

Electronic Supplementary Information

A DFT investigation of the potential of porous cages for the catalysis of ammonia borane dehydrogenation

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I. Computational Details

All the DFT calculations were carried out using the Turbomole suite of programs, using the Turbomole Version 6.0.¹ Geometry optimizations were performed using the BP-86 functional.²⁻³ The electronic configuration of the atoms was described by a triple-zeta basis set augmented by a polarization function (TURBOMOLE basis set TZVP).⁴⁻⁶ The dispersion correction⁷ was employed to incorporate dispersion effects. The resolution of identity (RI),⁸ along with the multipole accelerated resolution of identity (marij)⁹ approximations were employed for an accurate and efficient treatment of the electronic Coulomb term in the density functional calculations. Furthermore, for certain cases, single point ricc2 calculations have also been done with the DFT optimized structures.¹⁰⁻¹¹ The energy contributions were calculated by doing frequency calculations at 298 K: thus, the energies reported in the figures of the paper are the ΔG values. The calculations were done using atom centred basis sets. This is because the structures are self-contained and zero dimensional (0D) without any framework linkages between the individual cages, thus not necessitating the use of plane wave basis sets. It is also to be noted that the cage structures were optimized beginning from the experimental crystal structures for the *N*-cage. It is possible that the presence of hosts may alter the conformations of the cages.¹² This has not been considered in the current work. However, it is likely that the basic nature of the atoms in the cage with respect to the respective acidity and basicity of the phenyl group C atoms as well as the N (or P) atoms in the cage will not be altered by the conformational changes. In other word, the essential chemistry of the N- and P- cages will not be altered for different possible conformations of the cage.

Care was taken to ensure that the obtained transition state structures possessed only one imaginary frequency corresponding to the correct normal mode. The calculation of the barrier height for the first step of the ammonia borane dehydrogenation process (NH_3BH_3 giving two hydrogen atoms to the cage and becoming NH_2BH_2) was done by subtracting the free energy for the transition state structure from the free energy of the complex [*N*-cage][NH_3BH_3] or [*P*-cage][NH_3BH_3]. It is also to be noted that what is reported in the manuscript is the extraction of the hydridic and protic hydrogens from AB by N-C and P-C pairs where the C in question are the ones in unsubstituted positions of the phenyl ring. Alternate possibilities for the extraction of the hydridic and protic hydrogens from AB by different N-C and P-C combinations in the cage were also considered, and found to have higher barriers.

References

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II. Formation of P-cage

Calculations indicate that the making *P-cage* though the same synthetic route as for *N-cage*, as done by Tozawa *et al.* would be endothermic (ΔG calculated to be 11.7 kcal/mol). However, alternative routes can exist for synthesizing the *P-cage*. A suggested reaction by which this could be possible is shown in Equation 1 below:



For $X = \text{N}$, $\Delta G = -146.3$ kcal/mol

For $X = \text{P}$, $\Delta G = -90.3$ kcal/mol

A scheme showing the structures of the different reactants and products indicated in Equation 1 are shown in Figure S1 of the Electronic Supplementary Information file. As seen from Equation 1, the reaction is favourable for the synthesis of both the *N-cage* ($\Delta G = -146.3$ kcal/mol), as well as for the *P-cage* ($\Delta G = -90.3$ kcal/mol). This is because of the entropic gain in releasing 24 molecules of H_2S during the reaction. This example suggests that synthetic routes could be designed to make the *P-cage* 0D structure. It is also to be noted here that the *P-cage* structure represents a model for other, analogous structures that may be easier to prepare, such as the structure "*P-Me₂-cage*": having two methyl groups on each phosphorus atom. Such cage structures can also be potential AB dehydrogenation catalysts, since the electron donating methyl groups would enhance the ability of the phosphorus atoms to extract the protic hydrogen from AB. Shown in Figure S2 in the Electronic Supplementary Information File is the scheme for the dehydrogenation process for the formation of such a *P-Me₂-cage* structure from the easily accessible reagents $\text{Me}_2\text{PCH}_2\text{CH}_2\text{PMe}_2$, $(\text{BrCH}_2)_3\text{C}_6\text{H}_3$, and NaNH_2 , with the calculations indicating that such a process would also be a highly favoured exothermic process. ($\Delta G = -353.2$ kcal/mol)

III. Figures

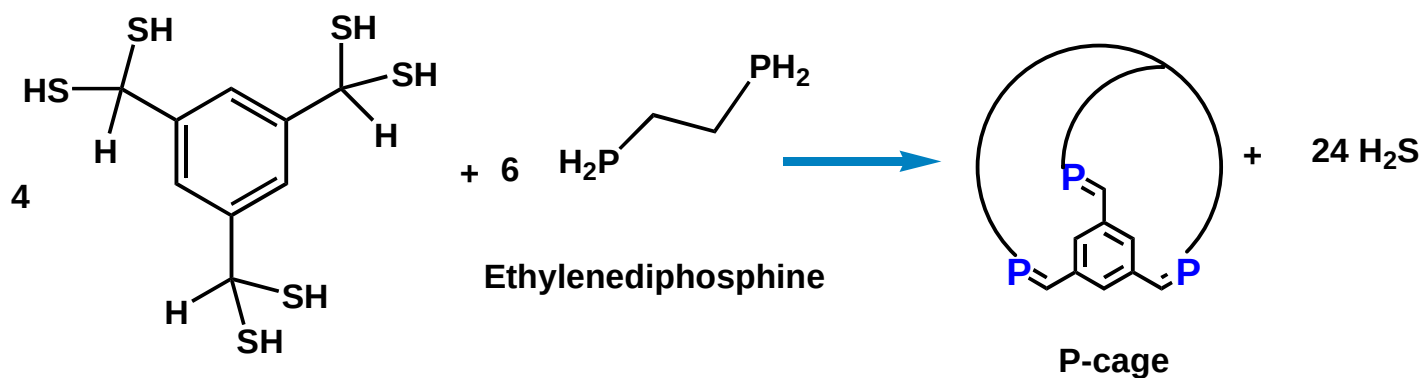


Fig. S1. The schematic representation of formation of the *P-cage* as indicated in Eq.1 in the manuscript.

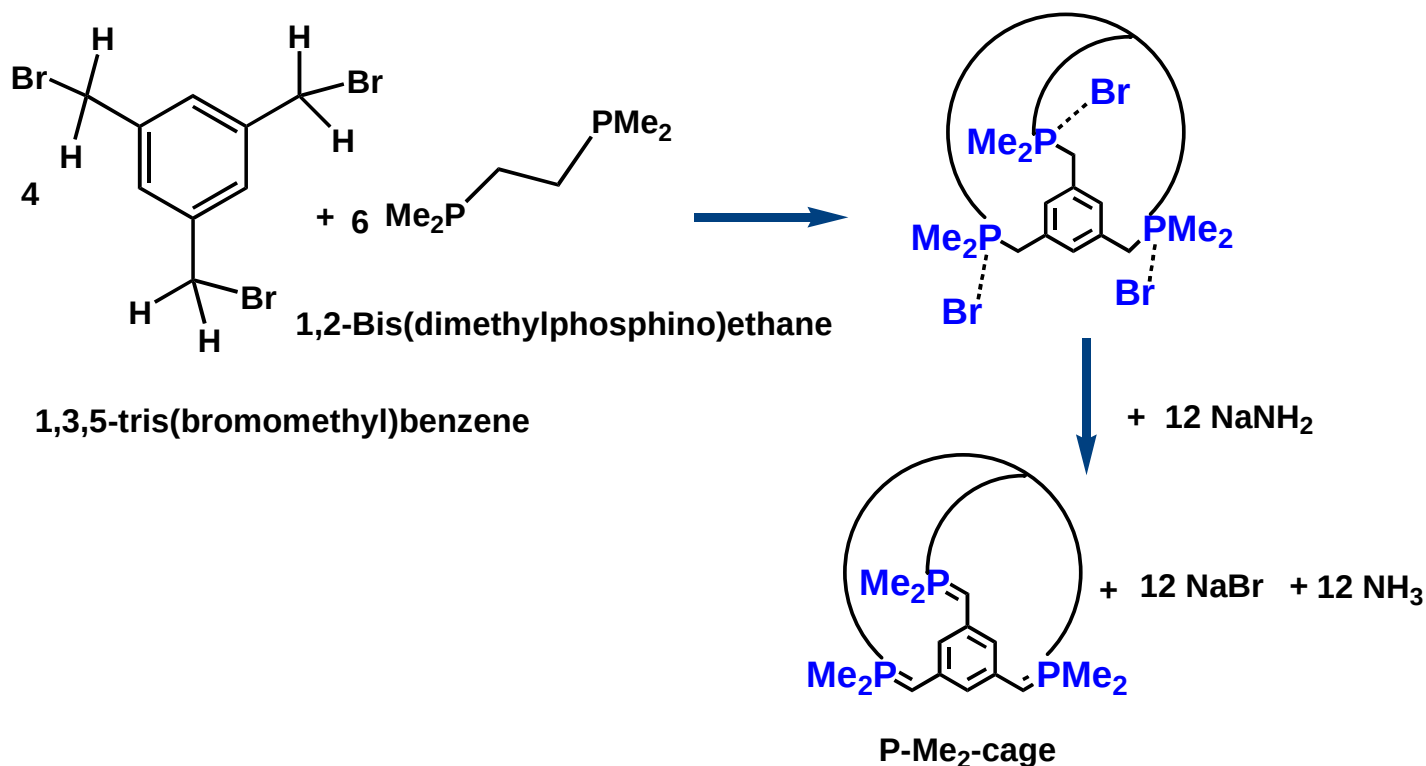


Fig. S2. The schematic representation of formation of the *P-cage* analogue: *P-Me₂-cage*, by easily accessible reagents.

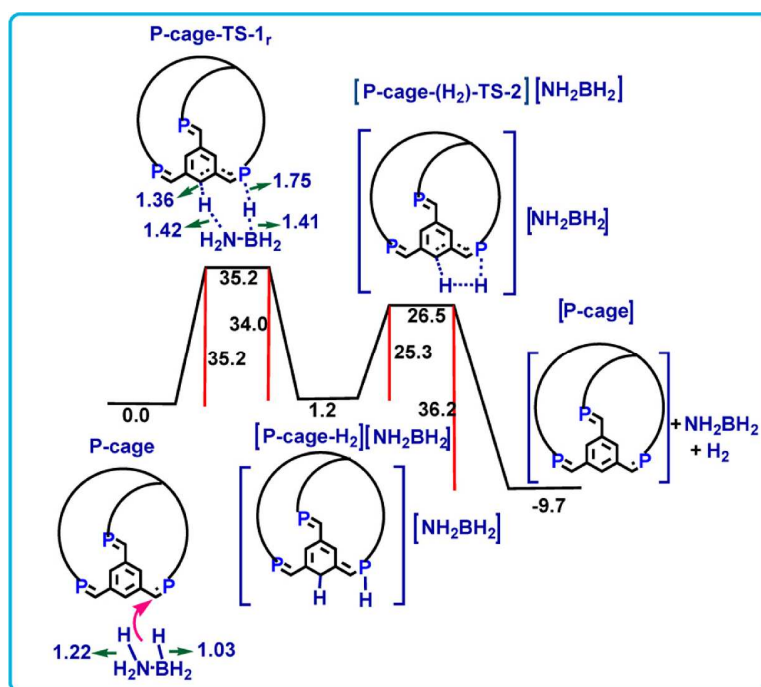


Fig.S3. The schematic representation of the catalytic AB dehydrogenation pathway for the *P-cage* – the protic hydrogen is transferred to the carbon of the P-C pair; all values are in kcal/mol; the arrows point to bond lengths in angstroms.

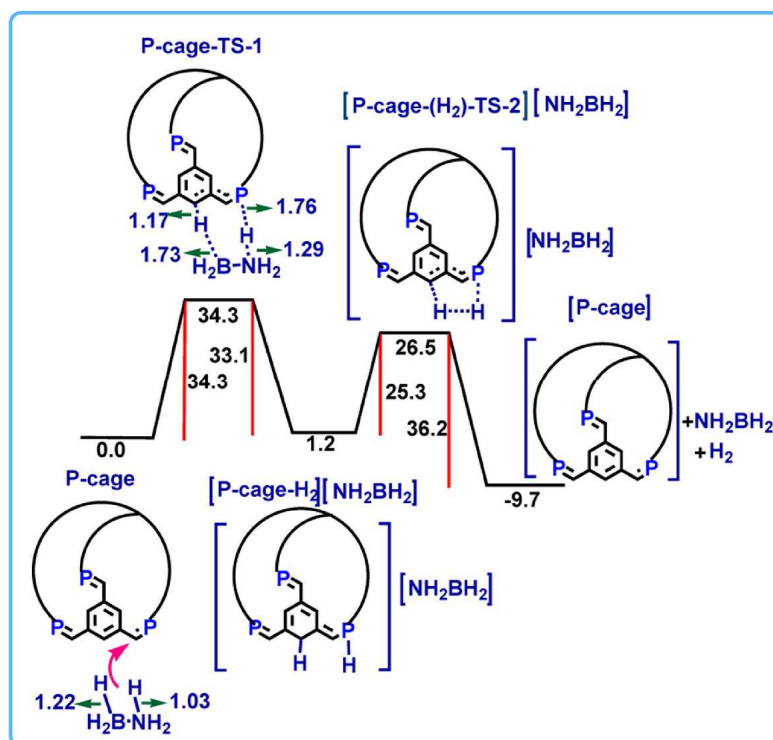


Fig. S4. The schematic representation of the catalytic AB dehydrogenation pathway for the *P-cage* – the protic hydrogen is transferred to the phosphorus of the P-C pair; all values are in kcal/mol.(ΔG)

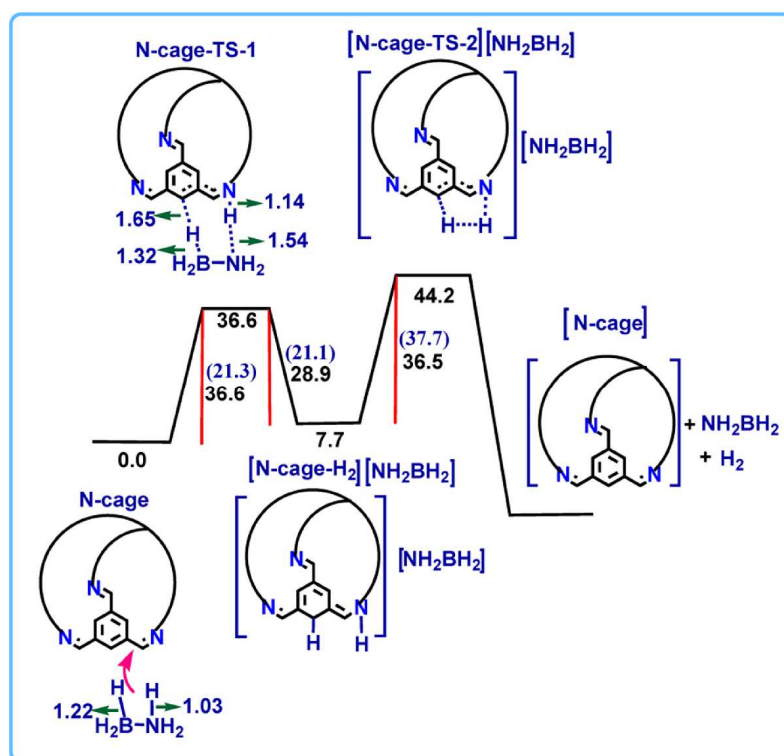


Fig. S5. The potential energy surface (ΔE values done by single point ricc2 calculations) for AB dehydrogenation with *N*-cage; all values are in kcal/mol; ΔE value done by BP-86 functional are shown in parentheses.

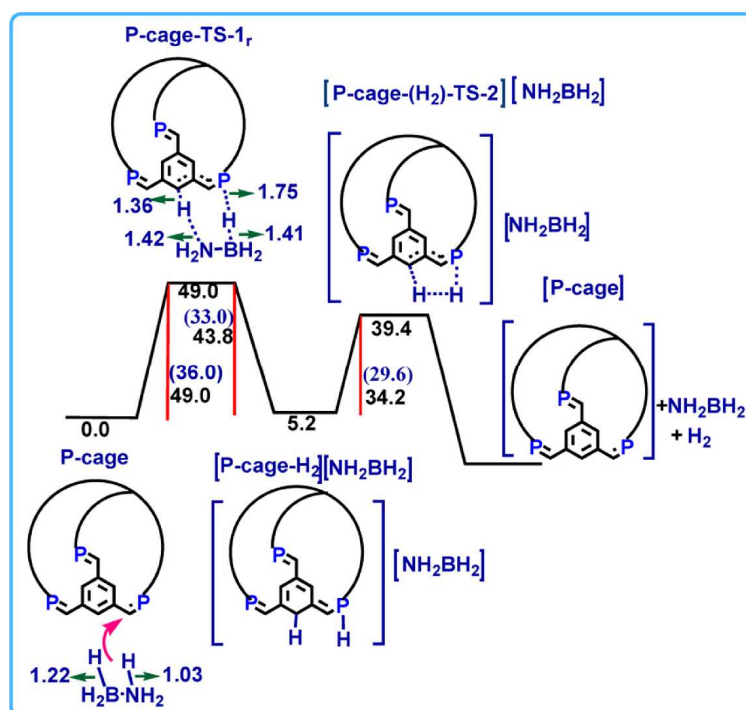


Fig. S6. The potential energy surface (ΔE values done by single point ricc2 calculations) for AB dehydrogenation with *P*-cage; the protic hydrogen is transferred to the carbon of the P-C pair; ΔE value done by BP-86 functional are shown in parentheses; all values are in kcal/mol.

