-1.9455
H	3.5717	2.7144	-1.2843
H	3.3237	1.7272	-2.7714
H	2.1939	3.077	-2.3854
C	-3.7897	0.5124	1.9517
H	-4.4857	0.4988	1.0837
H	-4.2084	-0.1542	2.7409
H	-3.7444	1.5423	2.3547
C	-3.3497	1.2269	-1.9554
H	-3.1956	2.0012	-2.7431

H	-3.7242	0.3051	-2.4402
H	-4.1342	1.5989	-1.2579
K	-0.0015	-0.1968	4.4262

4OH

C	2.16657	-3.64375	-0.34689
C	2.8245	-2.43691	-0.19571
C	2.13871	-1.22397	-0.392
C	0.76634	-1.2542	-0.6648
C	0.13654	-2.49337	-0.84931
C	0.82409	-3.69539	-0.69733
H	2.71203	-4.56829	-0.18822
H	3.86197	-2.44807	0.10762
H	0.33255	-4.65028	-0.82878
C	2.14685	1.21223	-0.39078
C	2.84277	2.41966	-0.19616
C	2.19331	3.63154	-0.34401
C	0.85003	3.6934	-0.68976
C	0.15312	2.49669	-0.84181
C	0.7744	1.25279	-0.66112
H	3.88175	2.42196	0.10227
H	2.74609	4.55194	-0.18652
H	0.36493	4.65197	-0.81834
C	-0.0806	0.00215	-0.68232
H	-0.68769	0.00591	-1.58768
C	-1.07044	0.00306	0.48558
C	-2.45579	0.00748	0.26714
C	-0.61059	-0.00128	1.809
C	-3.35098	0.00741	1.34118
C	-1.4962	-0.00131	2.88985
C	-2.85918	0.00305	2.63837
H	-4.42051	0.01086	1.17834
H	-1.13614	-0.00452	3.91039
H	-3.5558	0.00307	3.47032
C	4.27356	-0.01019	-0.32219
N	2.82068	-0.00812	-0.31073
O	-1.16043	2.43609	-1.16543
O	-1.17566	-2.42261	-1.17624
O	-2.86501	0.01148	-1.02224
O	0.73495	-0.00529	1.9586

C	1.29031	-0.01792	3.25497
C	-1.93569	-3.61058	-1.22179
C	-4.24859	0.0145	-1.29716
C	-1.91107	3.63011	-1.20878
H	4.7041	0.00735	0.68466
H	4.64157	-0.89052	-0.84418
H	4.6433	0.8508	-0.8754
H	-1.905	-4.13961	-0.26404
H	-2.95794	-3.30032	-1.42945
H	-1.59354	-4.27985	-2.01761
H	1.00709	0.87421	3.82253
H	0.99395	-0.91325	3.81059
H	2.36925	-0.02492	3.11166
H	-4.33761	0.01721	-2.38175
H	-4.73963	-0.87919	-0.89888
H	-4.73665	0.90797	-0.89476
H	-1.56498	4.29718	-2.00474
H	-2.9362	3.32838	-1.41479
H	-1.87432	4.1582	-0.25073

$\underline{4O^+}$

C	-3.98094	0.00747	0.24837
C	-3.23671	0.03812	1.41996
C	-1.84477	0.03417	1.33141
C	-1.22662	0.00034	0.08748
C	-1.98745	-0.03087	-1.07702
C	-3.37767	-0.0275	-1.00351
C	0.2603	-0.00063	0.008
C	0.9676	-1.22165	-0.02368
C	0.33156	-2.52739	-0.07109
C	1.09169	-3.67082	-0.16946
H	0.6239	-4.64302	-0.22458
C	2.48632	-3.58391	-0.22048
C	3.14253	-2.38581	-0.13556
C	2.39704	-1.1972	-0.01652
H	-5.06381	0.01079	0.31224
H	-3.74081	0.06522	2.37679
H	-3.9898	-0.05058	-1.89545
H	3.06248	-4.49483	-0.3356
H	4.21786	-2.36827	-0.21691

C	0.96693	1.21991	-0.05239
C	2.39644	1.19716	-0.03251
C	0.3298	2.52331	-0.13635
C	3.14162	2.38554	-0.15659
C	1.08964	3.66668	-0.23732
C	2.48501	3.58155	-0.2641
H	4.21787	2.36937	-0.22411
H	0.62134	4.637	-0.31595
H	3.06154	4.49194	-0.38164
N	3.04495	0.00105	0.10585
C	4.48425	0.00319	0.40288
H	4.72681	-0.86828	1.00114
H	5.07502	0.0045	-0.51383
H	4.7239	0.87508	1.00189
O	-0.9959	-2.5547	-0.02563
O	-1.00237	0.06155	2.39241
O	-1.27205	-0.06295	-2.22573
O	-0.99851	2.54846	-0.12317
C	-1.97595	-0.10569	-3.4542
H	-2.59569	-1.00429	-3.52333
H	-2.59964	0.78337	-3.58367
H	-1.21574	-0.13005	-4.23141
C	-1.68716	3.78624	-0.22276
H	-1.46466	4.28204	-1.1706
H	-2.74232	3.52915	-0.18196
H	-1.43498	4.4423	0.61376
C	-1.56207	0.10832	3.69286
H	-2.1629	1.01153	3.8325
H	-2.17403	-0.7759	3.89286
H	-0.719	0.12594	4.37971
C	-1.6844	-3.79405	-0.10507
H	-2.7391	-3.53811	-0.04869
H	-1.47648	-4.29587	-1.05304
H	-1.41759	-4.44399	0.73171

4O ·

C	2.6725	-3.555	0.3553
C	3.2507	-2.2657	0.2904
C	2.4495	-1.1378	0.033
C	1.0079	-1.2082	-0.0166

C	0.4916	-2.5532	-0.1364
C	1.2977	-3.6878	0.0982
H	3.2941	-4.4394	0.563
H	4.3365	-2.1474	0.4175
H	0.8484	-4.6903	0.0576
C	2.3817	1.314	0.0704
C	3.115	2.5067	0.2421
C	2.4527	3.7271	0.5023
C	1.0599	3.7221	0.6628
C	0.3289	2.5182	0.5568
C	0.9466	1.2689	0.1838
H	4.2105	2.4954	0.1619
H	3.0248	4.6634	0.5953
H	0.5367	4.6568	0.9098
C	0.2392	0.0136	-0.0092
C	-1.2389	-0.0068	-0.0743
C	-1.9421	0.7372	-1.0621
C	-2.0246	-0.7307	0.8643
C	-3.3513	0.7308	-1.1393
C	-3.4328	-0.7724	0.7831
C	-4.0873	-0.0374	-0.2202
H	-3.8782	1.3012	-1.9164
H	-4.0229	-1.3502	1.5078
H	-5.188	-0.0595	-0.2844
C	4.4376	0.1556	-0.6518
N	3.0447	0.1135	-0.2674
O	-1.0144	2.4819	0.83
O	-0.8132	-2.6713	-0.5471
O	-1.1581	1.4473	-1.9281
O	-1.3262	-1.347	1.8642
C	-2.0202	-2.2232	2.7272
C	-1.4145	-3.9437	-0.5588
C	-1.7882	2.2925	-2.869
C	-1.755	3.6805	0.8095
H	5.1482	0.2206	0.2084
H	4.6881	-0.7565	-1.228
H	4.6207	1.0346	-1.3027
H	-1.3826	-4.4417	0.4376
H	-2.4748	-3.7941	-0.8402
H	-0.9464	-4.6359	-1.2985

H	-2.7783	-1.6993	3.3545
H	-2.5368	-3.0386	2.173
H	-1.2679	-2.6785	3.3991
H	-0.9849	2.8074	-3.4292
H	-2.4186	1.7309	-3.5963
H	-2.4287	3.0634	-2.3835
H	-1.5784	4.2694	-0.1198
H	-2.8249	3.3954	0.8475
H	-1.538	4.343	1.6807

$4O^-$ with K^+

C	2.6081	-3.5239	0.6356
C	3.1944	-2.2414	0.5321
C	2.4113	-1.1325	0.1631
C	0.9728	-1.2068	0.0576
C	0.461	-2.5546	-0.034
C	1.2517	-3.6743	0.3007
H	3.2149	-4.3963	0.9223
H	4.2735	-2.1178	0.7026
H	0.8057	-4.6788	0.286
C	2.3578	1.3096	0.1055
C	3.0934	2.4997	0.29
C	2.4322	3.7209	0.5431
C	1.0389	3.722	0.6999
C	0.306	2.5206	0.5842
C	0.9194	1.2738	0.1935
H	4.1895	2.4848	0.223
H	3.0066	4.6556	0.6396
H	0.52	4.6569	0.9546
C	0.2059	0.0168	0.0036
C	-1.2702	0.0013	-0.0675
C	-1.9655	0.7693	-1.0462
C	-2.0715	-0.7322	0.851
C	-3.3729	0.7687	-1.1359
C	-3.478	-0.7659	0.7581
C	-4.1214	-0.0135	-0.2384
H	-3.8902	1.3531	-1.9089
H	-4.0762	-1.3474	1.4733
H	-5.2213	-0.0308	-0.3139
C	4.4331	0.1209	-0.493

N	3.018	0.0983	-0.2002
O	-1.0318	2.4735	0.8924
O	-0.8191	-2.6899	-0.5116
O	-1.1714	1.4907	-1.8922
O	-1.3938	-1.3655	1.8665
C	-2.079	-2.357	2.6126
C	-1.3757	-3.9797	-0.616
C	-1.7885	2.3599	-2.8211
C	-1.774	3.6731	0.9302
H	5.0832	0.2284	0.4103
H	4.718	-0.8181	-1.006
H	4.6627	0.9665	-1.1722
H	-1.4205	-4.5091	0.363
H	-2.4094	-3.8518	-0.9907
H	-0.8169	-4.6321	-1.328
H	-2.8535	-1.9292	3.2893
H	-2.569	-3.1061	1.954
H	-1.3223	-2.875	3.2332
H	-0.9767	2.8832	-3.3604
H	-2.4131	1.8167	-3.5667
H	-2.4306	3.1219	-2.3244
H	-1.6329	4.2827	0.0089
H	-2.8409	3.3855	1.0024
H	-1.5226	4.3129	1.8087
K	1.1286	0.3982	4.0684

PhAcrH

C	-2.70378	3.56435	0.04284
C	-2.83273	2.39847	0.78686
C	-2.19832	1.2201	0.3749
C	-1.43825	1.23022	-0.80489
C	-1.34074	2.40177	-1.54528
C	-1.96067	3.57455	-1.13096
C	-1.4533	-1.24733	-0.76171
C	-2.20848	-1.18852	0.41973
C	-2.84937	-2.34663	0.87651
H	-3.46193	-2.32258	1.76918
C	-2.73142	-3.5397	0.17459
C	-1.99418	-3.59771	-1.0014
C	-1.36756	-2.44505	-1.46005

H	-3.44931	2.41011	1.67702
H	-0.75035	2.39344	-2.45766
H	-0.78036	-2.47384	-2.37404
C	-0.69763	-0.02026	-1.22515
H	-0.6608	-0.04003	-2.31873
C	0.74489	-0.02896	-0.73452
C	1.06866	0.0514	0.62076
C	1.80029	-0.12313	-1.63516
C	2.38267	0.02926	1.05831
H	0.27821	0.13687	1.36068
C	3.12521	-0.14592	-1.21708
H	1.59287	-0.1772	-2.70069
C	3.45453	-0.08696	0.14897
H	2.56904	0.10541	2.12186
H	3.90003	-0.20989	-1.97017
N	-2.31023	0.02938	1.105
C	-2.87103	0.05755	2.43952
H	-3.9682	0.05959	2.44651
H	-2.51911	-0.80856	2.99905
H	-2.51617	0.94518	2.96224
H	-3.20331	4.46587	0.38187
H	-3.23498	-4.42493	0.54879
H	-1.90731	-4.52695	-1.55349
H	-1.8651	4.48253	-1.71604
H	4.47032	-0.12833	0.48266

PhAcr$^+$

C	1.76152	3.6009	-0.2041
C	2.4548	2.42595	-0.10543
C	1.75708	1.19799	-0.00591
C	0.33248	1.21013	-0.0374
C	-0.34518	2.46092	-0.13348
C	0.34887	3.6293	-0.20753
C	0.34031	-1.21235	0.00719
C	1.76508	-1.1882	0.02467
C	2.47159	-2.41336	-0.04555
H	3.54884	-2.43382	-0.11378
C	1.78712	-3.59689	-0.08134
C	0.37536	-3.63709	-0.03563
C	-0.32753	-2.47232	0.00223

H	3.53307	2.45467	-0.14966
H	-1.42713	2.46272	-0.16162
H	-0.17185	4.57526	-0.28864
H	-0.13851	-4.59022	-0.044
H	-1.40951	-2.4851	0.02297
C	-0.37034	-0.00306	0.0061
C	-1.85656	-0.00495	0.02756
C	-2.57406	-0.28868	-1.13371
C	-2.53292	0.27997	1.21283
C	-3.96328	-0.28433	-1.10695
H	-2.04654	-0.50745	-2.05604
C	-3.92216	0.27371	1.23552
H	-1.9733	0.50157	2.11535
C	-4.6381	-0.00643	0.07673
H	-4.51712	-0.5004	-2.01365
H	-4.44403	0.48953	2.16103
N	2.42245	0.00829	0.10486
C	3.87619	0.01596	0.32797
H	4.15438	-0.85047	0.91724
H	4.41047	0.01295	-0.62213
H	4.14653	0.89145	0.90754
H	2.34498	-4.52349	-0.15088
H	2.31338	4.52908	-0.29661
H	-5.72234	-0.00746	0.0962

PhAcr·

C	2.0956	-3.5738	-0.229
C	2.6512	-2.2719	-0.1157
C	1.8355	-1.1368	0.0355
C	0.3931	-1.2452	-0.0338
C	-0.1233	-2.5756	-0.1003
C	0.7039	-3.7129	-0.1913
C	-0.4092	-0.0431	0.0275
C	0.2554	1.2399	-0.075
C	1.6946	1.3114	0.0159
C	2.3682	2.5328	-0.1646
H	3.4664	2.5629	-0.1239
C	1.6588	3.7412	-0.3895
C	0.2616	3.6975	-0.4699
C	-0.4188	2.472	-0.3311

H	2.7577	-4.4475	-0.3296
H	3.7446	-2.1581	-0.1276
H	-1.213	-2.7201	-0.0643
H	0.2401	-4.7121	-0.2382
H	2.2099	4.6874	-0.5046
H	-0.3159	4.6182	-0.6547
H	-1.5148	2.4579	-0.4271
C	-1.8844	-0.0983	0.0525
C	-2.6265	0.6579	1.0063
C	-2.6461	-0.8845	-0.8591
C	-4.0266	0.6221	1.0555
H	-2.0764	1.2724	1.7367
C	-4.0487	-0.9276	-0.808
H	-2.1227	-1.4525	-1.6433
C	-4.7547	-0.1771	0.1504
H	-4.559	1.2122	1.8194
H	-4.5989	-1.5446	-1.5374
H	-5.8551	-0.213	0.1928
N	2.3962	0.1265	0.3256
C	3.7886	0.2111	0.7152
H	4.4954	0.2512	-0.1473
H	3.9474	1.1195	1.3285
H	4.0547	-0.6674	1.3344

PhAcr $^{-}$ with K^{+}

C	2.03	-3.6491	-0.2598
C	2.6045	-2.3642	-0.0721
C	1.8035	-1.223	0.1055
C	0.3631	-1.3035	-0.0045
C	-0.1748	-2.618	-0.1509
C	0.6356	-3.7646	-0.2713
C	-0.4226	-0.0932	0.0945
C	0.2573	1.1818	0.0773
C	1.6998	1.2277	0.1953
C	2.3906	2.4519	0.1214
H	3.4881	2.4644	0.1817
C	1.697	3.6862	-0.01
C	0.2999	3.667	-0.1092
C	-0.399	2.4423	-0.0848
H	2.6799	-4.5294	-0.3802

H	3.6994	-2.2699	-0.0477
H	-1.2676	-2.742	-0.1576
H	0.1571	-4.7518	-0.3816
H	2.261	4.6311	-0.0378
H	-0.2646	4.6073	-0.2193
H	-1.4942	2.4521	-0.189
C	-1.9006	-0.1337	0.0617
C	-2.6773	0.5353	1.0492
C	-2.626	-0.8241	-0.9498
C	-4.0787	0.5104	1.0386
H	-2.1592	1.0769	1.8561
C	-4.0296	-0.8582	-0.9616
H	-2.0709	-1.3248	-1.7577
C	-4.7707	-0.1931	0.0327
H	-4.6379	1.0333	1.8314
H	-4.5522	-1.3993	-1.7674
H	-5.8719	-0.2209	0.0248
N	2.3767	0.0182	0.4623
C	3.7563	0.0599	0.9035
H	4.4943	0.122	0.0694
H	3.9138	0.9408	1.5567
H	3.984	-0.8483	1.4948
K	0.6803	2.2406	3.8924

$\underline{Me_2N\text{-}AcrH}$

C	-2.70378	3.56435	0.04284
C	-2.83273	2.39847	0.78686
C	-2.19832	1.2201	0.3749
C	-1.43825	1.23022	-0.80489
C	-1.34074	2.40177	-1.54528
C	-1.96067	3.57455	-1.13096
C	-1.4533	-1.24733	-0.76171
C	-2.20848	-1.18852	0.41973
C	-2.84937	-2.34663	0.87651
H	-3.46193	-2.32258	1.76918
C	-2.73142	-3.5397	0.17459
C	-1.99418	-3.59771	-1.0014
C	-1.36756	-2.44505	-1.46005
H	-3.44931	2.41011	1.67702
H	-0.75035	2.39344	-2.45766

H	-0.78036	-2.47384	-2.37404
C	-0.69763	-0.02026	-1.22515
H	-0.6608	-0.04003	-2.31873
C	0.74489	-0.02896	-0.73452
C	1.06866	0.0514	0.62076
C	1.80029	-0.12313	-1.63516
C	2.38267	0.02926	1.05831
H	0.27821	0.13687	1.36068
C	3.12521	-0.14592	-1.21708
H	1.59287	-0.1772	-2.70069
C	3.45453	-0.08696	0.14897
H	2.56904	0.10541	2.12186
H	3.90003	-0.20989	-1.97017
N	-2.31023	0.02938	1.105
C	-2.87103	0.05755	2.43952
H	-3.9682	0.05959	2.44651
H	-2.51911	-0.80856	2.99905
H	-2.51617	0.94518	2.96224
H	-3.20331	4.46587	0.38187
H	-3.23498	-4.42493	0.54879
H	-1.90731	-4.52695	-1.55349
H	-1.8651	4.48253	-1.71604
N	4.76719	-0.15119	0.58324
C	5.82809	0.01206	-0.39029
H	6.79072	-0.06673	0.11221
H	5.79323	-0.77636	-1.1463
H	5.78597	0.98245	-0.9054
C	5.06566	0.20279	1.95679
H	6.13547	0.09595	2.12855
H	4.77861	1.23545	2.20149
H	4.55873	-0.46722	2.65565

Me_2N-Acr $^+$

C	-2.71261	-3.60016	-0.3352
C	-3.40328	-2.43241	-0.15625
C	-2.70721	-1.20652	-0.03178
C	-1.28471	-1.20672	-0.09857
C	-0.6135	-2.44669	-0.30616
C	-1.30423	-3.6163	-0.4116
C	-1.3077	1.21579	0.05196

C	-2.73138	1.17717	0.06486
C	-3.45352	2.39427	0.02524
H	-4.52962	2.39919	-0.0637
C	-2.78805	3.58932	0.04987
C	-1.38102	3.64314	0.14209
C	-0.66396	2.48481	0.14033
H	-4.48245	-2.4633	-0.15891
H	0.46357	-2.44267	-0.40458
H	-0.7818	-4.55009	-0.57865
H	-0.87848	4.60007	0.20903
H	0.41456	2.51607	0.21281
C	-0.57622	0.01074	-0.00634
C	0.89605	0.01694	0.00491
C	1.62926	0.66885	-0.99187
C	1.60716	-0.64278	1.01276
C	3.00992	0.65858	-0.99364
H	1.10968	1.17249	-1.80078
C	2.98732	-0.6381	1.04221
H	1.06872	-1.15256	1.80544
C	3.73576	0.01042	0.03252
H	3.52619	1.15813	-1.80241
H	3.48579	-1.14471	1.85777
N	-3.38113	-0.02561	0.12474
C	-4.82847	-0.05067	0.37761
H	-5.10452	0.80875	0.97826
H	-5.38565	-0.04817	-0.55953
H	-5.07711	-0.93275	0.95766
H	-3.3583	4.50999	0.0054
H	-3.26532	-4.5259	-0.44633
N	5.0988	0.00927	0.04669
C	5.8152	-0.67168	1.1075
H	6.8848	-0.56115	0.94544
H	5.5801	-0.24927	2.09039
H	5.5873	-1.74299	1.12929
C	5.83829	0.67632	-1.00705
H	6.90413	0.56846	-0.82023
H	5.62494	0.242	-1.98992
H	5.61111	1.74708	-1.0469

Me_2N-Acr ·

C	-2.7796	-3.6714	-0.4314
C	-3.4494	-2.4318	-0.2317
C	-2.7355	-1.243	-0.0056
C	-1.2892	-1.2302	-0.0425
C	-0.6526	-2.4932	-0.252
C	-1.3798	-3.6877	-0.4309
C	-1.3242	1.2509	0.0438
C	-2.7719	1.2142	0.0715
C	-3.5226	2.3933	-0.0684
H	-4.6202	2.3395	-0.1086
C	-2.8939	3.6681	-0.1403
C	-1.497	3.7322	-0.0799
C	-0.7312	2.5515	0.0057
H	-4.5486	-2.4139	-0.2498
H	0.4477	-2.5237	-0.2731
H	-0.8338	-4.6342	-0.5812
H	-0.9821	4.7073	-0.1026
H	0.3661	2.6265	0.0534
C	-0.5835	0.0184	0.0855
C	0.9029	0.0238	0.0644
C	1.6473	0.6216	-0.9829
C	1.6665	-0.5923	1.0869
C	3.0484	0.6164	-1.0148
H	1.1065	1.1071	-1.8114
C	3.0675	-0.6181	1.0756
H	1.1391	-1.0635	1.9326
C	3.8057	-0.0205	0.0118
H	3.5573	1.0995	-1.8602
H	3.5923	-1.1047	1.9088
N	-3.397	-0.0324	0.3011
C	-4.8049	-0.0645	0.6369
H	-5.0552	0.8074	1.2723
H	-5.4797	-0.0461	-0.2517
H	-5.0277	-0.983	1.2145
H	-3.5071	4.5781	-0.2297
H	-3.3638	-4.5921	-0.5837
N	5.1935	-0.0599	-0.0235
C	5.9243	-0.531	1.1397
H	7.0073	-0.5275	0.9166
H	5.7578	0.1002	2.0456

H	5.6456	-1.5741	1.4019
C	5.9047	0.7157	-1.0237
H	6.9897	0.5218	-0.9325
H	5.6035	0.4271	-2.0534
H	5.7406	1.8164	-0.9228

Me_2N-Acr $^-$ with K^+

C	-2.7722	-3.7304	-0.2953
C	-3.42	-2.5018	0.0081
C	-2.6917	-1.3071	0.1293
C	-1.268	-1.2785	-0.1107
C	-0.6558	-2.5281	-0.4324
C	-1.3879	-3.7299	-0.509
C	-1.3192	1.2051	-0.0504
C	-2.7514	1.1453	0.1749
C	-3.5381	2.3078	0.1366
H	-4.6273	2.2325	0.2659
C	-2.9503	3.5932	-0.0211
C	-1.5594	3.684	-0.1461
C	-0.7643	2.5193	-0.1701
H	-4.5074	-2.4981	0.1685
H	0.4275	-2.5428	-0.6261
H	-0.862	-4.6684	-0.7506
H	-1.0708	4.6685	-0.2376
H	0.3265	2.6219	-0.2661
C	-0.5584	-0.0221	-0.0517
C	0.9254	-0.0185	-0.0718
C	1.7068	0.6882	-1.0204
C	1.6623	-0.7318	0.9116
C	3.1094	0.7128	-0.9805
H	1.2016	1.2365	-1.8312
C	3.0598	-0.7282	0.9703
H	1.1082	-1.315	1.6671
C	3.8337	-0.0028	0.0155
H	3.6455	1.2876	-1.7484
H	3.554	-1.2916	1.7735
N	-3.3034	-0.1035	0.5488
C	-4.6393	-0.1484	1.1071
H	-4.799	0.7326	1.7594
H	-5.4492	-0.1549	0.3394

H	-4.751	-1.0595	1.7269
H	-3.5867	4.4916	-0.0272
H	-3.3604	-4.6589	-0.3608
N	5.2221	-0.0002	0.0562
C	5.9045	-0.576	1.2015
H	6.9975	-0.5172	1.0431
H	5.6682	-0.0529	2.1597
H	5.6482	-1.649	1.3341
C	5.9591	0.8951	-0.8169
H	7.0441	0.7309	-0.6781
H	5.7291	0.7027	-1.8873
H	5.7453	1.9736	-0.6175
K	-0.7602	1.2027	3.8028