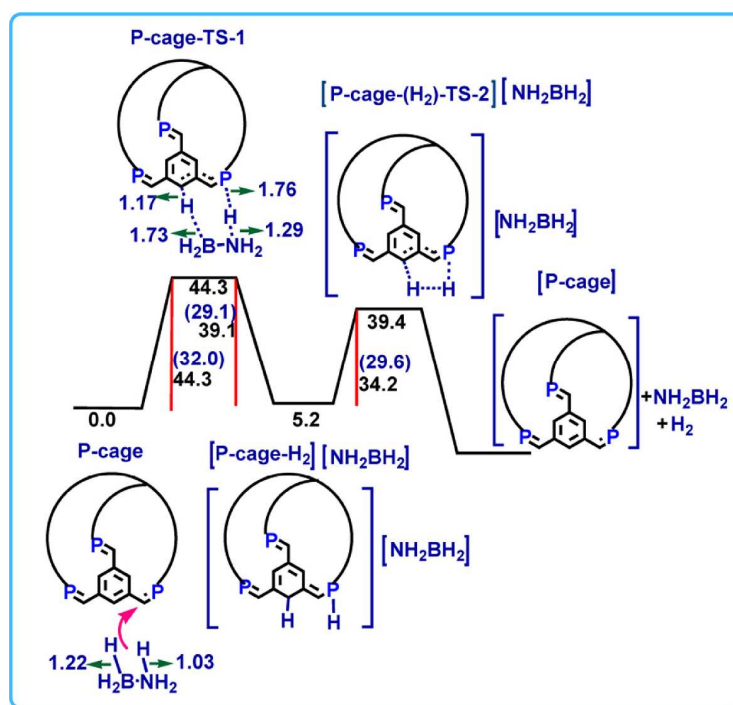


Fig. S7. The potential energy surface (ΔE values done by single point ricc2 calculations) for AB dehydrogenation with *P-cage*; the protic hydrogen is transferred to the phosphorus of the P-C pair; ΔE values done by BP-86 functional are shown in parentheses; all values are in kcal/mol.

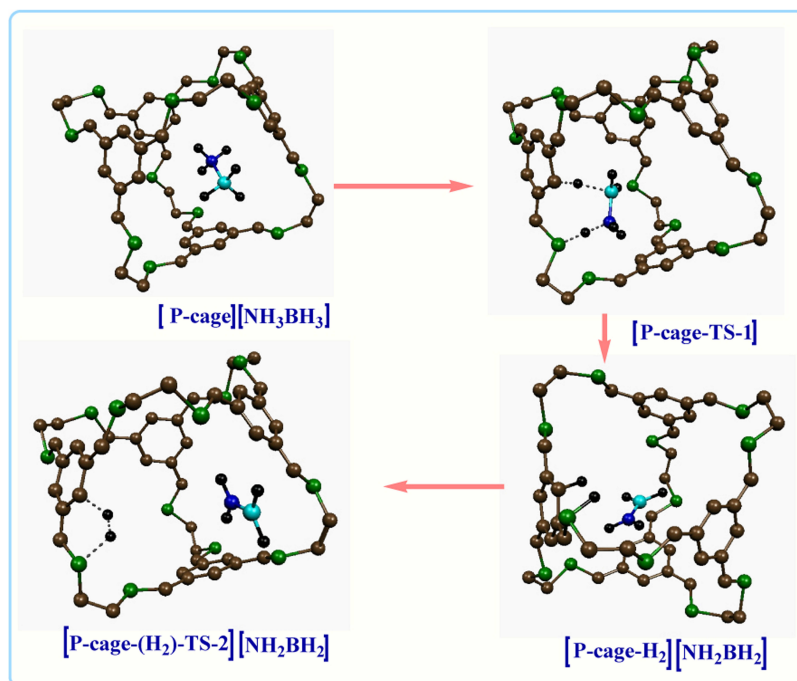


Fig. S8. The optimized structures obtained for the extraction of the protic and hydridic hydrogens from the *P-cage*; only the hydrogens of the NH_3BH_3 species are shown the rest have been removed for the purpose of clarity.

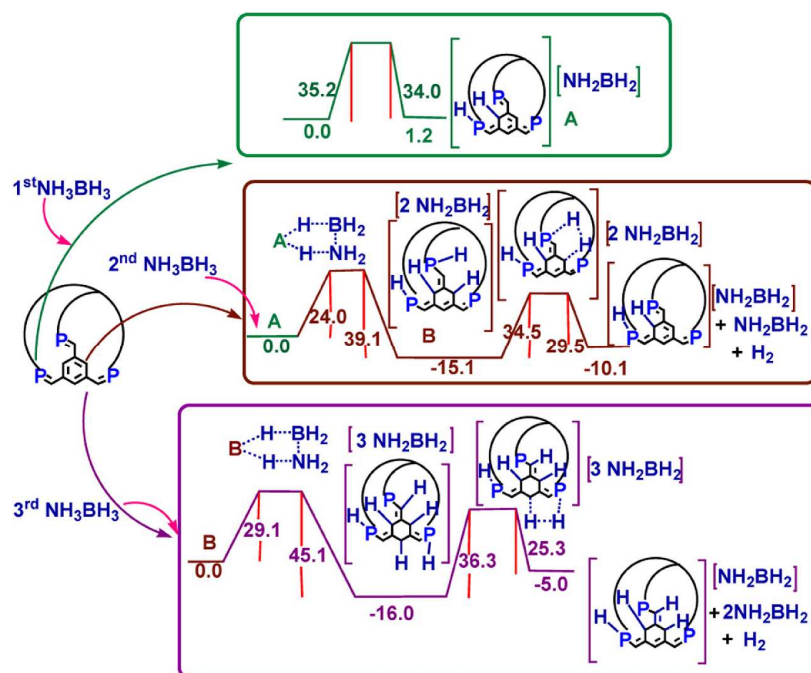


Fig. S9. The schematic representation for the second and third simultaneous dehydrogenations of AB molecules by different P-C pairs associated with one phenyl ring of the *P-cage*, considered for the case where the protic hydrogen of AB is being transferred to the carbon of the phenyl ring; the second AB dehydrogenation pathway is shown inside the middle box, while the third AB dehydrogenation pathway is shown in the lower box; all values are in kcal/mol.

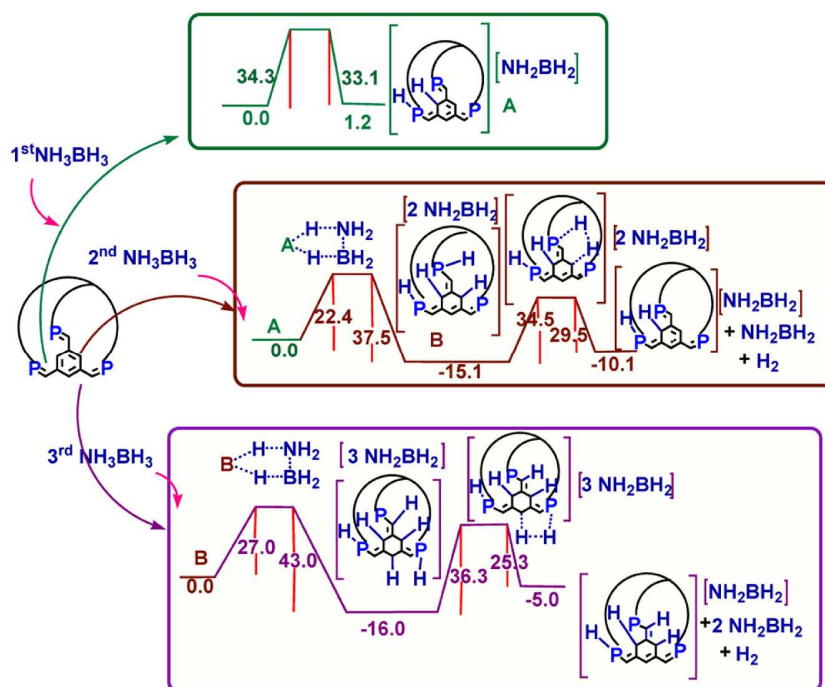


Fig.S10. The schematic representation for the second and third simultaneous dehydrogenations of AB molecules by different P-C pairs associated with one phenyl ring of the *P-cage*; considered for the case where the protic hydrogen of AB is being transferred to the phosphorus of the P-C pair; all values are in kcal/mol.

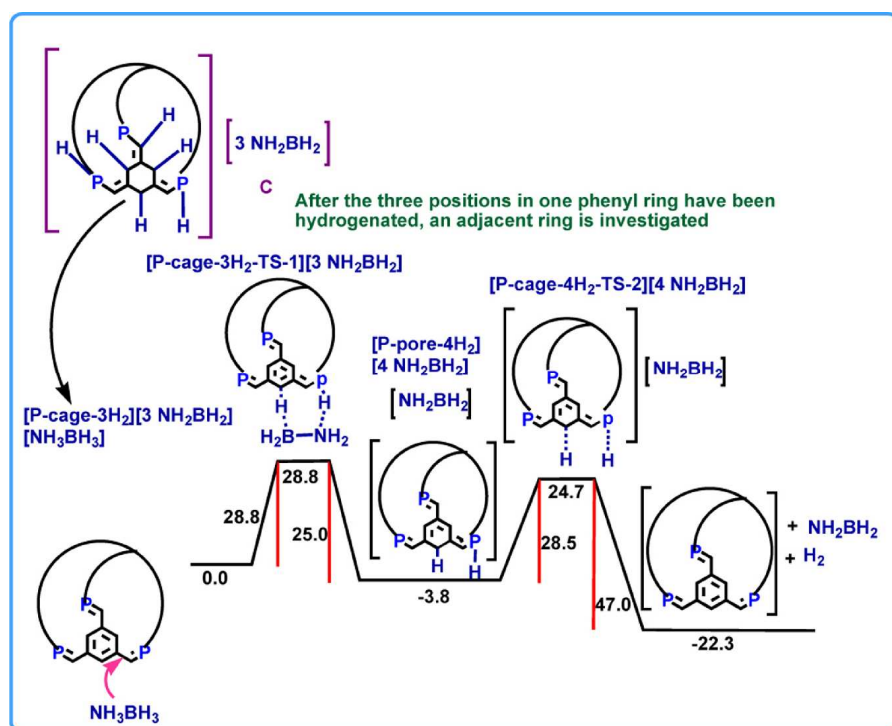


Fig. S11. The schematic representation of the catalytic AB dehydrogenation pathway for the P-C cage for the fourth AB dehydrogenation, where a phenyl ring adjacent to a phenyl ring where three dehydrogenation reactions have been completed in part, is taking part in the dehydrogenation process – the protic hydrogen is transferred to the phosphorus of the P-C pair; all values are in kcal/mol.

IV. The optimized geometries of the structures reported in the paper (the atomic symbol followed by the three Cartesian coordinates, in Å).

N-cage-only

C	2.946	3.789	-4.019
C	2.753	2.533	-4.603
C	3.336	1.398	-4.005
C	4.099	1.517	-2.839
C	4.283	2.790	-2.263
C	3.713	3.927	-2.844
C	1.949	2.423	-5.832
N	1.695	1.307	-6.401
C	0.892	1.326	-7.611
C	1.617	0.617	-8.766
N	2.770	1.383	-9.208
C	3.906	0.796	-9.230
C	5.147	1.465	-9.657
C	6.340	0.736	-9.698
C	7.543	1.349	-10.103
C	7.536	2.700	-10.463
C	6.342	3.449	-10.425
C	5.157	2.826	-10.022
C	6.319	4.874	-10.798
N	7.351	5.501	-11.219
C	7.202	6.905	-11.558
C	8.218	7.771	-10.795
N	7.899	7.824	-9.379
C	8.811	7.490	-8.547
C	8.610	7.501	-7.088
C	9.673	7.163	-6.246
C	9.510	7.158	-4.846
C	8.268	7.497	-4.302
C	7.186	7.841	-5.136
C	7.364	7.840	-6.522
C	10.620	6.798	-3.946
N	11.795	6.518	-4.366
C	12.804	6.175	-3.379
C	13.445	4.814	-3.693
N	12.502	3.730	-3.475
C	12.289	2.918	-4.439
C	11.357	1.783	-4.341
C	11.215	0.915	-5.428
C	10.330	-0.178	-5.365
C	9.588	-0.391	-4.199
C	9.717	0.474	-3.095
C	10.601	1.554	-3.174
C	8.940	0.264	-1.862
N	8.142	-0.721	-1.700
C	7.430	-0.821	-0.438
C	5.913	-0.921	-0.664
N	5.374	0.334	-1.156
C	4.697	0.311	-2.241
C	10.164	-1.100	-6.501
N	10.828	-0.996	-7.589
C	10.570	-1.969	-8.637
C	10.200	-1.275	-9.958
N	8.893	-0.647	-9.871
C	8.809	0.597	-10.151
C	5.869	8.197	-4.579
N	5.636	8.254	-3.323
C	4.294	8.617	-2.898
C	3.706	7.556	-1.955
N	3.418	6.323	-2.667
C	3.930	5.241	-2.217
H	10.649	6.893	-6.657
H	5.081	8.420	-5.327

H	8.146	8.796	-11.196
H	9.241	7.392	-10.990
H	7.414	7.017	-12.635
H	6.178	7.286	-11.365
H	4.518	-0.632	-2.795
H	5.336	5.377	-10.694
H	8.454	3.200	-10.777
H	9.700	1.185	-10.453
H	11.001	-0.560	-10.233
H	10.149	-2.055	-10.737
H	9.772	-2.688	-8.366
H	11.502	-2.534	-8.810
H	9.416	-1.906	-6.353
H	8.894	-1.230	-4.124
H	10.721	2.241	-2.334
H	12.806	3.027	-5.415
H	13.850	4.828	-4.724
H	14.287	4.675	-2.992
H	12.405	6.163	-2.345
H	13.601	6.937	-3.433
H	10.371	6.787	-2.866
H	7.752	-1.753	0.057
H	7.644	0.026	0.242
H	9.093	1.023	-1.068
H	5.446	-1.128	0.313
H	5.698	-1.772	-1.340
H	6.361	-0.318	-9.418
H	4.017	-0.265	-8.927
H	1.883	-0.412	-8.454
H	0.911	0.552	-9.611
H	0.617	2.353	-7.927
H	-0.036	0.766	-7.410
H	1.568	3.383	-6.239
H	4.883	2.868	-1.354
H	4.573	5.236	-1.313
H	4.394	7.405	-1.099
H	2.752	7.952	-1.566
H	3.603	8.774	-3.751
H	4.364	9.562	-2.331
H	2.508	4.686	-4.463
H	3.178	0.424	-4.473
H	4.219	3.383	-9.981
H	8.113	7.499	-3.220
H	11.788	1.070	-6.345

N-cage +NH₃BH₃

C	10.428	1.527	-2.946
C	11.186	1.752	-4.114
C	11.038	0.885	-5.203
C	10.144	-0.205	-5.136
C	9.401	-0.411	-3.971
C	9.538	0.453	-2.866
C	12.132	2.880	-4.208
N	12.338	3.684	-3.234
C	13.289	4.765	-3.438
C	12.651	6.123	-3.105
N	11.641	6.474	-4.087
C	10.463	6.742	-3.673
C	9.360	7.099	-4.584

C	7.232	7.791	-6.279
C	7.038	7.784	-4.895
C	8.112	7.433	-4.051
C	8.699	7.464	-8.295
N	7.781	7.803	-9.120
C	8.100	7.768	-10.537
C	7.077	6.915	-11.305
N	7.219	5.510	-10.969
C	6.189	4.883	-10.545
C	6.223	3.457	-10.172
C	7.424	2.717	-10.213
C	7.438	1.362	-9.862
C	6.237	0.741	-9.462
C	5.039	1.461	-9.417
C	5.042	2.825	-9.773
C	3.802	0.779	-9.000
N	2.663	1.359	-8.973
C	1.513	0.579	-8.548
C	0.769	1.274	-7.397
N	1.562	1.259	-6.180
C	1.801	2.377	-5.607
C	2.594	2.490	-4.370
C	2.782	3.747	-3.787
C	3.538	3.887	-2.606
C	4.103	2.751	-2.018
C	3.925	1.477	-2.593
C	3.171	1.356	-3.765
C	4.522	0.273	-1.990
N	5.203	0.302	-0.909
C	5.747	-0.950	-0.414
C	7.265	-0.844	-0.198
N	7.967	-0.740	-1.466
C	8.766	0.244	-1.629
C	3.751	5.203	-1.980
N	3.247	6.284	-2.440
C	3.533	7.521	-1.734
C	4.133	8.572	-2.680
N	5.474	8.198	-3.095
C	5.718	8.145	-4.349
C	8.706	0.609	-9.917
N	8.774	-0.638	-9.642
C	10.077	-1.278	-9.724
C	10.416	-1.995	-8.406
N	10.663	-1.034	-7.346
C	9.981	-1.132	-6.270
H	10.525	6.860	-6.388
H	4.939	8.376	-5.104
H	6.420	8.060	-6.958
H	9.704	7.147	-8.633
H	8.029	8.798	-10.925
H	9.120	7.387	-10.738
H	7.293	7.027	-12.381
H	6.055	7.301	-11.113
H	4.343	-0.672	-2.540
H	5.203	5.382	-10.438
H	8.340	3.219	-10.537
H	9.600	1.197	-10.203
H	10.888	-0.569	-9.976
H	10.025	-2.047	-10.514
H	9.607	-2.710	-8.156
H	11.347	-2.564	-8.569
H	9.224	-1.931	-6.129