CN-BNAH

C	0.66428	-1.64018	-0.32915
C	1.70725	-1.76333	-1.14613
C	2.91766	-0.86725	-1.08735
C	2.71897	0.17859	-0.00311
C	1.61424	0.22237	0.78105
H	3.82143	-1.45888	-0.89186
H	1.69105	-2.55154	-1.88967
H	-0.1979	-2.29342	-0.38411
H	1.50167	0.98183	1.54585
H	3.08469	-0.38811	-2.06033
C	-0.636	-0.52242	1.4399
H	-0.8726	-1.48354	1.9041
H	-0.43863	0.17712	2.25508
C	-1.81107	-0.04277	0.61195
C	-1.65417	0.97634	-0.32739
C	-3.07184	-0.60463	0.79549
C	-2.74137	1.42926	-1.06392
H	-0.67528	1.41734	-0.49041
C	-4.16332	-0.15015	0.06188
H	-3.20394	-1.40606	1.51663
C	-4.00023	0.86768	-0.87033
H	-2.60595	2.22117	-1.793
H	-5.13923	-0.59898	0.21358
H	-4.84855	1.22031	-1.44716
N	0.59154	-0.66118	0.67139

C	3.73347	1.14448	0.20475
N	4.58219	1.91759	0.34511

CN-BNA^{+}

C	-1.69312	1.90776	-0.87025
C	-0.62098	1.58766	-0.06994
C	-1.67206	-0.36827	0.66826
C	-2.77361	-0.0957	-0.12659
C	-2.78901	1.05869	-0.90811
H	-1.66547	2.81418	-1.45784
H	0.26563	2.20275	-0.0052
H	-1.61188	-1.24462	1.29715
H	-3.64387	1.28671	-1.53145
C	0.57166	0.16039	1.51979
H	0.72237	1.01781	2.17376
H	0.30705	-0.69311	2.14053
C	1.77902	-0.11977	0.66539
C	2.7884	0.83203	0.54158
C	1.88827	-1.33352	-0.01378
C	3.89698	0.5753	-0.25845
H	2.71549	1.77447	1.07555
C	2.99377	-1.58819	-0.8131
H	1.11174	-2.08596	0.08469
C	3.99904	-0.63278	-0.93687
H	4.67989	1.31998	-0.34766
H	3.07526	-2.53492	-1.33511
H	4.86408	-0.83431	-1.55906
N	-0.62769	0.46835	0.68028
C	-3.8781	-1.0078	-0.12709
N	-4.76685	-1.73661	-0.13178

CN-BNA $^{\cdot}$

C	1.7879	-0.4521	-0.8702
C	1.0444	-2.2205	0.4489
C	0.901	-1.4033	1.5616
C	1.0677	0.0037	1.4461
C	1.6486	0.4414	0.2129
H	2.4306	-0.2251	-1.7398
H	1.1724	-3.3172	0.5282
H	0.7872	-1.8619	2.5618
H	0.8987	0.6975	2.2798

C	2.1831	1.7579	0.0998
N	2.6118	2.8515	-0.0095
C	-0.3639	-1.5262	-1.493
H	-0.8167	-2.5404	-1.4557
H	-0.2104	-1.2607	-2.5617
C	-1.2536	-0.5142	-0.8222
C	-1.1796	0.851	-1.1842
C	-2.0746	-0.8766	0.2703
C	-1.8565	1.8299	-0.4416
H	-0.5661	1.1466	-2.0497
C	-2.7611	0.0979	1.0085
H	-2.1554	-1.9384	0.5522
C	-2.6381	1.4587	0.668
H	-1.7745	2.8909	-0.7278
H	-3.3896	-0.2014	1.8631
H	-3.1692	2.2261	1.2531
N	1.0043	-1.6503	-0.8797

CN-BNA$^-$ with K^+

C	1.6751	-0.1903	-0.7347
C	0.9548	-2.1136	0.5243
C	1.4866	-1.5817	1.6709
C	2.0558	-0.257	1.7367
C	2.2486	0.3445	0.409
H	1.8022	0.2845	-1.7215
H	0.6225	-3.1598	0.4364
H	1.552	-2.237	2.5586
H	2.7802	-0.0191	2.531
C	3.0462	1.5138	0.2512
N	3.666	2.5158	0.1736
C	-0.437	-1.2853	-1.3978
H	-0.775	-2.3336	-1.5363
H	-0.2569	-0.8561	-2.4053
C	-1.4718	-0.4824	-0.6552
C	-1.6597	0.893	-0.9295
C	-2.2012	-1.0637	0.4124
C	-2.5762	1.6579	-0.1908
H	-1.097	1.3616	-1.7531
C	-3.1037	-0.2967	1.1668
H	-2.0691	-2.1334	0.6364

C	-3.3063	1.0654	0.8633
H	-2.7345	2.7188	-0.4419
H	-3.6709	-0.7665	1.9862
H	-4.0392	1.6584	1.4331
N	0.8717	-1.3366	-0.6958
K	-0.2915	2.2206	3.2115

T-AcrH

C	-3.59173	3.50609	0.49426
C	-3.40796	2.33335	1.21726
C	-2.89652	1.19266	0.58992
C	-2.57187	1.25515	-0.77367
C	-2.78323	2.42651	-1.48607
C	-3.29043	3.56039	-0.86096
C	-2.57417	-1.21459	-0.82181
C	-2.89788	-1.20501	0.54338
C	-3.40949	-2.36891	1.12636
H	-3.68715	-2.38711	2.17293
C	-3.59497	-3.51243	0.35835
C	-3.29546	-3.51391	-0.99828
C	-2.78766	-2.35705	-1.57919
H	-3.68731	2.31064	2.26325
H	-2.52937	2.45383	-2.54184
H	-2.53488	-2.34319	-2.63545
C	-1.93622	0.03151	-1.40232
H	-2.09769	0.05324	-2.48424
N	-2.71643	-0.01995	1.27026
C	-2.83516	-0.04809	2.71385
H	-3.87637	-0.05326	3.06009
H	-2.33313	-0.93432	3.10029
H	-2.33018	0.82047	3.13499
H	-3.99204	4.37949	0.99822
H	-3.99537	-4.40435	0.8287
H	-3.44413	4.47447	-1.42337
H	-3.45101	-4.40497	-1.59601
C	-0.48533	0.02324	-1.15087
C	0.69486	0.01285	-0.90655
C	2.08743	-0.00316	-0.58253
C	2.51027	-0.11448	0.74776
C	3.07389	0.096	-1.57052

C	3.85169	-0.13119	1.08124
H	1.76854	-0.18616	1.53662
C	4.41948	0.08046	-1.25174
H	2.78017	0.19095	-2.61086
C	4.85158	-0.0419	0.08761
H	4.11923	-0.21489	2.12646
H	5.14017	0.16507	-2.05468
N	6.18318	-0.076	0.40879
C	6.58836	-0.07916	1.7998
H	7.67408	-0.11639	1.85868
H	6.24889	0.81804	2.33256
H	6.20003	-0.95654	2.32635
C	7.17925	0.14181	-0.62049
H	8.1711	0.0829	-0.1775
H	7.12082	-0.62259	-1.40179
H	7.07609	1.12549	-1.09553

T-Acr$^+$

C	-3.76063	-3.60297	-0.13239
C	-4.44198	-2.41964	-0.0237
C	-3.73606	-1.19526	0.04003
C	-2.31928	-1.22131	-0.04443
C	-1.65158	-2.4698	-0.14086
C	-2.35175	-3.63966	-0.1786
C	-1.59965	0.00001	-0.03715
C	-2.31931	1.22132	-0.04445
C	-3.73609	1.19523	0.04001
C	-4.44204	2.4196	-0.02374
H	-5.52173	2.43925	-0.02947
C	-3.76072	3.60294	-0.13245
C	-2.35184	3.63966	-0.17865
C	-1.65164	2.46982	-0.14089
H	-4.32221	-4.52792	-0.19513
H	-5.52167	-2.43932	-0.02942
H	-0.56958	-2.47299	-0.19735
H	-1.8361	-4.58838	-0.26039
H	-4.32232	4.52787	-0.1952
H	-1.83621	4.5884	-0.26045
H	-0.56964	2.47304	-0.19738
C	-0.2017	0.00003	-0.04709

C	1.012	0.00005	-0.03569
C	2.41685	0.00003	-0.01764
C	3.1404	1.20719	-0.00572
C	3.14038	-1.20715	-0.00566
C	4.51459	1.21352	0.01912
H	2.60412	2.14993	-0.01554
C	4.51457	-1.2135	0.01918
H	2.60408	-2.14987	-0.01543
C	5.2512	0.00001	0.03429
H	5.02629	2.16622	0.02762
H	5.02625	-2.16621	0.02774
N	6.6066	-0.00001	0.06253
C	7.33905	-1.25434	0.07252
H	8.40573	-1.04661	0.09812
H	7.09211	-1.856	0.95289
H	7.13195	-1.84722	-0.824
C	7.33906	1.25432	0.0725
H	8.40574	1.04657	0.09818
H	7.13203	1.84715	-0.82406
H	7.09208	1.85603	0.95282
N	-4.39546	-0.00002	0.17399
C	-5.83167	-0.00004	0.47739
H	-6.07399	0.8711	1.07672
H	-6.42387	-0.00008	-0.43843
H	-6.07395	-0.87117	1.07676

T-Acr

C	3.8782	3.6645	-0.2218
C	4.528	2.4173	-0.0554
C	3.7935	1.2201	0.0627
C	2.36	1.2475	-0.0515
C	1.7394	2.5127	-0.2185
C	2.4801	3.7079	-0.2931
C	1.6151	-0.0023	0.0007
C	2.3533	-1.2559	-0.0557
C	3.7869	-1.2367	0.0584
C	4.5149	-2.4373	-0.0646
H	5.6128	-2.4202	-0.0233
C	3.8583	-3.6803	-0.236
C	2.4599	-3.716	-0.3072

C	1.7258	-2.5171	-0.2278
H	4.4791	4.5841	-0.2958
H	5.6258	2.3939	-0.0137
H	0.6402	2.5413	-0.291
H	1.9551	4.6687	-0.4174
H	4.4541	-4.6029	-0.3142
H	1.9298	-4.6734	-0.4356
H	0.6264	-2.5391	-0.3008
C	0.2148	0.0011	-0.0136
C	-1.0333	0.0024	-0.0156
C	-2.4506	0.0037	0.0041
C	-3.2069	-1.2075	0.0322
C	-3.2056	1.216	-0.01
C	-4.6034	-1.2092	0.055
H	-2.6731	-2.1707	0.0328
C	-4.6021	1.2199	0.0134
H	-2.671	2.1781	-0.045
C	-5.3517	0.0063	0.0635
H	-5.1223	-2.1774	0.0718
H	-5.12	2.1886	-0.0047
N	-6.7385	0.008	0.1195
C	-7.4604	1.255	-0.0598
H	-8.5437	1.0708	0.0622
H	-7.1653	2.0101	0.7003
H	-7.3011	1.7105	-1.0671
C	-7.4618	-1.2439	-0.0153
H	-8.5448	-1.0544	0.1011
H	-7.3035	-1.7351	-1.0061
H	-7.1668	-1.9721	0.7706
N	4.4313	-0.0105	0.3256
C	5.8299	-0.0149	0.7108
H	6.0438	-0.9095	1.326
H	6.5299	-0.0146	-0.1567
H	6.0483	0.8755	1.3304

T-Acr$^-$ with K^+

C	3.8763	3.6649	-0.1832
C	4.5226	2.4173	-0.0026
C	3.7858	1.2207	0.105
C	2.3538	1.2471	-0.0318

C	1.7374	2.5126	-0.2165
C	2.4796	3.7075	-0.2812
C	1.6093	-0.001	0.0153
C	2.3465	-1.2534	-0.0347
C	3.7786	-1.2358	0.1019
C	4.5084	-2.4364	-0.0092
H	5.6054	-2.4199	0.0528
C	3.8547	-3.6797	-0.1935
C	2.4577	-3.7138	-0.2917
C	1.7227	-2.5147	-0.2235
H	4.4785	4.5844	-0.2484
H	5.6195	2.394	0.0595
H	0.64	2.5415	-0.3127
H	1.9571	4.6678	-0.4196
H	4.4515	-4.6024	-0.2617
H	1.9298	-4.6706	-0.4334
H	0.6252	-2.5365	-0.3206
C	0.2097	0.0025	0.0088
C	-1.0387	0.0042	0.011
C	-2.4555	0.0052	0.0247
C	-3.2127	-1.2059	0.0525
C	-3.2121	1.2167	0.0044
C	-4.6094	-1.2081	0.0776
H	-2.68	-2.1699	0.0494
C	-4.6089	1.2205	0.0301
H	-2.6791	2.1796	-0.0386
C	-5.3582	0.007	0.0868
H	-5.128	-2.1766	0.0939
H	-5.127	2.189	0.0072
N	-6.7449	0.0085	0.1476
C	-7.468	1.2554	-0.0261
H	-8.5508	1.0705	0.0994
H	-7.1706	2.0092	0.7346
H	-7.3128	1.7135	-1.0329
C	-7.4685	-1.2442	0.0252
H	-8.5512	-1.054	0.1431
H	-7.3132	-1.7435	-0.962
H	-7.1712	-1.9664	0.8162
N	4.4189	-0.0098	0.3803
C	5.8111	-0.0144	0.7874

H	6.0151	-0.9085	1.4067
H	6.5253	-0.015	-0.0686
H	6.0202	0.8766	1.4095
K	0.0067	-0.0352	5.4776

2OH

C	-3.52882	2.52408	0.06365
C	-2.27829	3.03809	0.38289
C	-1.13792	2.23199	0.24541
C	-1.29383	0.94945	-0.27439
C	-2.55899	0.41825	-0.516
C	-3.69732	1.21322	-0.36404
H	-4.40038	3.16114	0.17375
H	-2.19891	4.06592	0.71212
H	-4.69096	0.82228	-0.54278
C	1.27613	2.01752	0.12003
C	2.53219	2.64796	0.17871
C	3.65274	2.00773	-0.31739
C	3.56943	0.75126	-0.90738
C	2.32244	0.13985	-0.98405
C	1.17751	0.74288	-0.44792
H	2.6353	3.64524	0.58391
H	4.61501	2.50589	-0.26123
H	4.45863	0.27867	-1.30311
C	-0.14387	0.03625	-0.58016
H	-0.24777	-0.24301	-1.64093
N	0.13681	2.66997	0.60793
C	0.27603	3.87617	1.3992
H	1.15494	3.80014	2.03813
H	0.36224	4.78182	0.78743
H	-0.58523	3.97983	2.05725
N	-2.59533	-0.94914	-0.84955
C	-1.71222	-1.77386	-0.11739
C	-0.43	-1.26829	0.15189
C	0.42742	-2.00173	0.97837
C	0.05197	-3.26792	1.43456
C	-1.19641	-3.77537	1.09997
C	-2.09377	-3.03661	0.34493
H	0.7192	-3.85509	2.05244
H	-1.48451	-4.75676	1.46203

H	-3.08077	-3.43337	0.1453
C	-3.84589	-1.50841	-1.32226
H	-3.65561	-2.4683	-1.80142
H	-4.58408	-1.65405	-0.52283
H	-4.27179	-0.84238	-2.07226
O	2.10915	-1.06608	-1.56296
O	1.6077	-1.42487	1.30469
C	3.22684	-1.81688	-1.99142
H	3.76174	-1.31361	-2.80284
H	3.91612	-2.00821	-1.16325
H	2.8294	-2.76166	-2.35637
C	2.64405	-2.23547	1.81771
H	2.42922	-2.57339	2.83634
H	2.82364	-3.10352	1.17569
H	3.53295	-1.60676	1.83069

$2O^+$

C	1.63983	3.76316	0.50439
C	0.35332	3.69621	0.02557
C	-0.27768	2.4438	-0.07999
C	0.44156	1.26152	0.22686
C	1.73232	1.38961	0.82699
C	2.33388	2.62685	0.93073
C	-0.19839	0	0
C	-1.60389	0.00001	0
C	-2.3189	1.21248	-0.21761
C	-3.71244	1.19732	-0.21722
H	-4.28239	2.10559	-0.35006
C	-4.37657	0.00002	0
C	-3.71246	-1.19728	0.21722
C	-2.31891	-1.21246	0.21761
H	2.11412	4.73302	0.60388
H	-0.17475	4.60995	-0.20359
H	3.31411	2.7376	1.37287
H	-5.4608	0.00003	0
H	-4.28241	-2.10555	0.35006
C	0.44155	-1.26152	-0.22687
C	-0.27771	-2.4438	0.07999
C	1.7323	-1.38962	-0.82699
C	0.35328	-3.69622	-0.02557

C	2.33385	-2.62687	-0.93074
C	1.6398	-3.76318	-0.50439
H	-0.17479	-4.60995	0.2036
H	3.31408	-2.73763	-1.37287
H	2.11408	-4.73304	-0.60388
N	-1.59582	2.35332	-0.47238
C	-2.26843	3.51004	-1.05765
H	-2.69795	4.15782	-0.29026
H	-1.55877	4.07446	-1.65647
H	-3.05393	3.16444	-1.72483
N	-1.59584	-2.3533	0.47238
C	-2.26846	-3.51002	1.05765
H	-3.05396	-3.16441	1.72483
H	-2.69799	-4.15779	0.29026
H	-1.55881	-4.07445	1.65647
O	2.25822	-0.26385	-1.32096
O	2.25823	0.26383	1.32095
C	3.57504	-0.28805	-1.84817
H	3.6273	-0.90862	-2.74632
H	3.80515	0.74356	-2.10237
H	4.28887	-0.65048	-1.10388
C	3.57504	0.28803	1.84819
H	4.28889	0.65044	1.10392
H	3.62727	0.9086	2.74634
H	3.80513	-0.74358	2.1024

2O ·

C	4.457	0.1429	-0.0004
C	3.7187	1.3139	-0.274
C	2.3077	1.2607	-0.3115
C	1.6241	0.0522	0.0026
C	2.384	-1.1108	0.3139
C	3.7955	-1.0732	0.2736
H	5.5579	0.1783	-0.001
H	4.2497	2.2551	-0.4746
H	4.3866	-1.9783	0.4714
C	0.1971	2.4852	-0.1246
C	-0.409	3.7458	0.0592
C	-1.7287	3.834	0.5575
C	-2.4075	2.6694	0.9549

C	-1.7759	1.4124	0.8369
C	-0.4941	1.2725	0.2083
H	0.1294	4.666	-0.2041
H	-2.2157	4.8171	0.6525
H	-3.4152	2.7463	1.386
C	0.1785	0.0072	0.0061
N	1.4989	2.3647	-0.6874
C	2.1413	3.5411	-1.2335
H	1.409	4.1289	-1.8213
H	2.582	4.2164	-0.4597
H	2.9544	3.2359	-1.9202
N	1.6484	-2.2646	0.6895
C	0.3526	-2.4648	0.136
C	-0.4154	-1.2974	-0.191
C	-1.6917	-1.5167	-0.8076
C	-2.2455	-2.8102	-0.9194
C	-1.492	-3.9303	-0.529
C	-0.1758	-3.7605	-0.043
H	-3.2506	-2.9502	-1.3408
H	-1.9182	-4.9417	-0.6204
H	0.4207	-4.6457	0.2151
C	2.3662	-3.3995	1.2294
H	1.6747	-4.0345	1.8171
H	2.8464	-4.043	0.4522
H	3.1609	-3.0465	1.915
O	-2.3091	0.26	1.3484
O	-2.2996	-0.3999	-1.3143
C	-3.6333	0.2899	1.8366
H	-3.7471	0.9495	2.7279
H	-4.3613	0.6272	1.0644
H	-3.8914	-0.7445	2.1327
C	-3.6347	-0.5043	-1.7603
H	-3.7393	-1.164	-2.6528
H	-4.3161	-0.8886	-0.9678
H	-3.9624	0.5149	-2.0403

$\underline{2O^{-} \text{ with } K^{+}}$

C	4.4469	0.1417	0.1086
C	3.7133	1.3177	-0.1582
C	2.3021	1.2724	-0.196

C	1.6169	0.0641	0.1122
C	2.3725	-1.1023	0.4173
C	3.7831	-1.0731	0.3772
H	5.5479	0.1736	0.1052
H	4.2494	2.2567	-0.3547
H	4.3708	-1.9804	0.5748
C	0.1884	2.5002	-0.0222
C	-0.4258	3.759	0.1435
C	-1.754	3.8472	0.6182
C	-2.437	2.6854	1.0126
C	-1.7991	1.4321	0.9103
C	-0.5077	1.2884	0.3067
H	0.1126	4.6794	-0.1187
H	-2.2451	4.83	0.6949
H	-3.4509	2.7617	1.429
C	0.1681	0.0194	0.1176
N	1.4989	2.3826	-0.5629
C	2.1469	3.5598	-1.1022
H	1.4204	4.1485	-1.696
H	2.5803	4.233	-0.323
H	2.9656	3.2551	-1.782
N	1.6226	-2.2472	0.8134
C	0.3474	-2.4534	0.2034
C	-0.4214	-1.2847	-0.1148
C	-1.6859	-1.4988	-0.756
C	-2.2216	-2.795	-0.9132
C	-1.4629	-3.9176	-0.5391
C	-0.1602	-3.7485	-0.0206
H	-3.2164	-2.935	-1.3581
H	-1.875	-4.9302	-0.6718
H	0.4388	-4.6339	0.2308
C	2.3449	-3.3955	1.3242
H	1.6547	-4.0515	1.8893
H	2.8307	-4.0128	0.5296
H	3.1365	-3.0577	2.0205
O	-2.3329	0.2805	1.4463
O	-2.3025	-0.3743	-1.233
C	-3.7001	0.2823	1.8131
H	-3.9109	0.949	2.6805
H	-4.3562	0.5915	0.9696

H	-3.9576	-0.7547	2.1001
C	-3.6028	-0.4947	-1.7726
H	-3.6277	-1.1237	-2.6923
H	-4.3261	-0.9233	-1.0428
H	-3.9363	0.5262	-2.0382
K	0.2952	-0.4303	4.1202

HEH

C	0.00011	-0.90418	-0.33209
H	0.00274	-1.7221	0.39451
H	-0.00321	-1.40636	-1.30955
C	1.26225	-0.08469	-0.17427
C	-1.26131	-0.08543	-0.16499
C	-1.22325	1.26826	-0.14868
C	1.22383	1.26889	-0.16242
C	2.38696	2.21888	-0.08619
H	2.06728	3.23935	-0.30461
H	3.16902	1.94186	-0.78902
C	-2.38694	2.21635	-0.05569
H	-3.14531	1.9825	-0.79991
H	-2.06014	3.24672	-0.20529
H	2.83094	2.20469	0.91042
H	-2.86496	2.14474	0.92183
N	-0.00033	1.90433	-0.21895
C	-2.48264	-0.89129	-0.0865
O	-2.48096	-2.1005	-0.2168
C	2.48416	-0.89018	-0.09772
O	2.48469	-2.09782	-0.24117
O	-3.60834	-0.2026	0.14944
O	3.60686	-0.20329	0.1572
C	4.83032	-0.9514	0.20798
C	5.9437	0.03063	0.48793
H	4.97317	-1.4642	-0.7459
H	4.752	-1.70955	0.99046
H	6.89942	-0.49629	0.5338
H	6.00552	0.78521	-0.29936
H	5.78583	0.53645	1.4431
C	-4.83116	-0.9515	0.20091
C	-5.94644	0.03173	0.46887
H	-4.75573	-1.70398	0.98907

H	-4.96956	-1.47121	-0.74993
H	-6.90227	-0.4952	0.51228
H	-5.79407	0.54298	1.42204
H	-6.00387	0.7818	-0.32304
C	-0.00015	3.37374	-0.17734
H	-0.87542	3.74457	-0.66854
H	0.00324	3.70171	0.84116
H	0.87187	3.74452	-0.67434

$\underline{HE^+}$

C	-2.63404	-1.90507	0
C	-1.22716	-1.90507	0
C	-0.56047	-0.67847	0
C	-1.31455	0.49632	-0.00024
C	-2.71775	0.39352	-0.00038
N	-3.37728	-0.78144	-0.0002
H	0.53807	-0.63869	-0.00095
C	-3.42252	-3.22791	0.00017
H	-2.888	-3.9618	-0.56604
H	-4.38498	-3.06951	-0.43971
C	-3.6007	1.65526	-0.00049
H	-3.43025	2.20994	0.89849
H	-4.63057	1.36989	-0.05367
H	-3.35475	2.26262	-0.84638
H	-3.54242	-3.57153	1.00637
C	-0.63531	1.87844	-0.00038
O	-1.27847	2.92374	-0.00059
C	-0.44872	-3.23384	0.00037
O	0.77795	-3.27371	0.00038
O	0.7946	1.86293	-0.0002
O	-1.25015	-4.41816	0.00075
C	1.28654	3.20565	0
C	2.78671	3.22113	0.00334
H	0.88382	3.72448	0.90368
H	0.88779	3.72332	-0.9061
H	3.1714	4.26984	0.00344
H	3.18508	2.7033	0.90956
H	3.18914	2.70201	-0.90034
C	-0.40135	-5.56891	0.01531
C	-1.2156	-6.82895	0.00952

H	0.24061	-5.51724	0.92813
H	0.26323	-5.52347	-0.88151
H	-0.55292	-7.72812	0.02083
H	-1.8801	-6.87399	0.90645
H	-1.85763	-6.88022	-0.9033
C	-4.8463	-0.835	-0.00021
H	-5.23248	-0.03228	0.59259
H	-5.20656	-0.74281	-1.00351
H	-5.16916	-1.76889	0.41029