H	8.704	-1.248	-3.893
H	10.558	2.212	-2.105
H	12.648	2.992	-5.181
H	13.693	4.791	-4.468
H	14.128	4.612	-2.738
H	12.253	6.100	-2.070
H	13.448	6.885	-3.154
H	10.204	6.723	-2.594
H	7.595	-1.775	0.293
H	7.482	0.003	0.481
H	8.927	1.000	-0.834
H	5.286	-1.154	0.567
H	5.530	-1.805	-1.085
H	6.265	-0.317	-9.194
H	3.919	-0.285	-8.710
H	1.786	-0.450	-8.241
H	0.816	0.512	-9.400
H	0.484	2.298	-7.709
H	-0.153	0.700	-7.206
H	1.416	3.334	-6.016
H	4.695	2.830	-1.103
H	4.384	5.199	-1.069
H	4.212	7.373	-0.871
H	2.577	7.924	-1.356
H	3.448	8.728	-3.537
H	4.206	9.519	-2.119
H	2.347	4.643	-4.236
H	3.017	0.382	-4.233
H	4.099	3.375	-9.734
H	7.947	7.432	-2.971
H	11.621	1.029	-6.116
N	9.577	3.635	-7.308
B	10.939	3.844	-8.211
H	8.749	3.507	-7.902
H	9.652	2.810	-6.702
H	9.398	4.445	-6.702
H	10.758	4.858	-8.862
H	11.855	3.953	-7.413
H	11.034	2.848	-8.906

N-cage-TS-1

C	11.016	1.974	-1.991
C	11.710	2.090	-3.211
C	11.557	1.099	-4.186
C	10.719	-0.008	-3.962
C	10.043	-0.115	-2.743
C	10.188	0.872	-1.748
C	12.597	3.223	-3.509
N	12.783	4.221	-2.729
C	13.711	5.241	-3.185
C	13.058	6.631	-3.232
N	11.960	6.706	-4.198
C	10.785	7.172	-3.846
C	9.647	7.303	-4.688
C	8.401	7.551	-4.079
C	7.230	7.652	-4.832
C	7.320	7.501	-6.236
C	8.528	7.279	-6.887
C	9.732	7.118	-6.121
C	8.597	7.160	-8.348
N	7.581	7.318	-9.114
C	7.774	7.116	-10.539
C	6.776	6.080	-11.085
N	7.063	4.754	-10.568
C	6.123	4.134	-9.962
C	6.285	2.790	-9.381
C	5.172	2.142	-8.836

C	5.291	0.854	-8.276
C	6.541	0.227	-8.267
C	7.675	0.869	-8.803
C	7.540	2.147	-9.355
C	4.135	0.153	-7.695
N	2.953	0.642	-7.670
C	1.902	-0.162	-7.071
C	1.184	0.604	-5.948
N	2.045	0.766	-4.789
C	2.263	1.954	-4.369
C	3.116	2.253	-3.206
C	3.774	1.232	-2.492
C	4.584	1.537	-1.394
C	4.743	2.883	-1.007
C	4.100	3.908	-1.706
C	3.283	3.583	-2.808
C	4.300	5.306	-1.288
N	3.709	6.291	-1.850
C	3.993	7.627	-1.358
C	4.454	8.548	-2.499
N	5.785	8.198	-2.964
C	5.937	7.966	-4.216
C	5.266	0.452	-0.669
N	5.968	0.654	0.380
C	6.608	-0.489	1.004
C	8.120	-0.254	1.154
N	8.777	-0.255	-0.141
C	9.481	0.762	-0.460
C	8.996	0.217	-8.790
N	9.173	-0.977	-8.370
C	10.517	-1.526	-8.418
C	10.935	-2.097	-7.054
N	11.186	-1.033	-6.098
C	10.542	-1.046	-4.994
H	4.191	2.622	-8.836
H	9.835	0.831	-9.174
H	8.403	2.672	-9.770
H	5.115	4.584	-9.843
H	6.897	6.050	-12.182
H	5.743	6.413	-10.858
H	7.571	8.071	-11.054
H	8.806	6.797	-10.791
H	9.601	1.625	0.226
H	9.591	6.892	-8.757
H	6.425	7.603	-6.855
H	5.080	8.016	-4.919
H	3.699	8.527	-3.311
H	4.496	9.576	-2.097
H	4.751	7.634	-0.549
H	3.054	8.044	-0.955
H	5.003	5.455	-0.443
H	5.384	3.106	-0.152
H	3.638	0.198	-2.818
H	1.811	2.838	-4.865
H	0.814	1.571	-6.344
H	0.313	0.001	-5.639
H	2.276	-1.126	-6.672
H	1.155	-0.377	-7.853
H	4.354	-0.849	-7.272
H	6.188	-0.601	2.019
H	6.436	-1.433	0.450
H	5.135	-0.563	-1.095
H	8.530	-1.093	1.742
H	8.291	0.683	1.720
H	8.335	7.680	-2.996
H	10.662	7.452	-2.792
H	12.677	6.897	-2.235
H	13.830	7.368	-3.511
H	14.153	5.002	-4.174

H	14.542	5.307	-2.462
H	13.114	3.154	-4.487
H	9.388	-0.964	-2.537
H	9.810	-1.843	-4.752
H	10.164	-2.813	-6.706
H	11.880	-2.647	-7.199
H	11.272	-0.787	-8.754
H	10.511	-2.364	-9.137
H	12.073	1.175	-5.145
H	11.138	2.756	-1.239
H	10.677	7.377	-6.600
H	6.662	-0.769	-7.839
H	2.790	4.394	-3.346
H	12.207	6.367	-5.266
N	12.513	5.709	-6.629
B	11.225	4.860	-6.858
H	10.227	5.554	-6.332
H	10.865	4.769	-8.020
H	11.244	3.829	-6.216
H	12.750	6.319	-7.415
H	13.331	5.113	-6.485

[N-cage-H₂][NH₂BH₂]

C	3.291	1.396	-3.908
C	2.725	2.536	-4.514
C	2.935	3.792	-3.937
C	3.704	3.927	-2.764
C	4.261	2.787	-2.176
C	4.058	1.511	-2.744
C	1.928	2.429	-5.749
N	1.667	1.312	-6.313
C	0.881	1.333	-7.534
C	1.619	0.617	-8.677
N	2.773	1.382	-9.115
C	3.908	0.792	-9.144
C	5.148	1.459	-9.575
C	6.341	0.731	-9.619
C	7.543	1.342	-10.028
C	7.535	2.692	-10.388
C	6.341	3.442	-10.350
C	5.157	2.819	-9.944
C	6.314	4.864	-10.729
N	7.340	5.496	-11.158
C	7.177	6.896	-11.510
C	8.195	7.779	-10.772
N	7.891	7.856	-9.354
C	8.809	7.534	-8.525
C	8.615	7.564	-7.065
C	9.682	7.238	-6.224
C	9.520	7.242	-4.824
C	8.277	7.575	-4.278
C	7.190	7.904	-5.112
C	7.369	7.898	-6.498
C	10.624	6.892	-3.920
N	11.805	6.601	-4.321
C	12.797	6.274	-3.318
C	13.466	4.920	-3.604
N	12.563	3.789	-3.458
C	12.295	2.882	-4.432
C	11.444	1.804	-4.290
C	10.709	1.580	-2.976
C	9.740	0.409	-3.007
C	9.639	-0.385	-4.112
C	10.399	-0.168	-5.317
C	11.260	0.915	-5.375
C	10.219	-1.075	-6.447

N	10.865	-0.985	-7.555
C	10.575	-1.967	-8.584
C	10.192	-1.293	-9.912
N	8.886	-0.662	-9.826
C	8.808	0.588	-10.081
C	8.949	0.180	-1.803
N	8.091	-0.766	-1.659
C	7.399	-0.859	-0.388
C	5.875	-0.934	-0.578
N	5.340	0.324	-1.069
C	4.647	0.301	-2.143
C	5.869	8.238	-4.552
N	5.639	8.285	-3.294
C	4.295	8.627	-2.861
C	3.729	7.565	-1.905
N	3.433	6.327	-2.605
C	3.937	5.244	-2.148
H	10.656	6.966	-6.639
H	5.075	8.448	-5.297
H	6.543	8.144	-7.170
H	9.813	7.210	-8.866
H	8.113	8.798	-11.189
H	9.219	7.403	-10.972
H	7.376	6.997	-12.591
H	6.153	7.271	-11.310
H	4.449	-0.644	-2.688
H	5.328	5.364	-10.623
H	8.453	3.191	-10.703
H	9.702	1.179	-10.367
H	10.990	-0.581	-10.202
H	10.133	-2.081	-10.682
H	9.771	-2.673	-8.290
H	11.492	-2.554	-8.770
H	9.470	-1.880	-6.289
H	8.937	-1.224	-4.072
H	11.442	1.424	-2.155
H	12.810	3.053	-5.380
H	13.843	4.914	-4.635
H	14.331	4.805	-2.927
H	12.382	6.278	-2.286
H	13.593	7.039	-3.352
H	10.369	6.898	-2.840
H	7.709	-1.797	0.105
H	7.641	-0.017	0.292
H	9.131	0.899	-0.974
H	5.426	-1.126	0.411
H	5.632	-1.787	-1.242
H	6.364	-0.323	-9.336
H	4.018	-0.270	-8.844
H	1.882	-0.410	-8.356
H	0.919	0.544	-9.527
H	0.618	2.360	-7.856
H	-0.053	0.779	-7.343
H	1.564	3.391	-6.165
H	4.864	2.861	-1.269
H	4.584	5.240	-1.246
H	4.430	7.421	-1.058
H	2.779	7.958	-1.503
H	3.594	8.766	-3.709
H	4.354	9.576	-2.302
H	2.512	4.692	-4.388
H	3.121	0.422	-4.371
H	4.218	3.375	-9.903
H	8.122	7.579	-3.197
H	11.808	1.086	-6.306
H	10.155	2.500	-2.696
H	12.117	3.662	-2.552
N	7.244	2.416	-4.707
B	7.557	3.508	-5.520

H	6.730	4.364	-5.687
H	8.648	3.563	-6.024
H	6.344	2.303	-4.249
H	7.887	1.649	-4.520

[N-cage-TS-2][NH₂BH₂]

C	11.362	0.854	-5.271
C	11.629	1.649	-4.143
C	10.709	1.580	-2.976
C	9.508	0.766	-3.102
C	9.309	0.037	-4.262
C	10.227	0.041	-5.346
C	12.542	2.739	-4.288
N	12.563	3.789	-3.458
C	13.255	5.015	-3.856
C	12.460	6.280	-3.513
N	11.415	6.547	-4.486
C	10.252	6.874	-4.062
C	9.153	7.249	-4.966
C	9.332	7.254	-6.365
C	8.295	7.640	-7.216
C	7.058	8.023	-6.662
C	6.861	8.023	-5.278
C	7.918	7.634	-4.432
C	8.513	7.640	-8.673
N	7.625	8.029	-9.508
C	7.952	7.977	-10.922
C	6.940	7.110	-11.688
N	7.093	5.708	-11.342
C	6.061	5.081	-10.919
C	6.087	3.662	-10.528
C	7.287	2.923	-10.524
C	7.297	1.579	-10.142
C	6.088	0.962	-9.760
C	4.889	1.680	-9.761
C	4.897	3.036	-10.147
C	3.640	1.011	-9.357
N	2.500	1.591	-9.383
C	1.337	0.830	-8.962
C	0.560	1.571	-7.862
N	1.313	1.595	-6.621
C	1.544	2.728	-6.076
C	2.309	2.865	-4.823
C	2.882	1.738	-4.200
C	3.622	1.874	-3.021
C	3.786	3.154	-2.455
C	3.224	4.282	-3.060
C	2.484	4.129	-4.250
C	3.440	5.600	-2.440
N	2.961	6.688	-2.911
C	3.267	7.918	-2.201
C	3.944	8.940	-3.128
N	5.282	8.509	-3.501
C	5.550	8.435	-4.750
C	4.231	0.684	-2.402
N	4.904	0.740	-1.316
C	5.472	-0.493	-0.805
C	6.986	-0.358	-0.586
N	7.704	-0.256	-1.844
C	8.649	0.609	-1.927
C	8.571	0.838	-10.151
N	8.658	-0.402	-9.857
C	9.966	-1.033	-9.929
C	10.314	-1.756	-8.618
N	10.684	-0.825	-7.565
C	9.955	-0.804	-6.511
N	6.908	2.846	-4.827

B	7.218	3.647	-5.928
H	10.302	6.952	-6.766
H	4.793	8.690	-5.519
H	6.255	8.320	-7.341
H	9.508	7.282	-9.007
H	7.884	9.002	-11.323
H	8.976	7.595	-11.111
H	7.157	7.220	-12.765
H	5.915	7.489	-11.500
H	4.074	-0.270	-2.942
H	5.077	5.583	-10.822
H	8.209	3.426	-10.822
H	9.463	1.430	-10.444
H	10.774	-0.319	-10.184
H	9.919	-1.798	-10.724
H	9.461	-2.405	-8.334
H	11.186	-2.402	-8.817
H	9.063	-1.458	-6.418
H	8.428	-0.609	-4.307
H	11.221	1.488	-2.005
H	13.122	2.783	-5.221
H	13.488	5.024	-4.936
H	14.203	5.045	-3.294
H	12.084	6.219	-2.471
H	13.170	7.125	-3.560
H	10.017	6.914	-2.979
H	7.322	-1.281	-0.080
H	7.188	0.493	0.093
H	8.887	1.276	-1.071
H	5.010	-0.696	0.176
H	5.275	-1.359	-1.468
H	6.112	-0.087	-9.462
H	3.749	-0.042	-9.027
H	1.596	-0.186	-8.605
H	0.665	0.730	-9.832
H	0.291	2.585	-8.221
H	-0.372	1.010	-7.680
H	1.178	3.676	-6.521
H	4.367	3.243	-1.534
H	4.058	5.591	-1.519
H	3.909	7.749	-1.313
H	2.315	8.360	-1.861
H	3.295	9.123	-4.008
H	4.038	9.885	-2.566
H	2.057	5.019	-4.717
H	2.741	0.760	-4.664
H	3.954	3.585	-10.138
H	7.752	7.640	-3.352
H	12.025	0.898	-6.139
H	10.701	2.961	-2.745
H	11.209	3.757	-3.103
H	6.393	4.420	-6.337
H	8.304	3.541	-6.434
H	6.012	2.873	-4.347
H	7.553	2.165	-4.433

P-cage-only

C	2.599	-2.506	3.059
C	1.413	-2.762	3.764
C	0.493	-3.686	3.216
H	-0.429	-3.904	3.759
C	0.735	-4.330	1.993
C	1.942	-4.045	1.312
C	2.879	-3.134	1.823
C	4.100	-2.869	1.069
H	4.219	-3.478	0.166
H	2.150	-4.546	0.364

C	-0.260	-5.260	1.469
H	-1.108	-5.443	2.139
P	-0.230	-6.021	-0.056
C	-1.806	-7.062	-0.009
H	-1.488	-8.112	-0.117
H	-2.295	-6.969	0.972
C	-2.780	-6.711	-1.153
H	-3.547	-7.500	-1.226
H	-2.258	-6.674	-2.121
P	-3.707	-5.094	-0.845
H	1.215	5.847	-2.007
H	-2.611	-4.610	-2.965
C	-3.759	-2.830	-2.539
C	-4.741	-2.163	-1.770
C	-5.153	-0.857	-2.074
C	-4.571	-0.212	-3.191
C	-3.595	-0.841	-3.979
C	-3.206	-2.158	-3.640
H	-5.190	-2.678	-0.917
C	-6.159	-0.215	-1.231
H	-6.582	-0.863	-0.454
P	-6.677	1.406	-1.330
C	-7.979	1.489	0.036
H	-8.102	0.500	0.503
H	-8.933	1.737	-0.458
C	-7.663	2.569	1.091
H	-7.395	3.524	0.614
H	-8.564	2.751	1.700
P	-6.307	2.036	2.292
C	-5.144	3.266	2.083
C	-3.866	3.382	2.779
H	-5.331	4.053	1.342
C	-2.966	4.387	2.393
H	-3.245	5.070	1.587
C	-1.706	4.537	3.019
C	-1.372	3.658	4.061
C	-2.252	2.633	4.479
C	-3.493	2.516	3.833
H	-0.407	3.769	4.562
C	-1.918	1.698	5.550
H	-2.728	1.012	5.823
P	-0.418	1.567	6.351
C	-0.755	0.185	7.593
H	-1.808	-0.130	7.534
H	-0.603	0.625	8.594
C	0.198	-1.014	7.421
H	1.244	-0.682	7.338
H	0.131	-1.657	8.314
P	-0.259	-2.104	5.948
C	1.174	-2.068	5.025
H	2.012	-1.452	5.371
C	-0.748	5.564	2.619
P	-0.893	6.618	1.287
C	0.684	7.646	1.421
H	0.364	8.692	1.564
H	1.253	7.355	2.318
H	0.149	5.616	3.244
C	1.558	7.558	0.153
H	2.312	8.363	0.179
H	0.956	7.706	-0.755
P	2.519	5.936	0.045
P	-1.726	-0.637	-6.092
C	-3.019	-0.117	-5.109
H	-4.890	0.800	-3.447
H	-3.471	0.863	-5.299
C	-1.564	0.788	-7.320
H	-2.356	1.532	-7.144
H	-1.738	0.358	-8.320
C	-0.168	1.443	-7.290