HE ·

C	-1.2967	1.2214	0.2141
C	-0.9563	-0.1415	0.3872
C	0.4274	-0.4272	0.6577
C	1.3769	0.5434	0.172
C	0.9026	1.8677	0.0296
N	-0.2964	2.0934	0.8094
H	0.7343	-1.4522	0.896
C	-2.3323	1.8148	-0.7009
H	-2.9486	1.0291	-1.1714
H	-1.8545	2.4077	-1.5189
C	1.3723	2.9073	-0.9463
H	1.581	3.8928	-0.4712
H	0.6032	3.108	-1.7324
H	2.2986	2.5669	-1.4428
H	-3.0266	2.5204	-0.1877
C	2.724	0.1399	-0.2759
O	3.5474	0.8177	-0.8974
C	-1.873	-1.2898	0.2418
O	-1.5646	-2.469	0.4179
O	3.0248	-1.1419	0.1047
O	-3.1631	-0.9402	-0.0658
C	4.3282	-1.6241	-0.268
C	4.4692	-3.0472	0.2371
H	5.1084	-0.959	0.1612
H	4.4426	-1.5697	-1.3722
H	5.4676	-3.4453	-0.038
H	4.374	-3.0971	1.3414
H	3.7034	-3.7136	-0.2098
C	-4.0977	-2.0262	-0.204

C	-5.4478	-1.4463	-0.5807
H	-4.1498	-2.5921	0.7514
H	-3.73	-2.7408	-0.9725
H	-6.1931	-2.2625	-0.6743
H	-5.812	-0.7357	0.1894
H	-5.4043	-0.9142	-1.5531
C	-0.669	3.4468	1.1465
H	0.1648	3.9393	1.6923
H	-0.9357	4.1158	0.286
H	-1.5479	3.429	1.8268

HE^- with K^+

C	-1.3219	1.1908	0.2164
C	-0.9846	-0.1659	0.3683
C	0.398	-0.4715	0.6591
C	1.3576	0.5052	0.1872
C	0.9052	1.8307	0.0577
N	-0.3188	2.0716	0.7981
H	0.6905	-1.5186	0.7931
C	-2.4478	1.8019	-0.5692
H	-3.0232	1.0339	-1.114
H	-2.0641	2.5372	-1.3136
C	1.4893	2.9259	-0.7848
H	1.7716	3.8297	-0.1964
H	0.769	3.2822	-1.5584
H	2.3982	2.5606	-1.2942
H	-3.174	2.3685	0.0609
C	2.7167	0.0989	-0.2253
O	3.5541	0.7627	-0.8428
C	-1.9015	-1.3104	0.1814
O	-1.5796	-2.4947	0.2731
O	3.0137	-1.1695	0.1996
O	-3.2056	-0.9542	-0.0485
C	4.3295	-1.6541	-0.1222
C	4.4777	-3.045	0.464
H	5.0927	-0.956	0.2841
H	4.4651	-1.659	-1.2254
H	5.4859	-3.445	0.2305
H	4.3621	-3.0334	1.5674
H	3.7284	-3.7452	0.0414

C	-4.1372	-2.0387	-0.2197
C	-5.5056	-1.4496	-0.5026
H	-4.1451	-2.6656	0.6984
H	-3.7955	-2.6984	-1.0469
H	-6.2478	-2.2656	-0.6178
H	-5.8435	-0.7942	0.3262
H	-5.5067	-0.8553	-1.4393
C	-0.6928	3.441	1.089
H	0.127	3.943	1.6425
H	-0.9287	4.0808	0.2005
H	-1.5886	3.4488	1.7434
K	0.461	0.6002	4.2227

BNAH

C	-0.33575	2.11225	0.12994
C	-1.35438	2.29826	-0.70298
C	-2.48397	1.3161	-0.84509
C	-2.18357	0.05545	-0.06684
C	-1.12382	-0.02435	0.75874
H	-3.42383	1.76403	-0.49796
H	-1.38629	3.2128	-1.28172
H	0.45871	2.83877	0.24045
H	-0.93922	-0.90289	1.36527
H	-2.65727	1.07991	-1.90113
C	1.04821	0.70711	1.6091
H	1.4228	1.64706	2.01776
H	0.84608	0.04503	2.45234
C	2.07273	0.08811	0.686
C	2.14101	-1.29333	0.53174
C	2.92824	0.89109	-0.06149
C	3.04102	-1.86091	-0.35835
H	1.49019	-1.93353	1.1181
C	3.82805	0.32734	-0.95445
H	2.8954	1.96862	0.05961
C	3.88439	-1.05105	-1.10627
H	3.08731	-2.93816	-0.46596
H	4.4882	0.96486	-1.53041
H	4.58831	-1.49316	-1.80118
C	-3.15765	-1.04197	-0.1842
O	-4.27377	-0.84359	-0.66185

N	-2.8082	-2.2794	0.26366
H	-3.46782	-3.02212	0.10028
H	-1.84521	-2.54688	0.36811
N	-0.21955	0.98223	0.9415

BNA^+

C	1.22375	-2.0712	-0.87363
C	0.15556	-1.69114	-0.09956
C	1.31691	0.18267	0.67257
C	2.41437	-0.14311	-0.09358
C	2.37073	-1.29684	-0.86408
H	1.15271	-2.9687	-1.47007
H	-0.77004	-2.24755	-0.06003
H	1.2901	1.04151	1.32824
H	3.2368	-1.57644	-1.44974
C	-0.95778	-0.22093	1.49412
H	-1.15743	-1.06457	2.15249
H	-0.65579	0.62475	2.10839
C	-2.15446	0.11169	0.64506
C	-3.25511	-0.73513	0.62598
C	-2.16463	1.26926	-0.12813
C	-4.35834	-0.43006	-0.15974
H	-3.25573	-1.63504	1.23118
C	-3.26277	1.57066	-0.91565
H	-1.3135	1.9417	-0.11347
C	-4.36181	0.72046	-0.93245
H	-5.21341	-1.09476	-0.1668
H	-3.26501	2.4738	-1.51353
H	-5.22171	0.95954	-1.54632
C	3.67884	0.67647	-0.07715
O	4.75558	0.12039	-0.19758
N	3.5309	1.99974	0.08542
H	4.35646	2.57735	0.08247
H	2.64042	2.46055	0.00916
N	0.22054	-0.58718	0.66118

$BNA^{\cdot}$

C	1.3379	-2.2308	-0.4549
C	0.2482	-1.8963	0.4419
C	1.3025	0.3411	0.5886
C	2.4597	-0.0578	-0.0885

C	2.4224	-1.4232	-0.698
H	1.2937	-3.2295	-0.9287
H	-0.7635	-2.1993	0.0935
H	1.2018	1.3483	1.0249
H	3.2775	-1.7365	-1.3144
C	-0.94	0.0169	1.4708
H	-1.1825	-0.6856	2.3048
H	-0.7206	1.0061	1.9246
C	-2.1536	0.1382	0.5587
C	-3.443	0.2536	1.1169
C	-2.0088	0.1839	-0.8425
C	-4.5672	0.4372	0.2905
H	-3.5683	0.203	2.2113
C	-3.1328	0.3548	-1.6711
H	-1.0038	0.0897	-1.2824
C	-4.4151	0.4861	-1.106
H	-5.5668	0.5412	0.7412
H	-3.0051	0.3851	-2.7649
H	-5.2947	0.6252	-1.7536
C	3.6265	0.7861	-0.24
O	4.6813	0.403	-0.8015
N	3.5889	2.0959	0.3281
H	4.3303	2.6705	-0.0883
H	2.6906	2.5844	0.2329
N	0.2446	-0.4657	0.7989

$\underline{BNA^- \text{ with } K^+}$

C	1.1808	-2.1	-0.0458
C	0.1568	-1.6027	0.8597
C	1.2415	0.5831	0.6731
C	2.4141	0.0127	0.1723
C	2.2768	-1.3526	-0.3965
H	1.073	-3.1348	-0.4192
H	-0.8599	-2.0111	0.708
H	1.1563	1.6569	0.9142
H	3.0903	-1.7321	-1.0317
C	-1.0884	0.4845	1.3747
H	-1.3262	0.0278	2.3707
H	-0.8882	1.5613	1.5546
C	-2.2943	0.3362	0.4602

C	-3.5905	0.5648	0.965
C	-2.1392	0.0104	-0.9022
C	-4.7114	0.4888	0.1194
H	-3.7236	0.8107	2.0314
C	-3.2598	-0.0781	-1.7465
H	-1.1272	-0.1733	-1.2959
C	-4.5493	0.1645	-1.239
H	-5.7167	0.6817	0.5253
H	-3.1247	-0.3425	-2.8069
H	-5.4271	0.0973	-1.9003
C	3.6703	0.7476	0.0209
O	4.6254	0.3101	-0.6551
N	3.8156	1.9621	0.7147
H	4.4893	2.598	0.2762
H	2.9691	2.4441	1.0295
N	0.1118	-0.1313	0.8615
K	2.1831	-1.8229	3.9036

CAFH

C	-0.8542	-0.46392	0
H	-1.20159	-1.02464	0.90064
H	-1.31109	-0.94396	-0.89898
C	-2.01374	1.62283	-1.16151
H	-2.29227	2.68144	-0.93893
H	-1.37353	1.61563	-2.07701
H	-2.94971	1.05562	-1.3858
C	1.42194	-1.03183	1.17474
H	2.52505	-0.99321	1.00324
H	1.19275	-0.45401	2.10301
H	1.13269	-2.09714	1.34654
N	-1.28697	1.00958	-0.00113
N	0.68153	-0.46392	0
C	-0.00706	1.78946	-0.00029
C	1.06876	0.9839	0
C	0.56658	2.65193	1.13931
C	2.05355	2.72417	-1.50276
O	-0.06493	3.45588	2.0368
O	1.91404	2.86945	-2.77818
C	3.19146	2.07806	1.42665
H	2.97448	1.65152	2.43598

H	3.40322	1.23199	0.72851
H	4.11247	2.70565	1.50379
C	2.45703	-0.08495	-0.75444
H	3.56149	-0.17254	-0.89684
H	2.23245	-0.23079	0.33017
H	1.96511	-0.90888	-1.32648
N	2.03289	2.89445	0.93473
N	1.96552	1.25292	-1.22272

$\underline{CAF^{+}}$

C	-2.01374	1.62283	-1.16151
H	-2.29227	2.68144	-0.93893
H	-1.37353	1.61563	-2.07701
H	-2.94971	1.05562	-1.3858
C	1.42194	-1.03183	1.17474
H	2.52505	-0.99321	1.00324
H	1.19275	-0.45401	2.10301
H	1.13269	-2.09714	1.34654
N	0.68153	-0.46392	0
C	-0.00706	1.78946	-0.00029
C	1.06876	0.9839	0
C	0.56658	2.65193	1.13931
C	2.05355	2.72417	-1.50276
O	-0.06493	3.45588	2.0368
O	1.91404	2.86945	-2.77818
C	3.19146	2.07806	1.42665
H	2.97448	1.65152	2.43598
H	3.40322	1.23199	0.72851
H	4.11247	2.70565	1.50379
C	2.45703	-0.08495	-0.75444
H	3.56149	-0.17254	-0.89684
H	2.23245	-0.23079	0.33017
H	1.96511	-0.90888	-1.32648
N	2.03289	2.89445	0.93473
N	1.96552	1.25292	-1.22272
N	-1.28697	1.00958	-0.00113
C	-0.8542	-0.46392	0
H	-1.49131	-1.32132	-0.06208

$\underline{CAF^{\cdot}}$

C	1.8567	-2.1522	1.0745

H	1.9321	-1.335	1.8401
H	1.0309	-2.8327	1.3715
H	2.8028	-2.7349	1.1011
C	2.8294	1.836	-0.2264
H	2.3005	2.7739	-0.4628
H	3.3116	1.9343	0.7723
H	3.6377	1.7114	-0.9798
N	1.9881	0.6646	-0.3083
C	0.3759	-0.9053	-0.3312
C	0.6683	0.4758	-0.1528
C	-0.9286	-1.4279	-0.2188
C	-1.6957	0.9795	0.0893
O	-1.2966	-2.6207	-0.2251
O	-2.6126	1.7941	0.2533
C	-3.336	-0.7814	-0.0308
H	-3.3436	-1.8809	-0.144
H	-3.8127	-0.5003	0.931
H	-3.9187	-0.3105	-0.849
C	-0.0954	2.8222	0.291
H	-1.0555	3.271	0.5975
H	0.6499	2.9666	1.0966
H	0.2491	3.3345	-0.6303
N	-1.9392	-0.3728	-0.0719
N	-0.3433	1.4018	0.0611
N	1.6163	-1.6516	-0.2937
C	2.6151	-0.635	-0.7626
H	3.527	-0.7598	-0.1222

$\underline{CAF^{-} \text{ with } K^{+}}$

C	1.9904	-2.0501	1.2532
H	2.0942	-1.2067	1.9879
H	1.239	-2.7745	1.6352
H	2.9614	-2.5868	1.2113
C	2.8349	1.8394	-0.5857
H	2.2876	2.7292	-0.9374
H	3.3803	2.0917	0.3507
H	3.5886	1.585	-1.3609
N	1.9898	0.676	-0.423
C	0.3756	-0.8504	-0.062
C	0.6967	0.538	-0.1004