H	0.628	0.683	-7.325
H	-0.050	2.079	-8.183
P	0.072	2.575	-5.797
C	1.450	1.898	-5.055
C	2.114	2.385	-3.849
H	1.894	0.993	-5.483
C	3.148	1.623	-3.284
C	3.817	2.032	-2.108
C	3.434	3.244	-1.513
C	2.398	4.042	-2.051
C	1.975	5.298	-1.439
H	3.950	3.580	-0.610
C	4.882	1.243	-1.496
H	5.366	1.720	-0.636
P	5.384	-0.315	-1.972
C	6.786	-0.672	-0.758
H	6.952	0.192	-0.098
H	7.698	-0.798	-1.365
C	6.545	-1.958	0.059
H	6.233	-2.790	-0.590
H	7.488	-2.259	0.544
P	5.290	-1.706	1.447
H	3.442	0.687	-3.766
C	-3.302	-4.182	-2.228
C	1.757	3.600	-3.219
H	0.962	4.212	-3.654
H	-2.455	-2.665	-4.250
H	3.322	-1.800	3.474
H	-4.187	1.735	4.152

[P-cage][NH₃BH₃]

C	11.865	0.818	-3.616
C	11.822	1.594	-2.434
C	10.849	1.285	-1.470
C	9.937	0.218	-1.649
C	10.011	-0.527	-2.836
C	10.972	-0.242	-3.835
C	12.742	2.701	-2.183
P	14.083	3.146	-3.139
C	14.739	4.656	-2.212
C	16.207	4.492	-1.767
P	16.388	3.358	-0.268
C	17.402	2.128	-0.874
C	17.888	0.962	-0.142
C	17.657	0.779	1.242
C	18.118	-0.357	1.921
C	18.841	-1.329	1.190
C	19.091	-1.183	-0.182
C	18.609	-0.022	-0.831
C	17.835	-0.502	3.346
P	18.180	-1.866	4.310
C	17.557	-1.326	6.008
C	16.471	-2.272	6.562
P	14.788	-1.992	5.756
C	14.447	-3.527	5.095
C	13.242	-3.901	4.358
C	12.137	-3.029	4.218
C	10.985	-3.402	3.510
C	10.945	-4.690	2.923
C	12.024	-5.582	3.038
C	13.165	-5.173	3.770
C	11.929	-6.891	2.393
P	13.199	-8.019	2.200
C	12.304	-9.494	1.435
C	13.095	-10.157	0.286
P	12.870	-9.261	-1.359
C	14.298	-8.331	-1.441

C	14.628	-7.372	-2.494
C	15.946	-6.907	-2.615
C	16.322	-5.999	-3.633
C	15.334	-5.548	-4.523
C	13.988	-5.970	-4.417
C	13.655	-6.885	-3.402
C	12.939	-5.480	-5.307
P	13.110	-4.253	-6.479
C	11.390	-4.193	-7.251
C	10.776	-2.776	-7.222
P	10.076	-2.322	-5.528
C	11.062	-1.005	-5.077
C	17.693	-5.521	-3.793
P	19.000	-5.832	-2.743
C	20.428	-4.954	-3.612
C	21.115	-3.904	-2.714
P	20.112	-2.312	-2.565
C	19.828	-2.228	-0.885
C	9.878	-2.455	3.404
P	8.380	-2.731	2.638
C	7.503	-1.079	2.895
C	7.238	-0.336	1.568
P	8.768	0.548	0.904
C	8.927	-0.128	-0.652
N	12.079	-5.294	-0.715
B	10.549	-5.788	-1.057
H	17.105	1.543	1.795
H	20.202	-3.033	-0.241
H	19.215	-2.216	1.707
H	17.332	0.358	3.802
H	18.431	-1.348	6.680
H	17.199	-0.286	5.972
H	16.336	-2.074	7.639
H	16.772	-3.326	6.461
H	11.960	-5.950	-5.160
H	15.188	-4.329	5.195
H	12.178	-2.041	4.683
H	10.067	-1.482	3.874
H	8.070	-0.449	3.597
H	6.538	-1.314	3.373
H	6.830	-1.016	0.804
H	6.483	0.447	1.742
H	8.234	-0.918	-0.964
H	9.312	-1.352	-2.988
H	12.606	1.056	-4.383
H	12.531	3.267	-1.269
H	14.087	4.888	-1.356
H	14.670	5.505	-2.914
H	16.836	4.132	-2.596
H	16.602	5.475	-1.461
H	17.719	2.170	-1.923
H	9.927	-2.740	-7.925
H	11.505	-2.019	-7.550
H	11.856	-0.674	-5.758
H	11.514	-4.509	-8.301
H	10.727	-4.925	-6.766
H	10.065	-4.995	2.351
H	10.938	-7.128	1.988
H	11.294	-9.202	1.113
H	12.186	-10.223	2.255
H	14.165	-10.237	0.533
H	12.718	-11.180	0.132
H	15.070	-8.453	-0.671
H	15.611	-4.847	-5.314
H	17.856	-4.893	-4.677
H	20.083	-4.506	-4.557
H	21.158	-5.739	-3.871
H	21.330	-4.314	-1.715
H	22.082	-3.623	-3.164

H	16.706	-7.276	-1.923
H	12.619	-7.224	-3.310
H	14.002	-5.866	3.885
H	18.803	0.109	-1.899
H	10.796	1.884	-0.557
H	9.862	-5.437	-0.111
H	10.236	-5.233	-2.095
H	12.431	-5.746	0.139
H	12.731	-5.532	-1.473
H	10.610	-7.002	-1.168
H	12.127	-4.280	-0.573

P-cage-TS-1

C	-1.717	0.748	-4.011
C	-2.718	1.728	-4.103
C	-2.449	3.013	-3.577
C	-1.226	3.318	-2.962
C	-0.238	2.307	-2.898
C	-0.469	1.018	-3.403
C	-3.995	1.391	-4.727
P	-5.364	2.403	-4.825
C	-6.602	1.315	-5.746
C	-7.906	1.111	-4.949
P	-7.687	-0.101	-3.518
C	-8.239	0.807	-2.184
C	-8.309	0.348	-0.800
C	-8.665	1.256	0.208
C	-8.734	0.868	1.567
C	-8.443	-0.465	1.893
C	-8.077	-1.409	0.905
C	-8.027	-0.987	-0.431
C	-7.755	-2.798	1.220
P	-7.510	-3.460	2.772
C	-7.193	-5.280	2.371
C	-5.845	-5.789	2.920
P	-4.372	-5.231	1.877
C	-3.360	-4.520	3.051
C	-2.040	-3.939	2.829
C	-1.431	-3.228	3.874
C	-0.153	-2.630	3.734
C	0.513	-2.792	2.504
C	-0.077	-3.485	1.422
C	-1.344	-4.063	1.604
C	0.454	-1.851	4.802
P	-0.406	-1.235	6.163
C	0.937	-0.312	7.130
C	0.317	1.058	7.461
P	-0.607	1.517	5.895
C	-1.979	2.549	6.231
C	-2.602	3.348	5.262
C	-3.942	3.758	5.398
C	-4.572	4.608	4.479
C	-3.754	5.245	3.483
C	-2.436	4.917	3.263
C	-1.853	3.754	4.021
C	-1.582	5.603	2.327
P	-2.061	6.618	1.026
C	-0.388	7.245	0.402
C	-0.161	6.966	-1.097
P	0.280	5.164	-1.437
C	-1.025	4.652	-2.406
C	-5.986	4.900	4.511
P	-7.180	4.054	5.410
C	-8.762	4.948	4.889
C	-9.781	3.985	4.243
P	-9.309	3.484	2.484

C	-9.098	1.798	2.634
C	0.571	-3.603	0.120
P	1.940	-2.733	-0.408
C	2.188	-3.402	-2.157
C	2.170	-2.288	-3.223
P	0.426	-1.659	-3.589
C	0.578	0.010	-3.275
B	-0.946	1.874	2.164
N	0.189	1.347	2.995
H	-1.954	-3.139	4.829
H	0.076	-4.289	-0.576
H	-1.801	-4.617	0.781
H	-3.719	-4.449	4.085
H	-5.840	-6.892	2.894
H	-5.703	-5.488	3.969
H	-8.011	-5.846	2.847
H	-7.271	-5.449	1.286
H	-1.835	5.360	-2.618
H	-7.635	-3.445	0.343
H	-8.506	-0.783	2.937
H	-9.209	1.335	3.621
H	-9.923	3.087	4.864
H	-10.760	4.488	4.167
H	-8.523	5.784	4.214
H	-9.209	5.382	5.799
H	-6.309	5.693	3.827
H	-4.193	6.069	2.913
H	-0.786	3.915	4.249
H	-2.482	2.421	7.195
H	-0.426	0.972	8.268
H	1.055	1.815	7.759
H	1.841	-0.200	6.513
H	1.214	-0.871	8.036
H	1.508	-1.581	4.656
H	-0.380	8.335	0.568
H	0.426	6.823	1.011
H	-0.508	5.415	2.458
H	0.690	7.569	-1.455
H	-1.040	7.258	-1.693
H	-8.900	2.288	-0.062
H	-8.555	1.846	-2.338
H	-8.301	2.070	-4.580
H	-8.671	0.677	-5.614
H	-6.141	0.350	-6.008
H	-6.833	1.834	-6.692
H	-4.050	0.376	-5.137
H	0.726	2.534	-2.438
H	1.536	0.394	-2.904
H	2.824	-1.450	-2.934
H	2.560	-2.692	-4.172
H	1.435	-4.174	-2.376
H	3.174	-3.895	-2.167
H	-1.906	-0.245	-4.422
H	-3.217	3.787	-3.645
H	-7.761	-1.709	-1.206
H	1.516	-2.375	2.382
H	-4.512	3.396	6.258
H	0.215	0.321	3.058
H	1.116	1.694	2.738
H	-1.909	1.170	2.063
H	-0.725	2.816	1.463
H	-1.830	2.853	3.276
H	0.031	1.600	4.250

[P-cage-H₂][NH₂BH₂]

C	11.933	1.110	-3.546
C	11.813	1.891	-2.250
C	10.970	1.379	-1.217

C	10.161	0.264	-1.391
C	10.144	-0.394	-2.683
C	10.960	-0.039	-3.719
C	12.509	3.064	-2.081
P	13.366	3.930	-3.428
C	14.486	5.136	-2.503
C	15.899	4.650	-2.146
P	15.998	3.355	-0.774
C	17.174	2.300	-1.424
C	17.796	1.153	-0.769
C	18.556	0.262	-1.544
C	19.193	-0.862	-0.973
C	19.068	-1.063	0.409
C	18.319	-0.185	1.227
C	17.692	0.915	0.621
C	18.198	-0.375	2.670
P	18.803	-1.695	3.564
C	18.328	-1.239	5.332
C	17.441	-2.308	6.004
P	15.641	-2.196	5.447
C	15.382	-3.728	4.742
C	14.141	-4.194	4.131
C	14.112	-5.447	3.501
C	12.942	-5.934	2.871
C	11.788	-5.136	2.900
C	11.780	-3.866	3.523
C	12.958	-3.419	4.139
C	12.894	-7.224	2.189
P	14.217	-8.251	1.866
C	13.383	-9.708	0.999
C	14.000	-10.008	-0.381
P	13.459	-8.770	-1.702
C	14.955	-8.179	-2.267
C	15.156	-7.183	-3.316
C	14.096	-6.693	-4.115
C	14.305	-5.712	-5.096
C	15.619	-5.227	-5.290
C	16.697	-5.688	-4.518
C	16.445	-6.678	-3.539
C	18.024	-5.123	-4.740
P	19.421	-5.422	-3.808
C	20.710	-4.348	-4.674
C	21.308	-3.277	-3.737
P	20.138	-1.821	-3.459
C	19.978	-1.807	-1.762
C	13.164	-5.219	-5.861
P	13.170	-3.915	-6.962
C	11.361	-3.852	-7.505
C	10.700	-2.509	-7.138
P	10.469	-2.337	-5.270
C	10.980	-0.725	-4.993
C	10.606	-2.999	3.536
P	9.134	-3.261	2.715
C	8.154	-1.715	3.183
C	7.833	-0.832	1.961
P	9.349	0.096	1.317
C	9.276	-0.243	-0.358
N	14.105	-0.715	-0.866
B	14.361	-2.068	-1.101
H	15.015	-6.061	3.495
H	10.731	-2.076	4.115
H	12.964	-2.443	4.629
H	16.209	-4.447	4.706
H	17.440	-2.141	7.094
H	17.834	-3.321	5.831
H	19.276	-1.155	5.890
H	17.847	-0.249	5.356
H	11.440	-0.169	-5.820
H	17.650	0.418	3.192

H	19.570	-1.918	0.868
H	20.480	-2.583	-1.173
H	21.606	-3.715	-2.772
H	22.217	-2.860	-4.200
H	20.280	-3.890	-5.578
H	21.514	-5.027	-5.002
H	18.084	-4.417	-5.578
H	15.800	-4.468	-6.055
H	13.087	-7.082	-3.958
H	15.879	-8.534	-1.795
H	15.098	-10.048	-0.326
H	13.654	-10.998	-0.721
H	12.299	-9.533	0.922
H	13.526	-10.583	1.655
H	11.898	-7.515	1.835
H	11.346	-3.981	-8.599
H	10.807	-4.697	-7.067
H	12.220	-5.734	-5.653
H	9.699	-2.457	-7.600
H	11.282	-1.660	-7.529
H	18.659	0.445	-2.617
H	17.517	2.470	-2.452
H	16.422	4.283	-3.042
H	16.479	5.512	-1.772
H	13.933	5.454	-1.605
H	14.567	6.028	-3.143
H	12.399	3.608	-1.138
H	9.431	-1.210	-2.827
H	8.523	-0.957	-0.713
H	7.381	-1.424	1.151
H	7.095	-0.066	2.254
H	8.697	-1.144	3.953
H	7.211	-2.062	3.637
H	10.911	1.939	-0.280
H	11.836	1.806	-4.405
H	17.132	1.619	1.242
H	10.877	-5.501	2.421
H	17.275	-7.051	-2.934
H	13.442	-2.843	-1.088
H	14.829	-0.001	-0.855
H	15.493	-2.416	-1.311
H	13.176	-0.345	-0.678
H	14.348	2.935	-3.782
H	12.961	0.708	-3.627

[P-cage-(H₂)-TS-2][NH₂BH₂]

C	5.730	-0.731	-0.431
C	5.499	-2.101	-0.157
C	4.716	-2.878	-1.108
C	4.263	-2.256	-2.338
C	4.508	-0.900	-2.522
C	5.232	-0.112	-1.581
C	5.796	-2.658	1.104
P	5.145	-4.220	1.540
C	5.242	-4.196	3.430
C	3.883	-4.413	4.121
P	2.857	-2.831	4.235
C	1.273	-3.429	4.033
C	0.040	-2.653	4.135
C	0.009	-1.348	4.682
C	-1.183	-0.615	4.775
C	-2.376	-1.216	4.313
C	-2.388	-2.508	3.764
C	-1.166	-3.218	3.695
C	-1.153	0.723	5.357

P	-2.455	1.821	5.437
C	-1.683	3.288	6.340
C	-1.711	4.585	5.505
P	-0.369	4.623	4.178
C	-1.284	4.769	2.746
C	-0.756	4.853	1.387
C	0.628	4.947	1.115
C	1.119	5.009	-0.197
C	0.188	4.994	-1.262
C	-1.192	4.903	-1.033
C	-1.648	4.840	0.304
C	-2.102	4.880	-2.174
P	-3.787	4.620	-2.121
C	-4.265	4.764	-3.943
C	-5.008	3.515	-4.459
P	-3.844	2.056	-4.746
C	-4.532	0.848	-3.758
C	-4.037	-0.514	-3.590
C	-2.972	-1.037	-4.360
C	-2.488	-2.338	-4.160
C	-3.114	-3.145	-3.182
C	-4.174	-2.664	-2.398
C	-4.627	-1.343	-2.623
C	-4.756	-3.537	-1.384
P	-5.929	-3.105	-0.224
C	-6.145	-4.721	0.729
C	-5.731	-4.590	2.209
P	-3.857	-4.529	2.438
C	-3.651	-3.068	3.293
C	-1.355	-2.807	-4.952
P	-0.421	-4.199	-4.646
C	0.836	-4.183	-6.050
C	2.284	-4.202	-5.528
P	2.767	-2.561	-4.723
C	3.596	-3.089	-3.323
C	2.561	5.088	-0.413
P	3.367	4.975	-1.911
C	5.173	5.200	-1.408
C	6.065	4.027	-1.860
P	5.901	2.506	-0.751
C	5.442	1.301	-1.869
H	0.936	-0.906	5.056
H	-4.529	-2.447	3.504
H	-3.316	-0.664	4.391
H	-0.176	1.025	5.755
H	-2.282	3.435	7.254
H	-0.658	3.043	6.659
H	-1.515	5.444	6.168
H	-2.702	4.745	5.051
H	-1.073	-2.154	-5.786
H	-2.378	4.780	2.812
H	1.335	4.971	1.948
H	3.153	5.202	0.501
H	5.249	5.364	-0.322
H	5.516	6.125	-1.902
H	5.866	3.756	-2.909
H	7.123	4.335	-1.801
H	5.233	1.592	-2.905
H	4.168	-0.421	-3.445
H	4.966	-3.945	-1.184
H	6.273	-2.020	1.853
H	5.711	-3.260	3.768
H	5.918	-5.023	3.699
H	3.305	-5.216	3.639
H	4.062	-4.729	5.163
H	1.127	-4.486	3.779
H	2.972	-4.361	-6.376
H	2.441	-5.033	-4.823
H	3.622	-4.164	-3.104

H	0.650	-5.086	-6.655
H	0.659	-3.312	-6.700
H	0.554	5.058	-2.289
H	-1.616	5.024	-3.146
H	-3.375	4.979	-4.554
H	-4.934	5.638	-4.022
H	-5.822	3.225	-3.778
H	-5.465	3.746	-5.436
H	-5.412	1.091	-3.152
H	-2.770	-4.171	-3.033
H	-4.352	-4.556	-1.377
H	-5.591	-5.532	0.232
H	-7.216	-4.977	0.677
H	-6.198	-3.709	2.676
H	-6.083	-5.478	2.761
H	-5.457	-0.956	-2.027
H	-2.506	-0.407	-5.123
H	-2.721	4.781	0.500
H	-1.162	-4.233	3.290
H	6.319	-0.148	0.280
H	3.625	-3.710	0.658
H	3.627	-3.274	-0.192
N	-1.045	-6.651	-1.842
B	-1.472	-7.968	-2.027
H	-0.780	-6.031	-2.608
H	-0.956	-6.219	-0.927
H	-1.758	-8.630	-1.063
H	-1.544	-8.404	-3.146

[P-cage-H₂][NH₂BH₂][NH₃BH₃]

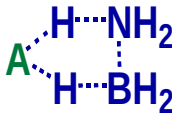
[A+ NH₃BH₃]

C	-1.640	4.690	4.490
C	-2.586	3.717	4.889
C	-3.921	3.883	4.489
C	-4.325	4.979	3.691
C	-3.358	5.925	3.317
C	-2.002	5.792	3.700
C	-2.224	2.552	5.692
P	-0.643	2.054	6.096
C	-0.970	0.525	7.156
C	-0.224	-0.721	6.637
P	-1.037	-1.459	5.101
C	0.255	-1.488	3.989
C	0.202	-1.981	2.615
C	1.305	-1.773	1.771
C	1.299	-2.203	0.423
C	0.164	-2.875	-0.054
C	-0.968	-3.096	0.761
C	-0.925	-2.656	2.093
C	-2.177	-3.745	0.261
P	-2.513	-4.117	-1.368
C	-4.220	-4.916	-1.251
C	-5.265	-4.190	-2.122
P	-5.856	-2.569	-1.354
C	-5.499	-1.438	-2.579
C	-5.777	-0.005	-2.541
C	-5.282	0.818	-3.565
C	-5.527	2.212	-3.584
C	-6.303	2.765	-2.552
C	-6.813	1.970	-1.498
C	-6.545	0.591	-1.514
C	-5.021	3.081	-4.646
P	-3.758	2.706	-5.728
C	-3.817	4.194	-6.888

C	-2.444	4.707	-7.349
P	-1.425	5.653	-6.067
C	-0.223	4.411	-5.514
C	0.511	4.506	-4.359
C	0.227	5.588	-3.334
C	1.248	5.718	-2.217
C	2.225	4.771	-2.080
C	2.346	3.624	-2.959
C	1.537	3.553	-4.084
C	3.340	2.615	-2.652
P	3.266	0.980	-3.148
C	4.896	0.265	-2.520
C	4.704	-1.097	-1.830
P	3.746	-0.933	-0.209
C	2.412	-1.959	-0.488
C	1.102	6.846	-1.325
P	1.675	6.939	0.288
C	1.216	8.712	0.759
C	0.566	8.782	2.154
P	-1.158	8.014	2.169
C	-0.975	6.748	3.297
C	-7.607	2.530	-0.406
P	-7.900	4.185	-0.117
C	-9.001	4.132	1.413
C	-8.414	4.937	2.592
P	-6.979	4.038	3.427
C	-5.702	5.153	3.236
N	0.174	0.248	-4.959
B	0.398	0.492	-6.568
N	-2.675	2.417	-1.064
B	-1.556	1.859	-1.680
H	-4.713	0.371	-4.383
H	-8.017	1.786	0.286
H	-6.951	-0.037	-0.718
H	-4.993	-1.780	-3.490
H	-6.160	-4.828	-2.218
H	-4.882	-4.013	-3.138
H	-4.108	-5.952	-1.612
H	-4.543	-4.971	-0.200
H	0.007	6.579	3.752
H	-2.931	-3.961	1.026
H	0.152	-3.231	-1.086
H	2.321	-2.460	-1.459
H	4.197	-1.810	-2.497
H	5.691	-1.524	-1.584
H	5.376	0.989	-1.843
H	5.560	0.145	-3.392
H	4.150	2.930	-1.982
H	2.961	4.883	-1.280
H	0.115	6.563	-3.847
H	0.019	3.610	-6.220
H	-1.816	3.881	-7.717
H	-2.586	5.394	-8.195
H	-4.413	5.002	-6.436
H	-4.375	3.847	-7.775
H	-5.507	4.062	-4.703
H	2.148	9.303	0.762
H	0.558	9.149	-0.007
H	0.502	7.678	-1.717
H	0.450	9.838	2.453
H	1.201	8.294	2.910
H	2.187	-1.262	2.163
H	1.226	-1.075	4.288
H	0.835	-0.498	6.439
H	-0.252	-1.505	7.413
H	-2.052	0.337	7.231
H	-0.608	0.765	8.170
H	-3.075	1.946	6.025
H	-3.660	6.785	2.714

H	-5.888	6.090	2.698
H	-8.101	5.942	2.272
H	-9.193	5.068	3.361
H	-9.199	3.089	1.703
H	-9.965	4.578	1.117
H	-4.666	3.145	4.797
H	-0.599	4.581	4.804
H	-1.787	-2.833	2.741
H	-6.522	3.836	-2.565
H	-3.593	2.456	-1.500
H	-2.658	2.802	-0.124
H	-2.344	5.611	-4.956
H	-1.685	1.416	-2.795
H	-0.507	1.832	-1.099
H	-0.763	5.399	-2.877
H	1.723	2.780	-4.834
H	-0.425	0.962	-4.528
H	-0.272	-0.655	-4.780
H	-0.714	0.531	-7.064
H	1.065	-0.447	-6.962
H	0.995	1.553	-6.670
H	1.067	0.260	-4.440

[P-cage-H₂-TS-1][NH₂BH₂]



C	-1.835	3.711	3.968
C	-2.522	3.366	5.239
C	-3.987	3.711	5.375
C	-4.475	4.877	4.543
C	-3.612	5.406	3.527
C	-2.370	4.907	3.222
C	-1.870	2.667	6.220
P	-0.437	1.649	5.908
C	0.587	1.444	7.469
C	1.266	0.081	7.227
P	-0.076	-0.975	6.397
C	0.751	-1.629	5.028
C	0.139	-2.510	4.048
C	-1.112	-3.140	4.277
C	-1.729	-3.957	3.319
C	-1.072	-4.167	2.084
C	0.165	-3.561	1.813
C	0.763	-2.752	2.807
C	-3.027	-4.543	3.633
P	-4.057	-5.382	2.562
C	-5.506	-5.827	3.692
C	-6.849	-5.263	3.187
P	-7.045	-3.412	3.513
C	-7.343	-2.809	1.947
C	-7.621	-1.422	1.583
C	-7.901	-0.419	2.540
C	-8.157	0.909	2.162
C	-8.152	1.229	0.784
C	-7.896	0.257	-0.196
C	-7.634	-1.066	0.226
C	-7.936	0.631	-1.607
P	-7.596	-0.393	-2.928
C	-7.888	0.744	-4.406
C	-6.636	0.879	-5.297
P	-5.332	1.995	-4.513
C	-3.968	0.974	-4.442
C	-2.660	1.333	-3.901
C	-1.662	0.352	-3.791
C	-0.389	0.645	-3.248

C	-0.132	1.959	-2.823
C	-1.116	2.971	-2.909
C	-2.361	2.645	-3.465
C	-0.897	4.330	-2.425
P	0.398	4.869	-1.457
C	-0.024	6.694	-1.224
C	-0.262	7.058	0.255
P	-1.939	6.490	0.911
C	-1.494	5.514	2.246
C	0.657	-0.362	-3.108
P	0.480	-2.045	-3.319
C	2.231	-2.671	-2.992
C	2.288	-3.705	-1.849
P	2.097	-2.908	-0.146
C	0.771	-3.765	0.501
C	-8.469	1.895	3.193
P	-8.476	3.593	3.021
C	-9.211	4.113	4.682
C	-8.549	5.322	5.360
P	-6.842	5.051	6.123
C	-5.718	5.416	4.738
B	-1.106	1.790	2.144
N	0.074	1.275	2.944
H	-1.611	-2.985	5.238
H	0.271	-4.518	-0.119
H	-1.535	-4.804	1.327
H	-3.358	-4.383	4.666
H	-5.564	-6.928	3.706
H	-5.298	-5.499	4.722
H	-7.674	-5.756	3.728
H	-6.992	-5.474	2.116
H	-1.689	5.040	-2.690
H	-7.301	-3.500	1.097
H	-7.927	-0.686	3.599
H	-8.713	1.463	4.172
H	-9.238	3.250	5.365
H	-10.261	4.373	4.460
H	-8.454	6.170	4.662
H	-9.193	5.672	6.181
H	-6.017	6.263	4.111
H	-3.951	6.306	3.005
H	-0.753	3.820	4.146
H	-2.355	2.563	7.198
H	-0.111	1.386	8.317
H	1.293	2.263	7.665
H	2.131	0.183	6.554
H	1.614	-0.392	8.156
H	1.762	-1.278	4.788
H	-0.248	8.156	0.362
H	0.540	6.664	0.896
H	-0.429	5.284	2.374
H	0.838	7.267	-1.600
H	-0.891	6.965	-1.845
H	-8.389	2.250	0.475
H	-8.207	1.676	-1.795
H	-8.243	1.729	-4.068
H	-8.702	0.287	-4.994
H	-6.206	-0.106	-5.533
H	-6.921	1.348	-6.253
H	-4.050	-0.059	-4.797
H	0.850	2.204	-2.415
H	1.632	0.033	-2.800
H	2.906	-1.824	-2.795
H	2.570	-3.147	-3.928
H	1.530	-4.491	-1.987
H	3.274	-4.199	-1.860
H	-1.873	-0.662	-4.137
H	-3.123	3.423	-3.553
H	-7.445	-1.837	-0.525

H	1.743	-2.310	2.610
H	-4.224	3.882	6.439
H	0.078	0.252	3.061
H	0.987	1.565	2.584
H	-2.082	1.097	2.132
H	-0.887	2.655	1.349
H	-1.890	2.810	3.210
H	0.049	1.610	4.112
H	-4.586	2.821	5.087
H	-6.812	3.613	6.082
N	-4.998	6.691	-1.281
B	-5.433	7.865	-1.899
H	-4.235	6.659	-0.604
H	-5.419	5.783	-1.455
H	-4.882	8.901	-1.632
H	-6.345	7.810	-2.683

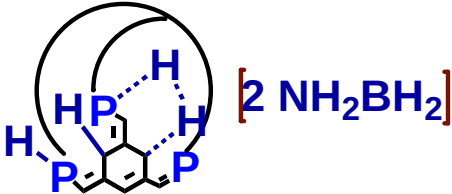
[P-cage-2H₂][2 NH₂BH₂]

B			
C	-1.676	4.798	4.926
C	-2.654	3.671	5.144
C	-4.096	4.098	5.008
C	-4.330	4.719	3.640
C	-3.269	5.566	3.142
C	-2.015	5.624	3.689
C	-2.320	2.388	5.371
P	-0.599	1.722	5.417
C	-0.780	0.395	6.758
C	0.138	-0.816	6.506
P	-0.579	-1.957	5.186
C	0.631	-1.947	3.986
C	0.562	-2.607	2.685
C	-0.555	-3.376	2.280
C	-0.632	-3.948	1.000
C	0.454	-3.761	0.114
C	1.581	-3.008	0.480
C	1.618	-2.442	1.776
C	-1.835	-4.687	0.624
P	-2.242	-5.219	-0.943
C	-3.896	-6.081	-0.652
C	-5.022	-5.514	-1.541
P	-5.684	-3.859	-0.915
C	-5.444	-2.844	-2.264
C	-5.796	-1.430	-2.359
C	-6.546	-0.763	-1.361
C	-6.858	0.600	-1.461
C	-6.412	1.307	-2.602
C	-5.662	0.684	-3.610
C	-5.373	-0.694	-3.476
C	-5.197	1.480	-4.742
P	-4.103	0.983	-5.951
C	-4.002	2.521	-7.043
C	-2.555	3.020	-7.225
P	-1.885	3.905	-5.696
C	-0.481	2.999	-5.355
C	0.475	3.246	-4.280
C	1.475	2.294	-4.028
C	2.425	2.468	-2.994
C	2.358	3.637	-2.218
C	1.366	4.621	-2.443
C	0.444	4.413	-3.482
C	1.271	5.840	-1.644
P	2.098	6.169	-0.188
C	1.490	7.913	0.214

C	0.778	7.991	1.578
P	-0.872	7.071	1.547
C	-0.939	6.417	3.129
C	3.468	1.484	-2.717
P	3.629	-0.046	-3.452
C	5.191	-0.720	-2.632
C	4.947	-2.062	-1.910
P	4.034	-1.833	-0.274
C	2.658	-2.817	-0.487
C	-7.606	1.245	-0.386
P	-8.001	2.902	-0.291
C	-8.920	3.027	1.351
C	-8.238	4.024	2.310
P	-6.765	3.276	3.240
C	-5.435	4.492	2.878
N	-2.275	-0.144	1.190
B	-3.437	0.181	1.891
H	-1.387	-3.516	2.975
H	2.520	-3.349	-1.436
H	0.413	-4.208	-0.881
H	-2.540	-4.860	1.447
H	-3.740	-7.144	-0.901
H	-4.168	-6.033	0.413
H	-5.876	-6.212	-1.526
H	-4.695	-5.424	-2.588
H	0.558	6.580	-2.027
H	-4.954	-3.252	-3.156
H	-6.890	-1.326	-0.490
H	-7.906	0.574	0.427
H	-9.038	2.034	1.810
H	-9.931	3.394	1.110
H	-7.904	4.920	1.764
H	-8.957	4.364	3.070
H	-5.503	5.016	1.917
H	-3.479	6.156	2.244
H	-1.693	5.470	5.807
H	-3.133	1.662	5.494
H	-1.830	0.073	6.831
H	-0.519	0.868	7.717
H	1.158	-0.502	6.234
H	0.214	-1.412	7.430
H	1.546	-1.366	4.153
H	0.567	9.047	1.819
H	1.416	7.595	2.382
H	-0.062	6.532	3.778
H	2.381	8.562	0.229
H	0.835	8.275	-0.592
H	-6.648	2.370	-2.697
H	-5.583	2.506	-4.764
H	-4.650	3.315	-6.641
H	-4.410	2.233	-8.027
H	-1.883	2.195	-7.508
H	-2.529	3.757	-8.045
H	-0.256	2.118	-5.968
H	3.095	3.795	-1.428
H	4.187	1.785	-1.946
H	5.614	0.028	-1.946
H	5.925	-0.875	-3.439
H	4.404	-2.769	-2.555
H	5.920	-2.522	-1.666
H	1.522	1.396	-4.648
H	-0.315	5.173	-3.678
H	-4.801	-1.196	-4.260
H	2.489	-1.854	2.077
H	-4.780	3.259	5.188
H	-1.723	-0.977	1.376
H	-1.900	0.426	0.439
H	-0.780	0.809	4.318
H	-3.815	-0.554	2.765

H	-4.029	1.187	1.600
H	-0.649	4.412	4.851
H	-6.396	2.349	2.202
H	-4.317	4.873	5.767
N	-7.390	1.360	6.380
B	-7.829	1.831	7.619
H	-7.183	0.381	6.203
H	-7.250	1.955	5.560
H	-7.967	1.051	8.526
H	-8.055	3.006	7.748

[P-cage-2H₂-TS-2][2 NH₂BH₂]



C	-4.649	-1.580	-2.732
C	-4.031	-0.834	-3.748
C	-2.982	-1.437	-4.479
C	-2.538	-2.737	-4.195
C	-3.192	-3.462	-3.171
C	-4.239	-2.899	-2.425
C	-4.474	0.533	-4.006
P	-3.764	1.623	-5.109
C	-4.829	3.165	-4.895
C	-4.000	4.385	-4.444
P	-3.556	4.327	-2.610
C	-1.853	4.417	-2.647
C	-0.967	4.457	-1.487
C	0.423	4.459	-1.682
C	1.325	4.525	-0.594
C	0.797	4.598	0.704
C	-0.596	4.587	0.942
C	-1.458	4.521	-0.162
C	-1.164	4.654	2.285
P	-0.296	4.658	3.753
C	-1.681	4.777	5.031
C	-1.717	3.561	5.981
P	-2.518	2.042	5.198
C	-1.217	0.941	5.140
C	-1.261	-0.426	4.631
C	-0.074	-1.172	4.569
C	-0.058	-2.504	4.092
C	-1.271	-3.083	3.688
C	-2.487	-2.360	3.725
C	-2.462	-1.041	4.206
C	1.165	-3.296	4.024
P	2.760	-2.721	4.194
C	3.778	-4.306	4.161
C	5.139	-4.130	3.461
P	5.044	-4.242	1.572
C	5.628	-2.648	1.086
C	5.320	-2.124	-0.163
C	5.524	-0.643	-0.429
C	5.147	-0.162	-1.816
C	4.398	-1.030	-2.671
C	4.117	-2.348	-2.369
C	4.590	-2.905	-1.095
C	3.455	-3.256	-3.284
P	2.589	-2.866	-4.710
C	2.213	-4.592	-5.391