C	-0.9124	-1.3182	0.2417
C	-1.6251	1.1205	0.3122
O	-1.2913	-2.5035	0.4425
O	-2.5145	1.9676	0.4533
C	-3.2914	-0.6039	0.5576
H	-3.3323	-1.7085	0.5548
H	-3.682	-0.2139	1.5205
H	-3.9336	-0.2009	-0.2517
C	0.0089	2.9365	0.138
H	-0.9008	3.4403	0.5056
H	0.8492	3.1511	0.8247
H	0.2414	3.333	-0.8706
N	-1.8957	-0.2369	0.3554
N	-0.2775	1.5044	0.104
N	1.6018	-1.6139	-0.0996
C	2.5705	-0.6706	-0.7547
H	3.5296	-0.7328	-0.1787
K	-1.3194	-2.3953	3.9774

Me-MNAH

C	3.50693	0.04143	-0.51717
C	3.05517	-1.38544	-0.3422
C	1.81874	-1.7044	0.05268
C	1.23892	0.57882	0.34628
C	2.44918	1.00515	-0.02729
H	1.50386	-2.73636	0.16245
H	3.75162	-2.18667	-0.56402
H	4.45127	0.22067	0.01945
H	3.74555	0.25478	-1.57259
H	0.47275	1.27171	0.67968
C	2.81602	2.45762	-0.01224
H	3.68358	2.63597	0.63453
H	3.10036	2.80048	-1.01483
H	1.99588	3.08788	0.34012
C	-0.37565	-1.1296	1.03308
H	-0.51504	-2.18868	0.97114
H	-0.30101	-0.83915	2.06019
N	0.844	-0.76004	0.33543
H	-1.20913	-0.63316	0.5817

Me-MNA$^+$

C	-0.94619	-1.47816	-0.13604
C	-2.04263	-1.64565	-0.9506
C	-3.04549	-0.68742	-0.94234
C	-2.94807	0.43178	-0.11515
C	-1.8224	0.53458	0.68169
N	-0.85568	-0.40085	0.66152
H	-3.91277	-0.8085	-1.58177
H	-0.12525	-2.18042	-0.09794
H	-2.10231	-2.52083	-1.58279
H	-1.66887	1.36538	1.35676
C	-4.01433	1.48637	-0.08316
H	-3.78624	2.26889	0.64027
H	-4.97744	1.04446	0.17995
H	-4.11984	1.94887	-1.06687
C	0.3597	-0.23979	1.50732
H	0.52353	-1.13477	2.07042
H	0.22147	0.5829	2.17738
H	1.2072	-0.0518	0.88179

Me-MNA $^{\cdot}$

C	1.1796	1.088	0.2759
C	0.0093	1.7966	0.1135
C	-1.1723	1.1293	-0.3909
C	-1.2098	-0.2949	-0.0955
C	-0.0138	-0.9638	0.0657
N	1.2075	-0.2527	-0.2958
H	-2.1278	1.6819	-0.4377
H	2.0388	1.4211	0.8867
H	-0.0407	2.8407	0.4776
H	0.0777	-1.9509	0.556
C	-2.5307	-0.9829	0.1675
H	-2.4136	-2.0715	0.3504
H	-3.2184	-0.866	-0.7015
H	-3.0668	-0.5432	1.0395
C	2.4258	-0.9893	-0.0613
H	3.3023	-0.4189	-0.4365
H	2.3993	-1.9619	-0.5964
H	2.6219	-1.2182	1.0275

Me-MNA^{-} with K^{+}

C	1.1916	1.0808	0.4012
C	0.0148	1.8006	0.2828
C	-1.2117	1.1517	-0.0671
C	-1.2298	-0.2748	0.1202
C	-0.0293	-0.9589	0.2396
N	1.2158	-0.285	-0.0609
H	-2.1594	1.7136	-0.0698
H	2.1645	1.5264	0.6577
H	0.0379	2.8809	0.5113
H	0.0358	-2.0504	0.3733
C	-2.5456	-1.0052	0.254
H	-2.4115	-2.0972	0.3929
H	-3.1725	-0.8529	-0.6534
H	-3.1446	-0.621	1.1089
C	2.3945	-1.0254	0.313
H	3.3117	-0.4967	-0.0144
H	2.392	-2.0306	-0.1526
H	2.4637	-1.1729	1.4391
K	0.1206	0.0186	3.9771

BIMH

C	1.76876	-0.70138	0.05536
C	1.76876	0.70138	0.05537
C	2.93987	1.41082	0.20262
C	4.13186	0.69122	0.36468
C	4.13187	-0.69122	0.36468
C	2.93987	-1.41082	0.2026
H	2.94789	2.49393	0.18768
H	5.06495	1.22987	0.47889
H	5.06495	-1.22986	0.47888
H	2.9479	-2.49393	0.18766
N	0.45239	1.13777	-0.0793
N	0.45239	-1.13777	-0.0793
C	0.16853	-2.42329	-0.67021
H	0.47013	-2.46995	-1.72682
H	0.68932	-3.20799	-0.12193
H	-0.90193	-2.62129	-0.60314
C	0.16853	2.42329	-0.67019
H	0.68932	3.20799	-0.12191
H	0.47012	2.46996	-1.72681

H	-0.90194	2.62129	-0.60312
C	-0.30548	0	-0.59356
H	-0.27447	0.00001	-1.70646
C	-1.75145	0	-0.16098
C	-2.07804	-0.00002	1.19144
C	-2.76517	0.00001	-1.107
C	-3.40432	-0.00002	1.58894
H	-1.28356	-0.00003	1.92864
C	-4.09793	0.00001	-0.71203
H	-2.51302	0.00002	-2.16239
C	-4.41779	0	0.63619
H	-3.65203	-0.00003	2.64393
H	-4.8827	0.00002	-1.45887
H	-5.45552	0	0.9484

$\underline{BIM^+}$

C	1.82832	0.68959	0.08323
C	1.82831	-0.68959	-0.08323
C	3.00682	-1.41674	-0.17286
C	4.18153	-0.69604	-0.08564
C	4.18154	0.69602	0.08551
C	3.00684	1.41672	0.17279
H	3.0071	-2.4907	-0.3025
H	5.12775	-1.21756	-0.1507
H	5.12777	1.21752	0.15054
H	3.00714	2.49068	0.30245
N	0.50152	-1.08312	-0.13443
N	0.50154	1.08313	0.13455
C	0.06018	2.45166	0.35007
H	0.59386	2.86251	1.20521
H	0.26696	3.04834	-0.5373
H	-1.00614	2.4577	0.55579
C	0.06013	-2.45166	-0.34983
H	0.59378	-2.86257	-1.20496
H	0.26693	-3.0483	0.53757
H	-1.00619	-2.45769	-0.55552
C	-1.73532	0.00002	-0.00002
C	-2.4259	0.6876	-0.99405
C	-2.42591	-0.68759	0.99399
C	-3.81075	0.68281	-0.99159

H	-1.88206	1.21442	-1.76884
C	-3.81076	-0.6828	0.9915
H	-1.88208	-1.21441	1.76878
C	-4.50115	0	-0.00005
H	-4.35048	1.21186	-1.76661
H	-4.3505	-1.21186	1.76651
H	-5.58423	0	-0.00006
C	-0.26904	0.00002	-0.00001

BIM ·

C	-1.8681	-0.7144	0.0131
C	-1.8721	0.7133	-0.0306
C	-3.0795	1.435	-0.0684
C	-4.2993	0.6885	-0.0523
C	-4.2953	-0.7078	0.0098
C	-3.0695	-1.445	0.0403
H	-3.0892	2.5351	-0.0799
H	-5.2571	1.2327	-0.0813
H	-5.2495	-1.2585	0.0291
H	-3.0695	-2.5451	0.0557
N	-0.5548	1.1365	-0.0421
N	-0.548	-1.1308	0.0469
C	-0.1826	-2.431	0.5763
H	-0.0249	-3.1939	-0.2166
H	0.7468	-2.3477	1.1701
H	-0.9886	-2.7974	1.2466
C	-0.1809	2.4499	-0.5277
H	0.0116	3.1781	0.2897
H	0.7299	2.3763	-1.1519
H	-0.9989	2.8555	-1.1586
C	1.7267	0.0054	0.0007
C	2.5236	-1.1636	-0.4051
C	2.5382	1.1669	0.3977
C	3.915	-1.1514	-0.4015
H	2.0101	-2.0638	-0.7737
C	3.9292	1.1397	0.3847
H	2.0377	2.0744	0.7661
C	4.6714	-0.0101	-0.0099
H	4.4421	-2.0624	-0.7385
H	4.4682	2.0462	0.7153

H	5.7721	-0.0158	-0.013
C	0.3292	0.0062	0.0107

BIM^- with K^+

C	-1.9235	-0.714	0.0278
C	-1.9579	0.7077	-0.0959
C	-3.1816	1.3961	-0.1986
C	-4.381	0.6266	-0.1531
C	-4.3486	-0.7622	0.0126
C	-3.1075	-1.4617	0.1162
H	-3.2174	2.4924	-0.2826
H	-5.3495	1.1459	-0.2325
H	-5.2901	-1.3308	0.0705
H	-3.086	-2.5536	0.2465
N	-0.6529	1.1629	-0.0872
N	-0.587	-1.1101	0.0886
C	-0.2503	-2.2861	0.8735
H	-0.7674	-3.1791	0.4716
H	0.8358	-2.483	0.8204
H	-0.5508	-2.1659	1.9437
C	-0.2822	2.4705	-0.5839
H	-0.0596	3.1986	0.2263
H	0.6099	2.389	-1.2354
H	-1.113	2.8823	-1.1915
C	1.6506	0.0863	0.0669
C	2.4532	-1.1016	-0.2814
C	2.4574	1.259	0.4373
C	3.8316	-1.1488	-0.0786
H	1.9571	-1.9607	-0.759
C	3.8337	1.1753	0.6205
H	1.9592	2.2141	0.6577
C	4.5654	-0.0372	0.4219
H	4.3691	-2.0745	-0.354
H	4.3711	2.0847	0.9437
H	5.6539	-0.0847	0.576
C	0.253	0.0607	0.0658
K	2.5676	-0.8973	3.8484

3NH

C	1.02315	-3.95883	-0.5148
C	-0.31232	-3.63149	-0.33418

C	-0.65117	-2.3289	0.05233
C	0.35704	-1.38044	0.24329
C	1.69843	-1.72184	0.05161
C	2.03295	-3.02534	-0.33578
C	-1.37364	0.38075	0.24324
C	-2.34037	-0.60976	0.05203
C	-3.63721	-0.24753	-0.33334
H	-4.39865	-0.99466	-0.51361
C	-3.94065	1.09377	-0.51277
C	-2.9887	2.08617	-0.33367
C	-1.69095	1.72785	0.05171
H	1.28343	-4.96596	-0.8237
H	-1.07397	-4.37819	-0.51536
H	3.06067	-3.30974	-0.51855
H	-4.94335	1.37228	-0.82007
H	-3.25488	3.11932	-0.51352
C	0.00017	-0.00022	0.73072
C	1.01724	0.99896	0.24354
C	2.34278	0.60036	0.05237
C	0.64223	2.33125	0.05162
C	3.30209	1.54506	-0.33306
C	1.60416	3.27245	-0.33586
C	2.91764	2.86501	-0.51426
H	4.33023	1.26021	-0.51274
H	1.33783	4.30472	-0.51982
H	3.65976	3.59391	-0.82311
H	0.00001	-0.00034	1.83576
C	4.07236	-1.12832	0.317
H	4.16838	-2.06963	0.8564
H	4.63423	-0.37916	0.87372
H	4.52587	-1.2431	-0.67534
N	2.67697	-0.74282	0.26434
C	-3.01527	-2.96035	0.31459
H	-3.87209	-2.57608	0.86698
H	-2.64483	-3.82963	0.85628
H	-3.35213	-3.2813	-0.67902
N	-1.98174	-1.94664	0.26533
C	-1.05911	4.0903	0.31419
H	-0.29439	4.64409	0.85715
H	-1.99181	4.20262	0.86565

H	-1.18112	4.53969	-0.67926
N	-0.69498	2.6891	0.26449

$\underline{3N^{+}}$

C	3.75853	-1.79153	0.07556
C	3.68631	-0.4076	0.0606
C	2.43391	0.20767	0.06214
C	1.26952	-0.60523	0.02554
C	1.37237	-2.02141	-0.00734
C	2.63774	-2.60655	0.05455
C	-0.11035	1.40059	-0.02724
C	1.06489	2.19646	-0.05924
C	0.9403	3.57427	-0.24099
H	1.80351	4.21441	-0.34524
C	-0.32536	4.12948	-0.34481
C	-1.48869	3.38283	-0.2418
C	-1.39559	2.0025	-0.05959
H	4.73665	-2.25856	0.10131
H	4.60179	0.16389	0.03305
H	2.76877	-3.67704	0.10149
H	-0.41012	5.19649	-0.51738
H	-2.44163	3.8792	-0.34715
C	-0.00007	-0.0005	0.01914
C	-1.1595	-0.7966	0.02718
C	-1.0386	-2.21128	-0.00485
C	-2.43674	-0.17611	0.06415
C	-2.19638	-2.98782	0.05848
C	-3.5769	-0.98075	0.06326
C	-3.43086	-2.35868	0.07965
H	-2.15694	-4.06553	0.10617
H	-4.57019	-0.55955	0.03371
H	-4.32396	-2.97304	0.10519
C	3.47808	2.40668	0.3107
H	4.16285	1.88987	0.97745
H	3.19363	3.33143	0.80337
H	3.98214	2.63176	-0.63147
C	-3.81206	1.83595	0.30299
H	-3.67797	2.78587	0.81163
H	-4.4209	1.21327	0.95232
H	-4.33127	1.9965	-0.64422