C	0.781	-4.710	-5.943
P	-0.511	-4.673	-4.571
C	-1.412	-3.276	-4.948
C	5.533	1.082	-2.245
P	6.750	2.116	-1.373
C	6.529	3.812	-2.165
C	5.393	4.706	-1.649
P	3.651	4.214	-2.190
C	2.773	4.560	-0.769
C	-3.757	-2.931	3.288
P	-3.983	-4.432	2.512
C	-5.858	-4.479	2.289
C	-6.276	-4.695	0.820
P	-6.016	-3.151	-0.236
C	-4.850	-3.688	-1.359
N	-1.145	-6.986	-1.655
B	-1.651	-8.284	-1.748
H	0.857	-0.717	4.911
H	-4.628	-2.289	3.466
H	-3.396	-0.477	4.257
H	-0.231	1.263	5.495
H	-2.331	3.812	6.862
H	-0.709	3.313	6.347
H	-1.480	5.687	5.621
H	-2.651	4.921	4.531
H	-1.102	-2.669	-5.807
H	-2.260	4.691	2.314
H	1.482	4.666	1.552
H	3.329	4.831	0.136
H	5.433	4.793	-0.553
H	5.541	5.724	-2.053
H	6.446	3.639	-3.250
H	7.489	4.330	-2.016
H	5.250	1.400	-3.253
H	4.111	-0.643	-3.654
H	4.810	-3.979	-1.117
H	6.083	-1.990	1.833
H	5.614	-3.182	3.759
H	5.808	-4.947	3.775
H	3.195	-5.125	3.714
H	3.949	-4.573	5.218
H	1.010	-4.362	3.817
H	2.930	-4.777	-6.209
H	2.404	-5.352	-4.618
H	3.514	-4.312	-2.992
H	0.666	-5.674	-6.466
H	0.569	-3.914	-6.673
H	0.819	4.433	-2.700
H	-1.339	4.443	-3.615
H	-3.090	4.495	-5.054
H	-4.600	5.300	-4.586
H	-5.657	2.965	-4.197
H	-5.276	3.377	-5.881
H	-5.325	0.862	-3.398
H	-2.877	-4.484	-2.952
H	-4.474	-4.715	-1.284
H	-5.745	-5.552	0.378
H	-7.354	-4.925	0.783
H	-6.310	-3.564	2.701
H	-6.224	-5.325	2.895
H	-5.466	-1.129	-2.163
H	-2.492	-0.871	-5.274
H	-2.538	4.533	0.004
H	-1.277	-4.116	3.335
H	4.945	-0.061	0.311
H	3.454	-3.765	0.706
H	3.432	-3.349	-0.107
H	-0.893	-6.417	-2.464
H	-0.978	-6.518	-0.768

H	-1.914	-8.883	-0.738
H	-1.813	-8.767	-2.838
H	6.582	-0.384	-0.230
H	6.049	2.353	-0.138
N	4.494	0.439	5.345
B	5.091	1.446	4.583
H	3.990	-0.352	4.945
H	4.524	0.424	6.360
H	5.013	1.389	3.384
H	5.667	2.341	5.145

[P-cage-2H₂] [2NH₂BH₂][NH₃BH₃]

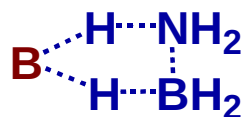
[B+NH₃BH₃]

C	-2.258	3.121	-3.120
C	-2.085	1.868	-3.753
C	-0.861	1.204	-3.585
C	0.183	1.752	-2.804
C	-0.027	2.994	-2.186
C	-1.249	3.696	-2.330
C	-3.117	1.252	-4.582
P	-4.692	1.846	-4.857
C	-5.400	0.553	-6.037
C	-6.699	-0.091	-5.508
P	-6.369	-1.347	-4.136
C	-7.061	-0.574	-2.782
C	-7.059	-1.063	-1.407
C	-7.555	-0.234	-0.389
C	-7.528	-0.629	0.968
C	-7.020	-1.898	1.284
C	-6.517	-2.765	0.285
C	-6.550	-2.333	-1.048
C	-5.948	-4.074	0.593
P	-5.697	-4.730	2.147
C	-4.938	-6.412	1.743
C	-3.564	-6.611	2.413
P	-2.189	-5.643	1.554
C	-1.529	-4.742	2.843
C	-0.401	-3.819	2.766
C	-0.080	-3.040	3.891
C	0.992	-2.116	3.872
C	1.740	-1.988	2.691
C	1.446	-2.752	1.537
C	0.382	-3.665	1.598
C	1.332	-1.275	5.017
P	0.545	-1.248	6.532
C	1.480	0.132	7.414
C	0.619	1.396	7.598
P	0.383	2.373	5.994
C	-1.160	3.084	6.264
C	-1.844	4.067	5.460
C	-1.221	4.845	4.514
C	-1.856	5.923	3.804
C	-3.313	6.208	4.134
C	-4.036	4.980	4.636
C	-3.325	4.272	5.759
C	-5.190	4.572	4.077
P	-6.145	3.069	4.566
C	-7.904	3.610	4.129
C	-8.765	2.416	3.669
P	-8.342	1.906	1.905
C	-7.967	0.249	2.047
C	-1.137	6.707	2.941
P	-1.614	8.339	2.292
C	-0.861	8.435	0.570
C	-1.368	7.493	-0.531
P	-0.504	5.808	-0.582

C	-1.479	5.007	-1.732
C	2.202	-2.607	0.296
P	3.412	-1.443	-0.002
C	3.925	-1.833	-1.774
C	3.681	-0.641	-2.723
P	1.870	-0.471	-3.229
C	1.472	1.082	-2.649
B	-3.103	0.054	4.205
N	-1.614	0.367	3.607
N	-4.871	0.739	7.242
B	-5.026	0.526	8.610
N	-6.265	4.449	0.063
B	-6.554	5.674	-0.540
H	-0.678	-3.147	4.799
H	1.921	-3.308	-0.497
H	0.147	-4.268	0.717
H	-1.989	-4.815	3.835
H	-3.280	-7.675	2.345
H	-3.601	-6.350	3.481
H	-5.638	-7.172	2.128
H	-4.874	-6.551	0.652
H	-2.389	5.506	-2.086
H	-5.639	-4.653	-0.285
H	-6.992	-2.214	2.329
H	-8.000	-0.218	3.038
H	-8.665	1.558	4.352
H	-9.827	2.711	3.668
H	-7.881	4.391	3.351
H	-8.343	4.062	5.030
H	-5.602	5.164	3.249
H	-3.835	6.628	3.263
H	-0.150	4.701	4.341
H	-1.728	2.742	7.139
H	-0.361	1.148	8.030
H	1.122	2.074	8.307
H	2.414	0.361	6.878
H	1.758	-0.260	8.405
H	2.172	-0.592	4.842
H	-1.043	9.479	0.269
H	0.229	8.354	0.700
H	-0.077	6.464	2.803
H	-1.164	7.957	-1.510
H	-2.457	7.353	-0.464
H	-7.963	0.744	-0.653
H	-7.532	0.406	-2.914
H	-7.409	0.673	-5.160
H	-7.187	-0.641	-6.329
H	-4.640	-0.210	-6.264
H	-5.621	1.083	-6.979
H	-2.818	0.306	-5.048
H	0.778	3.443	-1.602
H	2.225	1.658	-2.099
H	4.047	0.299	-2.284
H	4.245	-0.803	-3.657
H	3.414	-2.740	-2.132
H	5.004	-2.056	-1.744
H	-0.704	0.246	-4.086
H	-3.198	3.662	-3.256
H	-6.165	-2.992	-1.830
H	2.575	-1.283	2.665
H	-3.796	3.302	5.972
H	-1.088	-0.495	3.426
H	-1.663	0.887	2.726
H	-2.923	-0.577	5.237
H	-3.690	-0.592	3.359
H	-3.619	1.142	4.406
H	-1.050	0.928	4.266
H	-2.975	8.076	1.914
H	-3.337	6.988	4.921

H	-5.643	6.364	-0.923
H	-7.702	6.013	-0.659
H	-6.976	3.804	0.411
H	-5.320	4.100	0.191
H	-5.929	2.332	3.350
H	-3.412	4.873	6.685
H	-5.433	1.398	6.702
H	-4.197	0.248	6.654
H	-4.320	-0.278	9.165
H	-5.860	1.155	9.213

[P-cage-2H₂-TS-1][2 NH₂BH₂]

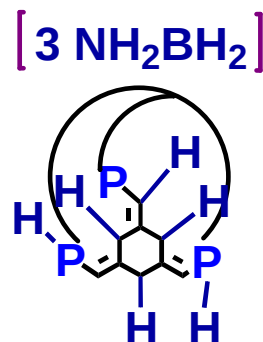


C	-1.839	3.842	4.103
C	-2.498	3.527	5.379
C	-3.876	4.144	5.593
C	-4.658	4.060	4.308
C	-4.007	4.839	3.182
C	-2.498	4.919	3.308
C	-1.907	2.769	6.369
P	-0.504	1.720	6.118
C	0.293	1.311	7.768
C	1.163	0.084	7.435
P	0.113	-1.036	6.320
C	1.199	-1.352	5.018
C	0.902	-2.166	3.849
C	-0.174	-3.092	3.820
C	-0.473	-3.853	2.681
C	0.328	-3.689	1.528
C	1.398	-2.781	1.508
C	1.682	-2.041	2.681
C	-1.595	-4.786	2.724
P	-2.224	-5.668	1.406
C	-3.612	-6.661	2.217
C	-4.984	-6.401	1.562
P	-5.733	-4.753	2.093
C	-6.003	-3.976	0.600
C	-6.594	-2.654	0.414
C	-7.165	-1.923	1.481
C	-7.711	-0.644	1.293
C	-7.697	-0.093	-0.009
C	-7.138	-0.786	-1.094
C	-6.597	-2.074	-0.863
C	-7.127	-0.159	-2.413
P	-6.340	-0.753	-3.804
C	-6.780	0.545	-5.101
C	-5.533	1.130	-5.795
P	-4.634	2.395	-4.719
C	-3.106	1.667	-4.508
C	-1.987	2.211	-3.744
C	-0.809	1.457	-3.619
C	0.305	1.933	-2.890
C	0.212	3.194	-2.280
C	-0.958	3.981	-2.377
C	-2.037	3.482	-3.124
C	-1.077	5.294	-1.749
P	-0.081	5.929	-0.518
C	-0.763	7.683	-0.365
C	-1.042	8.161	1.068
P	-2.523	7.410	1.970
C	-1.783	5.915	2.740
C	1.546	1.172	-2.767
P	1.807	-0.433	-3.278
C	3.622	-0.699	-2.829

C	3.828	-1.859	-1.834
P	3.300	-1.407	-0.076
C	2.158	-2.625	0.272
C	-8.257	0.062	2.447
P	-8.831	1.669	2.493
C	-9.312	1.845	4.309
C	-8.485	2.894	5.078
P	-6.678	2.443	5.461
C	-5.790	3.353	4.126
B	-1.215	1.872	2.391
N	0.055	1.373	3.143
H	-0.777	-3.224	4.722
H	1.912	-3.357	-0.506
H	0.111	-4.279	0.634
H	-2.068	-4.887	3.708
H	-3.349	-7.724	2.090
H	-3.642	-6.461	3.299
H	-5.693	-7.181	1.887
H	-4.920	-6.456	0.465
H	-1.922	5.895	-2.107
H	-5.690	-4.472	-0.326
H	-7.184	-2.367	2.480
H	-8.263	-0.524	3.373
H	-9.262	0.864	4.806
H	-10.370	2.157	4.317
H	-8.472	3.856	4.543
H	-8.968	3.086	6.049
H	-6.238	3.329	3.125
H	-4.288	4.411	2.204
H	-0.754	3.986	4.213
H	-2.398	2.748	7.349
H	-0.494	1.047	8.491
H	0.876	2.143	8.188
H	2.074	0.385	6.897
H	1.471	-0.465	8.337
H	2.154	-0.812	4.978
H	-1.222	9.247	1.051
H	-0.166	8.011	1.719
H	-0.695	5.924	2.865
H	0.009	8.336	-0.808
H	-1.662	7.786	-0.990
H	-8.134	0.894	-0.176
H	-7.661	0.796	-2.469
H	-7.397	1.339	-4.653
H	-7.404	0.033	-5.853
H	-4.840	0.333	-6.107
H	-5.847	1.666	-6.706
H	-2.915	0.687	-4.962
H	1.073	3.588	-1.735
H	2.363	1.712	-2.273
H	4.058	0.235	-2.444
H	4.141	-0.936	-3.773
H	3.298	-2.765	-2.166
H	4.901	-2.108	-1.790
H	-0.748	0.483	-4.110
H	-2.940	4.089	-3.224
H	-6.170	-2.630	-1.701
H	2.543	-1.367	2.685
H	-4.398	3.643	6.417
H	0.141	0.347	3.122
H	0.928	1.759	2.771
H	-2.113	1.075	2.370
H	-0.992	2.618	1.476
H	-1.830	2.853	3.276
H	0.031	1.600	4.250
H	-3.157	6.793	0.835
H	-4.410	5.872	3.188
N	-4.806	3.046	-0.506
B	-5.540	4.163	-0.908

H	-4.949	5.148	-1.272
H	-6.741	4.122	-0.868
H	-5.233	2.173	-0.207
H	-3.791	3.001	-0.537
H	-6.689	1.156	4.820
H	-3.764	5.212	5.867
N	-5.639	1.997	9.022
B	-5.808	2.887	10.083
H	-5.958	2.180	8.067
H	-5.189	1.091	9.125
H	-5.401	2.582	11.175
H	-6.355	3.939	9.879

[P-pore-3H₂][3 NH₂BH₂]

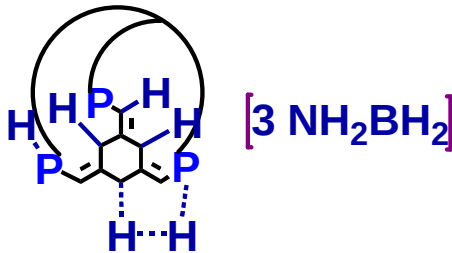


C	0.396	4.056	-3.495
C	0.478	2.894	-4.299
C	1.489	1.960	-4.023
C	2.395	2.143	-2.951
C	2.282	3.307	-2.174
C	1.278	4.274	-2.422
C	-0.455	2.626	-5.389
P	-1.919	3.445	-5.685
C	-2.574	2.592	-7.234
C	-4.033	2.121	-7.071
P	-4.176	0.614	-5.939
C	-5.196	1.195	-4.701
C	-5.639	0.452	-3.525
C	-6.313	1.135	-2.501
C	-6.724	0.480	-1.316
C	-6.466	-0.893	-1.193
C	-5.793	-1.617	-2.205
C	-5.397	-0.932	-3.363
C	-5.486	-3.039	-2.078
P	-5.709	-3.999	-0.686
C	-5.112	-5.693	-1.270
C	-4.005	-6.269	-0.362
P	-2.338	-5.426	-0.636
C	-1.982	-4.823	0.919
C	-0.791	-4.069	1.300
C	-0.734	-3.474	2.570
C	0.378	-2.703	2.982
C	1.458	-2.567	2.095
C	1.438	-3.153	0.807
C	0.313	-3.904	0.433
C	0.429	-2.033	4.279
P	-0.881	-1.836	5.352
C	-0.109	-0.899	6.797
C	-0.965	0.317	7.197
P	-0.714	1.773	6.010
C	-2.415	2.489	5.964
C	-2.703	3.800	5.868

C	-1.681	4.919	5.828
C	-1.843	5.710	4.542
C	-3.250	6.235	4.332
C	-4.233	5.079	4.400
C	-4.132	4.280	5.684
C	-5.031	4.781	3.357
P	-6.129	3.307	3.228
C	-7.695	4.057	2.480
C	-8.446	3.053	1.584
P	-7.613	2.869	-0.100
C	-7.374	1.184	-0.214
C	-0.834	5.831	3.661
P	-0.965	6.619	1.996
C	0.735	7.438	1.850
C	1.234	7.454	0.392
P	1.916	5.773	-0.120
C	1.116	5.469	-1.594
C	2.533	-2.998	-0.146
P	3.899	-1.991	0.028
C	4.843	-2.331	-1.571
C	5.120	-1.047	-2.379
P	3.581	-0.403	-3.265
C	3.430	1.167	-2.619
N	-1.210	2.133	-0.509
B	-2.450	2.741	-0.320
N	-6.289	0.428	5.581
B	-6.943	0.402	6.815
H	-1.573	-3.606	3.257
H	2.417	-3.579	-1.068
H	0.290	-4.372	-0.553
H	-2.710	-4.966	1.726
H	-3.861	-7.335	-0.603
H	-4.292	-6.210	0.698
H	-5.988	-6.362	-1.239
H	-4.779	-5.640	-2.318
H	0.372	6.185	-1.963
H	-5.042	-3.492	-2.972
H	-6.786	-1.415	-0.288
H	-7.688	0.540	0.615
H	-8.553	2.073	2.075
H	-9.463	3.434	1.391
H	-7.439	4.966	1.913
H	-8.336	4.367	3.319
H	-4.987	5.431	2.475
H	-3.481	6.947	5.149
H	-1.873	5.592	6.687
H	-3.252	1.780	5.965
H	-2.030	0.042	7.240
H	-0.679	0.665	8.201
H	0.926	-0.608	6.563
H	-0.065	-1.608	7.640
H	1.400	-1.589	4.529
H	0.633	8.467	2.224
H	1.461	6.926	2.501
H	0.131	5.382	3.923
H	2.069	8.168	0.300
H	0.446	7.782	-0.302
H	-6.511	2.203	-2.616
H	-5.541	2.235	-4.738
H	-4.675	2.937	-6.704
H	-4.424	1.817	-8.056
H	-1.913	1.757	-7.509
H	-2.521	3.334	-8.048
H	-0.181	1.780	-6.031
H	2.985	3.470	-1.354
H	4.138	1.497	-1.850
H	5.548	-0.259	-1.741
H	5.862	-1.269	-3.164
H	4.304	-3.075	-2.178