C	0.33128	-4.21036	-0.35616
H	-0.51734	-4.54622	-0.94474
H	0.37548	-4.77199	0.57928
H	1.22189	-4.41014	-0.94456
N	-2.51162	1.2029	0.09878
N	2.29197	1.58114	0.09892
N	0.2186	-2.77443	-0.11222

3N ·

C	3.683	-2.1336	-0.0063
C	3.6939	-0.723	0.0113
C	2.4764	-0.0108	0.0816
C	1.2374	-0.7188	0.0627
C	1.2347	-2.142	-0.0411
C	2.4618	-2.8423	-0.0201
C	0.0073	1.426	-0.0266
C	1.2447	2.1315	-0.1173
C	1.2458	3.5033	-0.4463
H	2.1928	4.0484	-0.5659
C	0.022	4.1911	-0.6173
C	-1.2091	3.5162	-0.4468
C	-1.2226	2.1446	-0.1175
H	4.634	-2.6878	-0.014
H	4.6543	-0.1899	-0.0159
H	2.4821	-3.9409	-0.029
H	0.0277	5.2611	-0.8746
H	-2.1503	4.0713	-0.5668
C	-0.0002	0.0044	0.1207
C	-1.2454	-0.7056	0.0628
C	-1.2575	-2.1287	-0.0411
C	-2.4768	0.0155	0.0813
C	-2.4919	-2.8161	-0.0208
C	-3.7017	-0.6839	0.0107
C	-3.7055	-2.0945	-0.0072
H	-2.524	-3.9144	-0.0303
H	-4.6565	-0.1409	-0.017
H	-4.6622	-2.6388	-0.0154
C	3.659	2.1346	0.4193
H	4.3146	1.5707	1.1127
H	3.4354	3.1106	0.8923

H	4.2405	2.3311	-0.5147
C	-3.6371	2.1732	0.4174
H	-3.4039	3.1472	0.89
H	-4.2992	1.6164	1.1104
H	-4.2156	2.3751	-0.5173
C	-0.0232	-4.2179	-0.5104
H	-0.9128	-4.4614	-1.1228
H	-0.031	-4.8812	0.3865
H	0.8673	-4.4733	-1.1163
N	-2.415	1.4326	0.1994
N	2.4295	1.4069	0.1995
N	-0.015	-2.8061	-0.1874

$3N^-$ with K^+

C	3.695	-2.1032	-0.0161
C	3.7075	-0.6935	-0.0065
C	2.4891	0.0156	0.07
C	1.254	-0.6958	0.0694
C	1.2466	-2.1176	-0.0274
C	2.4762	-2.815	-0.0168
C	0.0242	1.4482	-0.0683
C	1.2618	2.1492	-0.1773
C	1.2618	3.5118	-0.5395
H	2.2079	4.0564	-0.6698
C	0.0348	4.1946	-0.7191
C	-1.1968	3.5281	-0.5163
C	-1.2055	2.166	-0.1537
H	4.6462	-2.6572	-0.0305
H	4.6675	-0.16	-0.0414
H	2.5009	-3.9134	-0.0186
H	0.039	5.2574	-1.0046
H	-2.1385	4.0846	-0.6266
C	0.0154	0.0325	0.149
C	-1.2331	-0.6789	0.0778
C	-1.2468	-2.1006	-0.024
C	-2.4587	0.0488	0.0966
C	-2.4865	-2.7791	-0.0119
C	-3.6879	-0.6403	0.0223
C	-3.6955	-2.0498	-0.0001
H	-2.5279	-3.877	-0.0207

H	-4.6402	-0.0921	0.0019
H	-4.6543	-2.5907	-0.0139
C	3.6622	2.1666	0.4136
H	4.318	1.6106	1.1126
H	3.4331	3.1468	0.8756
H	4.243	2.357	-0.5222
C	-3.5924	2.212	0.4951
H	-3.3435	3.1874	0.957
H	-4.2446	1.6606	1.2013
H	-4.1862	2.4125	-0.4308
C	-0.0163	-4.2059	-0.4259
H	-0.9051	-4.4635	-1.0328
H	-0.0257	-4.8445	0.4879
H	0.8725	-4.4791	-1.0255
N	-2.3775	1.4636	0.261
N	2.4348	1.4328	0.2003
N	-0.0051	-2.7854	-0.1366
K	-0.2117	0.9104	3.8734

3. Calculated Reduction Potentials

Calculated reduction potentials are obtained using the ωB97X-D3/Def2-TZVP/SMD (DMSO), as described in the main text. First electron reduction potentials ($R^+ \rightarrow R^{\cdot}$) for the NAD^+ analogs are listed in Table S1 as follows: E_1^{exp} are experimental values obtained from cyclic voltammetry; E_1^{calc} are calculated values from DFT calculations; $E_1^{calc,ion}$ are calculated values in the presence of stabilizing ion (K^+). Second electron reduction potentials ($R^{\cdot} \rightarrow R^-$) for the NADH analogs are listed in Table S1 as follows: E_2^{exp} are experimental values obtained from cyclic voltammetry; E_2^{calc} are calculated values from DFT calculations; $E_2^{calc,ion}$ are calculated values in the presence of stabilizing counter ion (K^+).

Table S1. Experimental and calculated reduction potentials (in V vs. NHE) for model compounds in dimethyl sulfoxide.

Compound	E_1^{exp}	E_1^{calc}	$E_1^{calc,ion}$	E_2^{exp}	E_2^{calc}	$E_2^{calc,ion}$
6OH	+0.24	0.08	0.01	-1.24	-1.54	-1.27
4OH	-0.38	-0.61	-0.46	-1.41	-1.55	-1.48
PhAcrH	-0.29	-0.25	-0.39	-1.23	-1.30	-1.17
Me_2N-AcrH	-0.30	-0.30	-0.38	-1.42	-1.34	-1.20
CN-BNAH	*-0.50**	-0.69	-0.76	N/A	-1.86	-1.42
T-AcrH	-0.22	-0.09	-0.15	-1.07	-1.03	-1.02
2OH	-0.50	-0.58	-0.61	-1.39	-1.59	-1.40
HEH	*-0.68**	-1.04	-1.08	N/A	-1.96	-1.50
BNAH	*-0.76**	-0.94	-1.14	N/A	-2.15	-1.84
CAFH	*-1.38**	-1.87	-1.92	N/A	-1.78	-1.65
Me-MNAH	*-1.02**	-1.24	-1.30	N/A	-2.13	-1.63
BIMH	*-1.30**	-1.51	-1.65	N/A	-2.10	-1.69
3NH	-0.80	-1.07	-1.17	*-1.62**	-1.96	-1.75

** Obtained from the irreversible/quasireversible peaks*

4. pKa determination of NADH analogs

The pKa values of NADH analogs were determined using the indicator anion method, which has been previously reported.[1-2] Generally, potassium dimsyl solution was used to generate an indicator anion. First, the extinction coefficient of the indicator anion was obtained using Beer's law plot, generated from adding several aliquots of indicator solution in DMSO to the potassium dimsyl solution (Figure S2a and S2b). An excess of indicator solution was added to ensure that all potassium dimsyl reacted. The concentration of the indicator anion was calculated from the observed absorbance and determined extinction coefficient. Then, the colored indicator anion was quenched upon addition of aliquots of NADH analog solutions in DMSO (Figure S2c). All procedures were carried under inert conditions. The pKa values of the model compounds were estimated from known indicator pKa value and experimentally obtained equilibrium constant of the reaction between indicator anion and the model compounds.

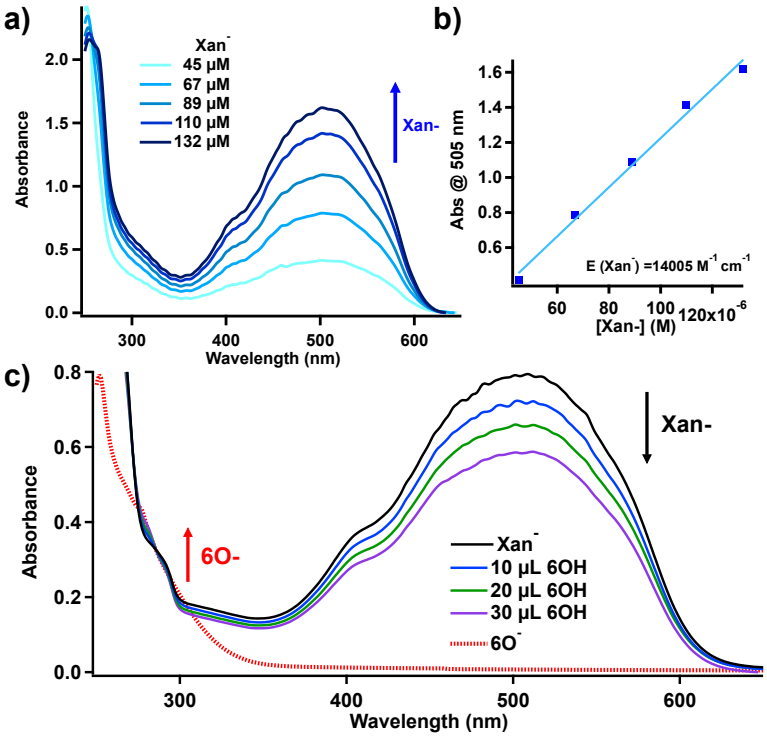

Figure S2. The example for pKa determination using indicator anion method: a) Addition of indicator solution (XanH) in DMSO to the potassium dimsyl to generate the indicator

anion (Xan^-); b) Beer's law plot for determination of the extinction coefficient of indicator anion at maximum absorbance (505 nm); c) Titration of 24 mM 6OH with indicator anion.

The equilibrium constants (K_{eq}) for the reactions between the indicator anion and model compounds (R-H + In^- ⇄ R^- + In-H), were obtained from experimental data and following equations:

$K_{eq} = \frac{[R^-][InH]}{[RH][In^-]}$, where

$[R^-] = \frac{A_0 - A_{obs}}{\varepsilon^{In-}}$; $[InH] = C_0^{InH} - \frac{A_{obs}}{\varepsilon^{In-}}$; $[In^-] = \frac{A_{obs}}{\varepsilon^{In-}}$; $[RH] = (\frac{C^{RH}\, V^{RH}}{V^{tot}} - \frac{A_0 - A_{obs}}{\varepsilon^{In-}})$,

where A_0 and A_{obs} represent the initial absorbance and the absorbance upon addition of NADH analog; ε^{In-} represents the molar extinction coefficient of the indicator anion; C_0^{InH} represents a total starting concentration of InH/In^-; C^{RH} represents a concentration of titrating stock solution of NADH analog; V^{tot} represents a total volume of the solution and V^{RH} represents a volume of NADH solution added.

In case of Me_2N-AcrH, the absorption of the formed Me_2N-Acr^- was taken into account when deriving the equilibrium constant:

$[R^-] = \frac{A_0 - A_{obs}}{\Delta\varepsilon}$; $[InH] = C_0^{InH} - (\frac{A_0}{\varepsilon^{In-}} - \frac{A_0 - A_{obs}}{\Delta\varepsilon})$; $[In^-] = \frac{A_0}{\varepsilon^{In-}} - \frac{A_0 - A_{obs}}{\Delta\varepsilon}$;

$[RH] = (\frac{C^{RH}\, V^{RH}}{V^{tot}} - \frac{A_0 - A_{obs}}{\Delta\varepsilon})$,

where $\Delta\varepsilon$ represent the difference in molar extinction coeffitients of indicator anion and Me_2N-Acr^-, at the indicator anion absorption maximum.

5. Hydride Transfer Method for Hydricity Determination

The hydricities of model compounds listed in Table 3 were determined using the hydride transfer method. As an example, the hydricity of 2OH in acetonitrile was determined using BNAH, whose hydricity was previously determined.[3] The reaction between BNAH and $2O^+$ went cleanly at room temperature over the course of 14 days in acetonitrile (Figure S3). An equilibrium constant of 9.61 was calculated for the reaction by integration of ^1H NMR spectrum. Using the obtained free energy for hydride transfer (-1.3 kcal/mol) and the previously reported hydricity of BNAH in acetonitrile (ΔG_{H^-}= 59 kcal/mol), we obtain ΔG_{H^-}= 60.3 kcal/mol as the hydricity of 2OH in acetonitrile.

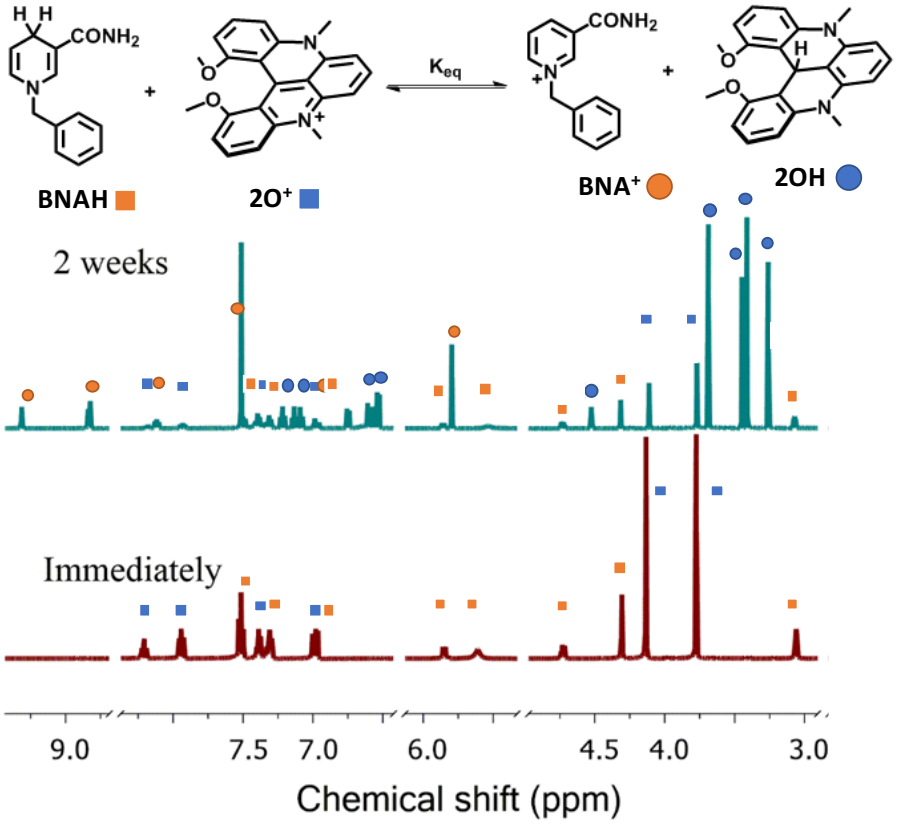

Figure S3. Hydride transfer method for determination of hydricity of 2OH using the BNAH as a standard.

6. Internal Validation of Experimental Values by Cross-Referencing Hydride Transfers

The validation of the experimental hydricity values was achieved by cross-referencing selected model compounds. The cross-referencing reaction was performed using hydride transfer method, as described in the Experimental Section of the manuscript and the results are summarized in Figure S4. The hydricities colored in blue represent the values that were obtained during the initial hydricity determination experiments. The ΔΔG values shown in red represent the difference in hydricities obtained during cross-referencing. For example, the ΔΔG value difference between 4OH and NMe_2AcrH was expected to be 0.1 kcal/mol, while cross-referencing provided a value of 0.5 kcal/mol.

For DMSO values, model compounds whose hydricities were obtained using potential-pKa method (PhAcrH, 4OH, Me_2NAcrH and 2OH) were chosen as reference hydrides. Reactions involving sterically burdened PhAcrH, Me_2NAcrH and 4OH took place only upon heating (80°C). For these measurements, reaction mixtures were cooled down to room temperature before the NMR spectrum was collected. The reference hydrides for the values obtained in ACN were NADH-analogs already reported in literature. In general, the cross-referencing hydride transfer reactions showed a good agreement for both experimental values, giving difference in hydridicty ($\Delta\Delta G_{H-}$) within the experimental error.

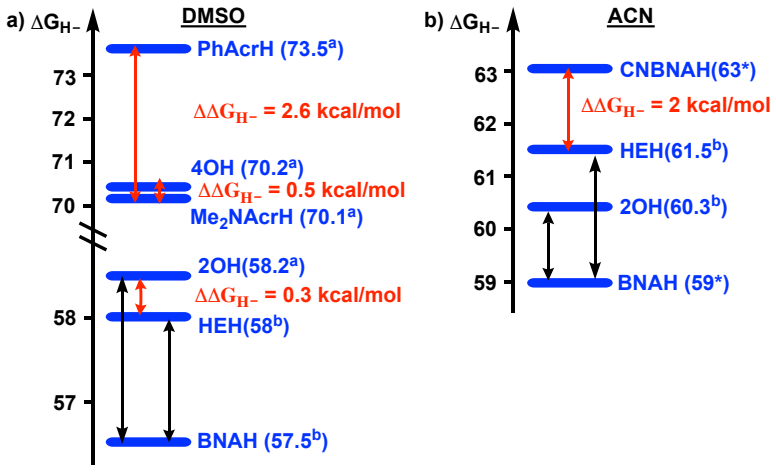

Figure S4. Cross-referencing model hydrides in: a) DMSO and b) ACN. Red two-sided arrows indicate a hydride pair used for cross-referencing and the differences in their

hydricity are described with $\Delta\Delta G_{H-}$, where black two-sided arrows represent a reaction pairs used in the hydride transfer method. Superscirpts: [a] represent result obtained potential-pKa method, [b] using hydride transfer method and * are reported values in Ref 3.

7. Enthalpy Contribution

The enthalpy contribution of metal free hydride donors ($T\Delta S_{H^-}$) was estimated by comparing calculated and experimental ΔG_{H^-} and ΔH_{H^-} values obtained by us and others.[3-10] Figure S4 lists relevant parameters used to construct Figure 4: thermodynamic hydricity ΔG_{H^-} and the enthalpy change for hydride-ion release reaction ΔH_{H^-} were used to derive entropic contribution $T\Delta S_{H^-}$ according to the relationship: $T\Delta S_{H^-} = \Delta H_{H^-} - \Delta G_{H^-}$. The ΔG_{H^-} and ΔH_{H^-} values are obtained from either experiments or calculations (in italics). For hydrides studied here, the ΔH_{H^-} was calculated using the method described in Computational Section, with dihydroacridine 10-methyl-9,10-dihydroacridine as a reference. In the case of hydride donors denoted with *, ΔG_{H^-} was obtained using the equilibrium constant for a hydride transfer to a referent hydride, which was derived by measuring rates for forward and back-reactions. From the derived values, it is clear that using enthalpy parameter to describe hydride donor ability introduces the uncertainty of up to 10%.

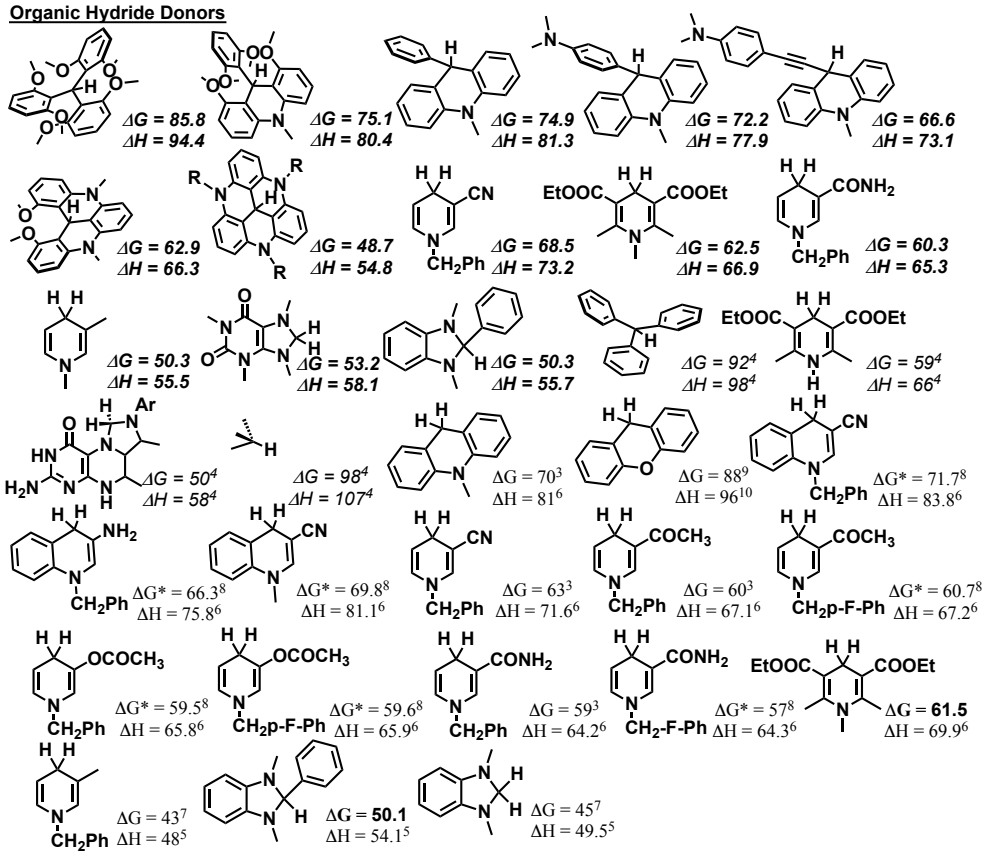

Figure S5. Metal-free hydride donors used to evaluate entropic contributions. Values in italics are calculated values, while values in bold are determined in this work.

8. The Effect of Structural Changes on Reduction Potentials

Previous reports showed that the structural changes, caused by the one-electron reductions, can result in a decrease of the second electron reduction potentials.[11] In our case, $PhAcr^+$ and BIM^+ can undergo structural changes over phenyl group upon first electron reduction. While a negligible change in dihedral angle is observed for the $PhAcr^+$ (Figure S5a, from 106.8° to 102.0°), much more prominent difference in the dihedral angle is present for BIM^+ (Figure S5b, from 90.0° to -151.7°). As a result, the difference for first and second reduction potential ($\Delta E = E_2 - E_1$) is dramatically lower for BIM^+ which undergoes a significant structural change upon reduction ($\Delta E = 0.92$V for $PhAcr^+$ and $\Delta E = 0.18$ V for BIM^+).

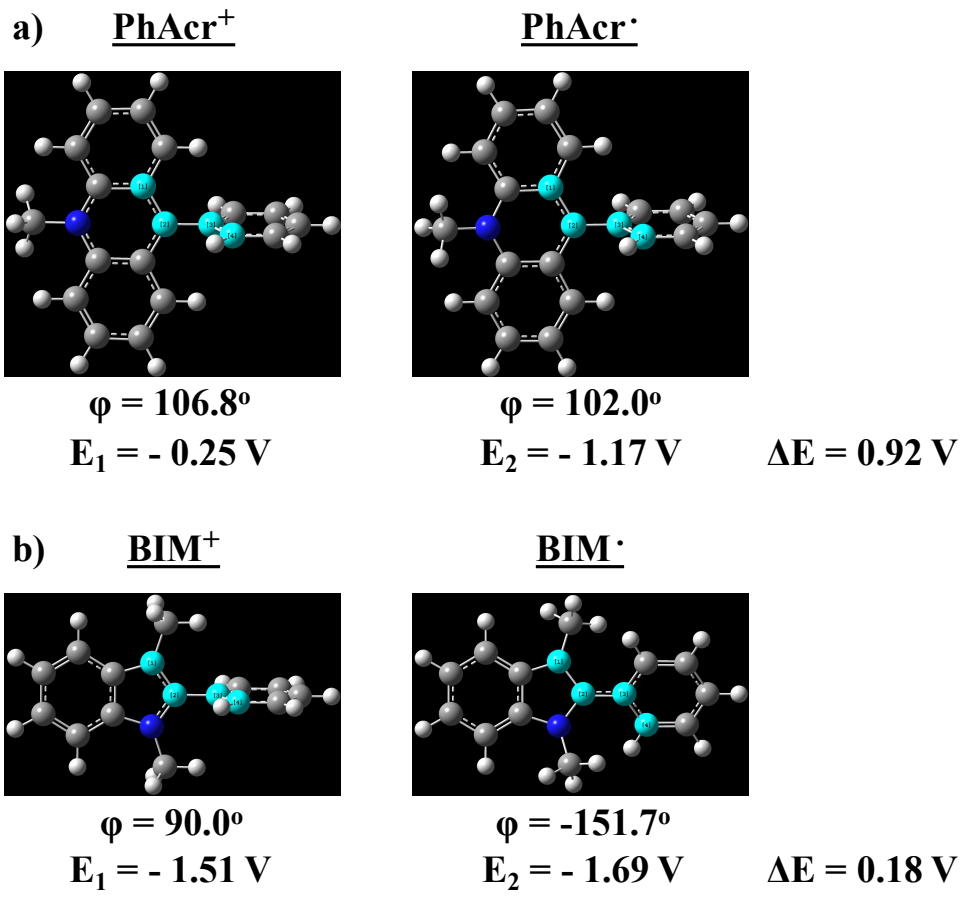

Figure S6. The effect of structural changes on the differences in reduction potentials ($\Delta E = E_2 - E_1$) for: a) $PhAcr^+$; b) BIM^+. The dihedral angles (φ) correspond to atoms colored in light-blue.

5. References

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