H	5.804	-2.784	-1.277
H	1.573	1.066	-4.645
H	-0.368	4.804	-3.711
H	-4.882	-1.479	-4.156
H	2.331	-1.989	2.405
H	-4.833	3.435	5.687
H	-0.963	1.232	-0.111
H	-0.465	2.545	-1.066
H	-0.873	0.974	4.819
H	-3.283	2.189	0.347
H	-2.652	3.811	-0.836
H	-0.660	4.526	5.926
H	-5.594	2.837	1.978
H	-4.398	4.947	6.527
H	-5.763	-0.361	5.217
H	-6.300	1.232	4.949
H	-6.881	-0.591	7.491
H	-7.550	1.379	7.171
H	-0.589	5.439	1.257
H	-3.334	6.771	3.378
N	-3.588	5.774	-3.238
B	-4.072	7.057	-3.501
H	-4.025	7.475	-4.629
H	-4.521	7.711	-2.596
H	-3.196	5.163	-3.955
H	-3.593	5.348	-2.314

[P-cage-3H₂-TS-2][3 NH₂BH₂]



C	-4.649	-1.580	-2.732
C	-4.031	-0.834	-3.748
C	-2.982	-1.437	-4.479
C	-2.538	-2.737	-4.195
C	-3.192	-3.462	-3.171
C	-4.239	-2.899	-2.425
C	-4.474	0.533	-4.006
P	-3.764	1.623	-5.109
C	-4.829	3.165	-4.895
C	-4.000	4.385	-4.444
P	-3.556	4.327	-2.610
C	-1.853	4.417	-2.647
C	-0.967	4.457	-1.487
C	0.423	4.459	-1.682
C	1.325	4.525	-0.594
C	0.797	4.598	0.704
C	-0.596	4.587	0.942
C	-1.458	4.521	-0.162
C	-1.164	4.654	2.285
P	-0.296	4.658	3.753
C	-1.681	4.777	5.031
C	-1.717	3.561	5.981
P	-2.518	2.042	5.198
C	-1.217	0.941	5.140
C	-1.261	-0.426	4.631
C	-0.074	-1.172	4.569
C	-0.058	-2.504	4.092
C	-1.271	-3.083	3.688
C	-2.487	-2.360	3.725
C	-2.462	-1.041	4.206

C	1.165	-3.296	4.024
P	2.760	-2.721	4.194
C	3.778	-4.306	4.161
C	5.139	-4.130	3.461
P	5.044	-4.242	1.572
C	5.628	-2.648	1.086
C	5.320	-2.124	-0.163
C	5.524	-0.643	-0.429
C	5.147	-0.162	-1.816
C	4.398	-1.030	-2.671
C	4.117	-2.348	-2.369
C	4.590	-2.905	-1.095
C	3.455	-3.256	-3.284
P	2.589	-2.866	-4.710
C	2.213	-4.592	-5.391
C	0.781	-4.710	-5.943
P	-0.511	-4.673	-4.571
C	-1.412	-3.276	-4.948
C	5.533	1.082	-2.245
P	6.750	2.116	-1.373
C	6.529	3.812	-2.165
C	5.393	4.706	-1.649
P	3.651	4.214	-2.190
C	2.773	4.560	-0.769
C	-3.757	-2.931	3.288
P	-3.983	-4.432	2.512
C	-5.858	-4.479	2.289
C	-6.276	-4.695	0.820
P	-6.016	-3.151	-0.236
C	-4.850	-3.688	-1.359
N	-1.145	-6.986	-1.655
B	-1.651	-8.284	-1.748
H	0.857	-0.717	4.911
H	-4.628	-2.289	3.466
H	-3.396	-0.477	4.257
H	-0.231	1.263	5.495
H	-2.331	3.812	6.862
H	-0.709	3.313	6.347
H	-1.480	5.687	5.621
H	-2.651	4.921	4.531
H	-1.102	-2.669	-5.807
H	-2.260	4.691	2.314
H	1.482	4.666	1.552
H	3.329	4.831	0.136
H	5.433	4.793	-0.553
H	5.541	5.724	-2.053
H	6.446	3.639	-3.250
H	7.489	4.330	-2.016
H	5.250	1.400	-3.253
H	4.111	-0.643	-3.654
H	4.810	-3.979	-1.117
H	6.083	-1.990	1.833
H	5.614	-3.182	3.759
H	5.808	-4.947	3.775
H	3.195	-5.125	3.714
H	3.949	-4.573	5.218
H	1.010	-4.362	3.817
H	2.930	-4.777	-6.209
H	2.404	-5.352	-4.618
H	3.514	-4.312	-2.992
H	0.666	-5.674	-6.466
H	0.569	-3.914	-6.673
H	0.819	4.433	-2.700
H	-1.339	4.443	-3.615
H	-3.090	4.495	-5.054
H	-4.600	5.300	-4.586
H	-5.657	2.965	-4.197
H	-5.276	3.377	-5.881
H	-5.325	0.862	-3.398

H	-2.877	-4.484	-2.952
H	-4.474	-4.715	-1.284
H	-5.745	-5.552	0.378
H	-7.354	-4.925	0.783
H	-6.310	-3.564	2.701
H	-6.224	-5.325	2.895
H	-5.466	-1.129	-2.163
H	-2.492	-0.871	-5.274
H	-2.538	4.533	0.004
H	-1.277	-4.116	3.335
H	4.945	-0.061	0.311
H	3.454	-3.765	0.706
H	3.432	-3.349	-0.107
H	-0.893	-6.417	-2.464
H	-0.978	-6.518	-0.768
H	-1.914	-8.883	-0.738
H	-1.813	-8.767	-2.838
H	6.582	-0.384	-0.230
H	6.049	2.353	-0.138
N	4.494	0.439	5.345
B	5.091	1.446	4.583
H	3.990	-0.352	4.945
H	4.524	0.424	6.360
H	5.013	1.389	3.384
H	5.667	2.341	5.145

[P-cage-3H₂][3 NH₂BH₂][NH₃BH₃]

C	-1.199	4.842	4.233
C	-2.130	4.055	4.952
C	-3.498	4.264	4.719
C	-3.954	5.219	3.782
C	-3.001	5.985	3.094
C	-1.613	5.800	3.295
C	-1.721	3.029	5.905
P	-0.127	2.502	6.206
C	-0.394	1.186	7.537
C	0.200	-0.180	7.140
P	-0.856	-1.081	5.863
C	0.266	-1.397	4.619
C	-0.016	-2.087	3.363
C	-1.234	-2.767	3.126
C	-1.509	-3.386	1.897
C	-0.524	-3.331	0.883
C	0.699	-2.671	1.080
C	0.941	-2.065	2.337
C	-2.798	-4.045	1.705
P	-3.405	-4.671	0.240
C	-5.079	-5.366	0.766
C	-6.245	-4.793	-0.064
P	-6.688	-3.025	0.435
C	-6.460	-2.175	-1.025
C	-6.657	-0.743	-1.232
C	-7.249	0.092	-0.257
C	-7.396	1.473	-0.463
C	-6.961	2.019	-1.693
C	-6.369	1.222	-2.684
C	-6.237	-0.163	-2.439
C	-5.899	1.850	-3.917
P	-4.968	1.099	-5.133
C	-4.740	2.482	-6.398
C	-3.259	2.656	-6.787
P	-2.303	3.648	-5.487
C	-0.647	2.828	-5.566
C	0.536	3.450	-5.392
C	1.835	2.667	-5.284
C	2.482	2.954	-3.945

C	2.714	4.435	-3.701
C	1.394	5.169	-3.835
C	0.714	4.940	-5.174
C	0.796	5.879	-2.860
P	1.404	6.043	-1.127
C	1.092	7.874	-0.775
C	0.833	8.125	0.723
P	-0.906	7.593	1.231
C	-0.606	6.537	2.537
C	2.750	2.047	-2.986
P	2.252	0.294	-2.815
C	3.907	-0.572	-2.496
C	3.724	-1.939	-1.809
P	3.120	-1.729	-0.032
C	1.646	-2.590	-0.027
C	-7.979	2.288	0.597
P	-7.968	3.990	0.686
C	-8.911	4.333	2.283
C	-8.149	5.290	3.223
P	-6.664	4.454	4.041
C	-5.369	5.418	3.487
N	0.405	1.000	0.270
B	-0.709	2.192	0.398
H	-1.984	-2.804	3.919
H	1.324	-3.103	-0.940
H	-0.720	-3.812	-0.077
H	-3.423	-4.091	2.605
H	-5.025	-6.457	0.607
H	-5.239	-5.202	1.843
H	-7.146	-5.403	0.112
H	-6.026	-4.840	-1.142
H	-0.174	6.338	-3.084
H	-6.095	-2.717	-1.906
H	-7.593	-0.345	0.682
H	-8.419	1.719	1.424
H	-9.150	3.385	2.788
H	-9.868	4.797	1.990
H	-7.829	6.198	2.689
H	-8.824	5.608	4.034
H	-5.580	6.252	2.808
H	-3.339	6.732	2.372
H	-0.130	4.691	4.402
H	-2.550	2.550	6.440
H	-1.464	1.099	7.780
H	0.117	1.548	8.444
H	1.233	-0.074	6.774
H	0.233	-0.832	8.029
H	1.291	-1.022	4.715
H	0.902	9.207	0.924
H	1.589	7.628	1.351
H	0.428	6.332	2.834
H	1.986	8.427	-1.102
H	0.245	8.235	-1.379
H	-7.088	3.088	-1.878
H	-6.155	2.912	-4.016
H	-5.174	3.424	-6.028
H	-5.318	2.187	-7.289
H	-2.785	1.673	-6.941
H	-3.183	3.210	-7.735
H	-0.640	1.737	-5.679
H	3.163	4.608	-2.714
H	3.183	2.428	-2.053
H	4.490	0.102	-1.850
H	4.467	-0.674	-3.437
H	3.043	-2.593	-2.376
H	4.700	-2.448	-1.759
H	1.656	1.595	-5.436
H	-0.247	5.465	-5.226
H	-5.792	-0.800	-3.207

H	1.894	-1.559	2.512
H	-4.228	3.665	5.269
H	0.521	0.649	-0.691
H	1.331	1.340	0.563
H	-1.790	1.698	0.142
H	-0.378	3.053	-0.397
H	-0.647	2.579	1.560
H	0.180	0.193	0.863
H	2.524	3.010	-6.081
H	2.077	-0.074	-4.189
H	1.365	5.331	-5.981
H	-2.774	2.866	-4.372
H	3.409	4.827	-4.470
H	0.187	5.579	-0.515
B	3.207	2.973	2.260
N	2.196	3.514	1.462
H	2.373	4.163	0.694
H	1.194	3.359	1.607
H	4.354	3.244	2.016
H	2.906	2.232	3.160
B	-6.270	7.319	-2.205
N	-5.810	6.281	-1.392
H	-4.829	6.028	-1.312
H	-6.421	5.705	-0.812
H	-7.450	7.552	-2.237
H	-5.476	7.950	-2.853
B	1.784	3.671	-9.479
N	0.567	3.123	-9.069
H	0.249	3.115	-8.100
H	-0.092	2.697	-9.714
H	2.508	4.158	-8.650
H	2.079	3.639	-10.644

[P-cage-3H₂-TS-1][3 NH₂BH₂]

C	-1.810	3.775	4.001
C	-2.564	3.396	5.241
C	-3.869	3.905	5.423
C	-4.458	4.821	4.545
C	-3.632	5.384	3.515
C	-2.349	4.960	3.250
C	-1.964	2.579	6.205
P	-0.623	1.471	5.939
C	0.274	1.466	7.602
C	1.255	0.305	7.803
P	0.444	-1.401	7.693
C	0.910	-1.905	5.981
C	0.149	-2.652	5.158
C	-1.203	-3.219	5.520
C	-2.204	-3.087	4.378
C	-1.801	-2.081	3.325
C	-0.449	-2.448	2.732
C	0.579	-2.949	3.740
C	-3.349	-3.791	4.346
P	-4.631	-3.674	3.024
C	-6.030	-4.654	3.825
C	-7.387	-4.386	3.150
P	-8.017	-2.640	3.507
C	-8.187	-2.005	1.933
C	-8.578	-0.645	1.576
C	-8.873	0.344	2.544
C	-9.175	1.665	2.179
C	-9.202	1.990	0.802
C	-8.923	1.035	-0.186
C	-8.616	-0.283	0.222
C	-8.922	1.436	-1.590

P	-8.559	0.433	-2.921	H	0.535	-0.284	-2.447	C	0.274	-1.945	3.946
C	-8.707	1.629	-4.375	H	1.443	-2.358	-2.420	C	-0.995	-2.504	3.739
C	-7.414	1.670	-5.217	H	0.605	-3.788	-3.049	C	-2.164	-1.708	3.713
P	-6.025	2.630	-4.371	H	-0.063	-4.388	-0.617	C	-2.030	-0.325	3.912
C	-4.839	1.425	-4.145	H	1.652	-4.523	-1.029	C	1.435	-2.829	3.967
C	-3.523	1.612	-3.538	H	-3.038	-0.490	-3.648	P	3.077	-2.370	4.048
C	-2.691	0.498	-3.338	H	-3.672	3.761	-3.302	C	3.919	-4.060	4.181
C	-1.400	0.627	-2.775	H	-8.385	-1.036	-0.535	C	5.289	-4.116	3.479
C	-0.945	1.909	-2.430	H	0.683	-4.045	3.614	P	5.172	-4.223	1.593
C	-1.763	3.051	-2.592	H	-4.430	3.584	6.305	C	5.806	-2.671	1.101
C	-3.039	2.883	-3.152	H	0.492	0.553	3.060	C	5.453	-2.114	-0.146
C	-1.340	4.389	-2.196	H	1.171	2.060	2.811	C	5.656	-0.737	-0.404
P	0.107	4.830	-1.414	H	-1.755	1.099	2.142	C	5.074	-0.098	-1.503
C	-0.091	6.688	-1.185	H	-0.772	2.826	1.440	C	4.302	-0.875	-2.414
C	-0.218	7.093	0.298	H	-1.801	2.867	3.242	C	4.082	-2.236	-2.245
P	-1.915	6.694	1.039	H	0.100	1.721	4.331	C	4.620	-2.880	-1.063
C	-1.485	5.582	2.279	H	1.574	-2.521	3.543	C	3.324	-3.038	-3.191
C	-0.529	-0.522	-2.548	H	1.498	-2.104	8.374	P	2.380	-2.442	-4.488
P	-1.032	-2.142	-2.372	H	-1.095	-4.284	5.792	C	1.752	-4.031	-5.292
C	0.614	-3.054	-2.225	H	-5.153	-2.369	3.337	C	0.269	-3.902	-5.685
C	0.825	-3.806	-0.901	H	-1.729	-1.088	3.814	P	-0.846	-3.813	-4.168
P	1.374	-2.696	0.536	H	1.837	-3.767	1.374	C	-1.821	-2.449	-4.481
C	-0.211	-2.370	1.409	B	-3.817	-5.881	-1.006	C	5.182	1.333	-1.743
C	-9.408	2.653	3.228	N	-3.661	-4.580	-0.525	P	5.754	2.524	-0.660
P	-9.617	4.333	3.019	H	-3.920	-4.295	0.421	C	5.432	4.102	-1.649
C	-9.771	4.928	4.804	H	-3.279	-3.823	-1.088	C	4.241	4.909	-1.098
C	-8.526	5.707	5.282	H	-3.485	-6.133	-2.136	P	2.575	4.084	-1.435
P	-7.055	4.572	5.642	H	-4.277	-6.721	-0.276	C	1.494	5.073	-0.316
C	-5.828	5.271	4.669	B	3.482	3.126	1.423	C	-3.493	-2.274	3.503
B	-0.887	1.922	2.216	N	3.229	3.402	0.083	P	-3.857	-3.908	3.174
N	0.306	1.562	3.055	H	3.942	3.325	-0.635	C	-5.738	-3.874	3.026
H	-1.584	-2.711	6.421	H	2.325	3.713	-0.279	C	-6.234	-4.124	1.584
H	-1.009	-1.997	0.756	H	2.581	3.259	2.219	P	-6.124	-2.582	0.502
H	-2.553	-1.992	2.529	H	4.575	2.770	1.772	C	-4.962	-3.041	-0.658
H	-3.547	-4.514	5.145	B	-3.322	-1.828	10.447	N	-0.469	-6.110	-1.191
H	-5.770	-5.720	3.729	N	-2.999	-1.375	9.166	B	-0.532	-7.505	-1.223
H	-6.078	-4.420	4.900	H	-2.056	-1.416	8.772	H	1.346	-0.099	4.333
H	-8.133	-5.088	3.557	H	-3.682	-0.972	8.532	H	-4.312	-1.547	3.557
H	-7.332	-4.558	2.064	H	-4.460	-1.741	10.829	H	-2.927	0.298	3.916
H	-2.071	5.178	-2.409	H	-2.451	-2.293	11.135	H	0.396	2.015	4.656
H	-7.956	-2.649	1.075	[P-pore-4H₂][4 NH₂BH₂]				H	-0.524	4.195	5.883
H	-8.838	0.082	3.604	C	-4.990	-0.936	-2.045	H	-0.057	4.615	4.227
H	-9.399	2.244	4.245	C	-4.490	-0.152	-3.095	H	-1.434	6.367	5.730
H	-9.981	4.076	5.468	C	-3.447	-0.682	-3.890	H	-2.836	5.399	5.316
H	-10.650	5.593	4.837	C	-2.899	-1.950	-3.635	H	-1.621	-1.851	-5.378
H	-8.239	6.481	4.554	C	-3.430	-2.707	-2.565	H	-3.359	5.006	2.301
H	-8.772	6.224	6.225	C	-4.466	-2.217	-1.756	H	-0.000	6.469	1.289
H	-6.093	6.113	4.018	C	-5.078	1.162	-3.334	H	1.952	5.461	0.600
H	-4.029	6.234	2.952	P	-4.457	2.396	-4.336	H	4.356	5.087	-0.017
H	-0.737	3.890	4.229	C	-5.844	3.675	-4.232	H	4.202	5.894	-1.590
H	-2.446	2.528	7.188	C	-5.380	5.125	-4.025	H	5.288	3.861	-2.713
H	-0.509	1.442	8.376	P	-4.758	5.494	-2.277	H	6.343	4.717	-1.574
H	0.805	2.423	7.711	C	-2.932	5.348	-2.477	H	4.784	1.659	-2.712
H	2.092	0.364	7.090	C	-2.074	4.913	-1.534	H	3.890	-0.377	-3.296
H	1.692	0.375	8.811	C	-0.578	4.882	-1.772	H	4.858	-3.947	-1.167
H	1.881	-1.552	5.613	C	0.197	5.348	-0.546	H	6.317	-2.028	1.824
H	-0.087	8.185	0.377	C	-0.619	6.157	0.437	H	5.907	-3.247	3.755
H	0.577	6.632	0.904	C	-1.859	5.414	0.900	H	5.823	-5.022	3.806
H	-0.432	5.278	2.340	C	-2.449	4.465	-0.142	H	3.247	-4.849	3.812
H	0.808	7.156	-1.617	C	-2.433	5.562	2.111	H	4.068	-4.244	5.258
H	-0.956	7.041	-1.767	P	-2.042	6.762	3.445	H	1.188	-3.896	3.914
H	-9.432	3.016	0.502	C	-1.824	5.670	4.971	H	2.356	-4.206	-6.198
H	-9.158	2.493	-1.763	C	-0.920	4.430	4.883	H	1.912	-4.889	-4.621
H	-8.984	2.633	-4.019	P	-1.848	2.889	4.291	H	3.347	-4.119	-3.004
H	-9.535	1.265	-5.006	C	-0.620	1.708	4.383	H	-0.040	-4.790	-6.260
H	-7.075	0.654	-5.470	C	-0.769	0.277	4.132	H	0.102	-3.022	-6.325
H	-7.617	2.193	-6.166	C	0.367	-0.547	4.147	H	-0.279	3.850	-2.026
H	-5.054	0.397	-4.459					H	-2.519	5.674	-3.439
H	0.054	2.023	-2.007					H	-4.613	5.409	-4.763

H	-6.237	5.799	-4.178
H	-6.566	3.381	-3.455
H	-6.368	3.611	-5.201
H	-6.003	1.352	-2.777
H	-3.036	-3.708	-2.373
H	-4.505	-4.035	-0.590
H	-5.693	-4.961	1.116
H	-7.300	-4.402	1.616
H	-6.134	-2.927	3.424
H	-6.111	-4.681	3.678
H	-5.809	-0.546	-1.436
H	-3.066	-0.095	-4.730
H	-3.536	4.376	-0.019
H	-1.085	-3.585	3.601
H	6.263	-0.159	0.296
H	3.619	-3.724	0.755
H	3.577	-3.290	-0.086
H	-0.588	-5.518	-2.013
H	-0.298	-5.582	-0.340
H	-0.376	-8.121	-0.201
H	-0.739	-8.053	-2.275
H	-0.948	7.086	-0.070
H	-0.641	6.942	3.176
H	-0.316	5.501	-2.645
H	2.768	2.961	-0.558
H	-2.015	3.459	0.018
H	-4.819	6.925	-2.423
B	4.492	5.719	6.573
N	5.756	5.593	7.152
H	4.143	6.798	6.172
H	3.792	4.744	6.493
H	6.404	6.368	7.255
H	6.121	4.716	7.512
B	-8.242	3.443	-0.175
N	-7.361	4.475	0.145
H	-9.163	3.200	0.558
H	-8.055	2.818	-1.189
H	-6.560	4.735	-0.436
H	-7.458	5.046	0.980
B	2.290	5.177	-5.840
N	1.991	4.030	-5.103
H	1.640	3.176	-5.525
H	2.105	3.965	-4.087
H	2.129	5.168	-7.033
H	2.701	6.149	-5.259

[P-cage-4H₂-TS-2][4 NH₂BH₂]

C	-4.990	-0.936	-2.045
C	-4.490	-0.152	-3.095
C	-3.447	-0.682	-3.890
C	-2.899	-1.950	-3.635
C	-3.430	-2.707	-2.565
C	-4.466	-2.217	-1.756
C	-5.078	1.162	-3.334
P	-4.457	2.396	-4.336
C	-5.844	3.675	-4.232
C	-5.380	5.125	-4.025
P	-4.758	5.494	-2.277
C	-2.932	5.348	-2.477
C	-2.074	4.913	-1.534
C	-0.578	4.882	-1.772
C	0.197	5.348	-0.546
C	-0.619	6.157	0.437
C	-1.859	5.414	0.900
C	-2.449	4.465	-0.142
C	-2.433	5.562	2.111
P	-2.042	6.762	3.445

C	-1.824	5.670	4.971
C	-0.920	4.430	4.883
P	-1.848	2.889	4.291
C	-0.620	1.708	4.383
C	-0.769	0.277	4.132
C	0.367	-0.547	4.147
C	0.274	-1.945	3.946
C	-0.995	-2.504	3.739
C	-2.164	-1.708	3.713
C	-2.030	-0.325	3.912
C	1.435	-2.829	3.967
P	3.077	-2.370	4.048
C	3.919	-4.060	4.181
C	5.289	-4.116	3.479
P	5.172	-4.223	1.593
C	5.806	-2.671	1.101
C	5.453	-2.114	-0.146
C	5.656	-0.737	-0.404
C	5.074	-0.098	-1.503
C	4.302	-0.875	-2.414
C	4.082	-2.236	-2.245
C	4.620	-2.880	-1.063
C	3.324	-3.038	-3.191
P	2.380	-2.442	-4.488
C	1.752	-4.031	-5.292
C	0.269	-3.902	-5.685
P	-0.846	-3.813	-4.168
C	-1.821	-2.449	-4.481
C	5.182	1.333	-1.743
P	5.754	2.524	-0.660
C	5.432	4.102	-1.649
C	4.241	4.909	-1.098
P	2.575	4.084	-1.435
C	1.494	5.073	-0.316
C	-3.493	-2.274	3.503
P	-3.857	-3.908	3.174
C	-5.738	-3.874	3.026
C	-6.234	-4.124	1.584
P	-6.124	-2.582	0.502
C	-4.962	-3.041	-0.658
N	-0.469	-6.110	-1.191
B	-0.532	-7.505	-1.223
H	1.346	-0.099	4.333
H	-4.312	-1.547	3.557
H	-2.927	0.298	3.916
H	0.396	2.015	4.656
H	-0.524	4.195	5.883
H	-0.057	4.615	4.227
H	-1.434	6.367	5.730
H	-2.836	5.399	5.316
H	-1.621	-1.851	-5.378
H	-3.359	5.006	2.301
H	-0.000	6.469	1.289
H	1.952	5.461	0.600
H	4.356	5.087	-0.017
H	4.202	5.894	-1.590
H	5.288	3.861	-2.713
H	6.343	4.717	-1.574
H	4.784	1.659	-2.712
H	3.890	-0.377	-3.296
H	4.858	-3.947	-1.167
H	6.317	-2.028	1.824
H	5.907	-3.247	3.755
H	5.823	-5.022	3.806
H	3.247	-4.849	3.812
H	4.068	-4.244	5.258
H	1.188	-3.896	3.914
H	2.356	-4.206	-6.198
H	1.912	-4.889	-4.621

H	3.347	-4.119	-3.004
H	-0.040	-4.790	-6.260
H	0.102	-3.022	-6.325
H	-0.279	3.850	-2.026
H	-2.519	5.674	-3.439
H	-4.613	5.409	-4.763
H	-6.237	5.799	-4.178
H	-6.566	3.381	-3.455
H	-6.368	3.611	-5.201
H	-6.003	1.352	-2.777
H	-3.036	-3.708	-2.373
H	-4.505	-4.035	-0.590
H	-5.693	-4.961	1.116
H	-7.300	-4.402	1.616
H	-6.134	-2.927	3.424
H	-6.111	-4.681	3.678
H	-5.809	-0.546	-1.436
H	-3.066	-0.095	-4.730
H	-3.536	4.376	-0.019
H	-1.085	-3.585	3.601
H	6.263	-0.159	0.296
H	3.619	-3.724	0.755
H	3.577	-3.290	-0.086
H	-0.588	-5.518	-2.013
H	-0.298	-5.582	-0.340
H	-0.376	-8.121	-0.201
H	-0.739	-8.053	-2.275
H	-0.948	7.086	-0.070
H	-0.641	6.942	3.176
H	-0.316	5.501	-2.645
H	2.768	2.961	-0.558
H	-2.015	3.459	0.018
H	-4.819	6.925	-2.423
B	4.492	5.719	6.573
N	5.756	5.593	7.152
H	4.143	6.798	6.172
H	3.792	4.744	6.493
H	6.404	6.368	7.255
H	6.121	4.716	7.512
B	-8.242	3.443	-0.175
N	-7.361	4.475	0.145
H	-9.163	3.200	0.558
H	-8.055	2.818	-1.189
H	-6.560	4.735	-0.436
H	-7.458	5.046	0.980
B	2.290	5.177	-5.840
N	1.991	4.030	-5.103
H	1.640	3.176	-5.525
H	2.105	3.965	-4.087
H	2.129	5.168	-7.033
H	2.701	6.149	-5.259

P-cage-TS-1^r

C	-4.008	0.954	-3.100
C	-4.335	-0.415	-3.227
C	-3.305	-1.359	-3.092
C	-1.972	-0.973	-2.818
C	-1.688	0.395	-2.690
C	-2.699	1.376	-2.818
C	-5.695	-0.878	-3.488
P	-7.105	0.080	-3.493
C	-8.442	-1.185	-3.909
C	-9.549	-1.245	-2.837
P	-8.995	-2.148	-1.273
C	-9.282	-0.977	-0.067
C	-9.053	-1.134	1.366

C	-9.206	-0.022	2.208
C	-8.984	-0.109	3.602
C	-8.613	-1.351	4.141
C	-8.448	-2.495	3.325
C	-8.682	-2.369	1.947
C	-8.053	-3.795	3.862
P	-7.501	-4.115	5.443
C	-7.243	-5.986	5.397
C	-5.809	-6.404	5.782
P	-4.572	-6.091	4.391
C	-3.388	-5.144	5.171
C	-2.174	-4.605	4.563
C	-1.422	-3.655	5.270
C	-0.270	-3.055	4.709
C	0.122	-3.446	3.420
C	-0.603	-4.408	2.680
C	-1.740	-4.981	3.270
C	0.494	-2.019	5.393
P	0.213	-1.393	6.956
C	1.498	-0.009	7.038
C	0.833	1.378	7.118
P	-0.216	1.761	5.591
C	-1.373	2.922	6.206
C	-2.183	3.642	5.300
C	-1.625	4.045	4.003
C	-2.507	4.737	3.060
C	-3.846	4.904	3.371
C	-4.384	4.512	4.638
C	-3.528	3.957	5.596
C	-5.806	4.698	4.878
P	-6.720	3.932	6.102
C	-8.444	4.648	5.822
C	-9.510	3.542	5.687
P	-9.422	2.652	4.023
C	-9.132	1.038	4.493
C	-1.928	5.206	1.811
P	-2.771	5.487	0.349
C	-1.387	6.084	-0.791
C	-1.437	5.362	-2.151
P	-1.044	3.520	-1.990
C	-2.438	2.803	-2.664
C	-0.220	-4.805	1.327
P	1.010	-4.094	0.384
C	0.936	-5.109	-1.204
C	0.719	-4.227	-2.451
P	-1.068	-3.642	-2.618
C	-0.893	-1.946	-2.671
N	0.046	2.445	2.548
B	1.359	2.642	3.296
H	-1.749	-3.351	6.267
H	-0.819	-5.619	0.902
H	-2.311	-5.727	2.712
H	-3.540	-4.856	6.219
H	-5.792	-7.489	5.980
H	-5.481	-5.900	6.704
H	-7.950	-6.412	6.129
H	-7.521	-6.383	4.409
H	-3.263	3.453	-2.982
H	-8.100	-4.618	3.139
H	-8.453	-1.438	5.218
H	-9.015	0.806	5.558
H	-9.433	2.815	6.509
H	-10.513	3.996	5.745
H	-8.445	5.313	4.944
H	-8.678	5.270	6.702
H	-6.320	5.336	4.149
H	-4.508	5.395	2.654
H	-0.637	4.523	4.112
H	-1.597	2.948	7.276

H	0.164	1.444	7.990
H	1.594	2.164	7.236
H	2.173	-0.073	6.172
H	2.105	-0.173	7.943
H	1.310	-1.594	4.797
H	-1.526	7.167	-0.946
H	-0.409	5.948	-0.304
H	-0.837	5.325	1.821
H	-0.681	5.797	-2.826
H	-2.418	5.492	-2.631
H	-9.506	0.934	1.775
H	-9.652	0.011	-0.363
H	-9.914	-0.238	-2.585
H	-10.407	-1.812	-3.238
H	-7.991	-2.176	-4.071
H	-8.885	-0.867	-4.868
H	-5.783	-1.957	-3.661
H	-0.660	0.711	-2.499
H	0.106	-1.508	-2.563
H	1.405	-3.365	-2.453
H	0.936	-4.819	-3.355
H	0.160	-5.887	-1.126
H	1.907	-5.624	-1.293
H	-3.539	-2.420	-3.207
H	-4.795	1.703	-3.218
H	-8.572	-3.248	1.307
H	1.014	-2.995	2.977
H	-3.923	3.710	6.585
H	2.094	1.682	3.348
H	1.838	3.743	3.144
H	-0.242	1.474	2.406
H	-0.029	2.940	1.657
H	-0.971	3.072	3.304
H	0.967	2.629	4.645

[P-cage-H₂-TS-1^r][NH₂BH₂]

C	-3.356	4.801	5.791
C	-2.067	4.097	5.415
C	-1.529	4.299	4.089
C	-2.351	4.995	3.086
C	-3.690	5.236	3.327
C	-4.288	5.066	4.620
C	-1.388	3.317	6.324
P	-0.383	1.965	5.746
C	0.772	1.646	7.208
C	1.578	0.346	7.037
P	0.433	-1.144	6.856
C	0.931	-1.799	5.362
C	0.321	-2.929	4.670
C	-0.778	-3.641	5.202
C	-1.403	-4.674	4.488
C	-0.888	-5.020	3.216
C	0.204	-4.339	2.656
C	0.802	-3.298	3.404
C	-2.579	-5.318	5.064
P	-3.619	-6.421	4.283
C	-4.915	-6.739	5.618
C	-6.312	-6.219	5.218
P	-6.471	-4.341	5.357
C	-6.976	-3.914	3.784
C	-7.304	-2.575	3.302
C	-7.380	-1.450	4.156
C	-7.707	-0.173	3.670
C	-7.968	-0.031	2.286
C	-7.908	-1.125	1.408
C	-7.575	-2.393	1.938

C	-8.216	-0.929	-0.006
P	-8.113	-2.113	-1.230
C	-8.701	-1.170	-2.756
C	-7.639	-1.130	-3.875
P	-6.284	0.130	-3.515
C	-4.879	-0.834	-3.484
C	-3.523	-0.357	-3.224
C	-3.220	1.017	-3.105
C	-1.926	1.464	-2.799
C	-0.899	0.502	-2.656
C	-1.155	-0.872	-2.790
C	-2.479	-1.283	-3.075
C	-0.053	-1.818	-2.643
P	-0.172	-3.519	-2.616
C	1.634	-4.038	-2.438
C	1.882	-4.909	-1.189
P	1.847	-3.893	0.401
C	0.661	-4.706	1.319
C	-1.699	2.896	-2.634
P	-0.403	3.632	-1.805
C	-0.789	5.466	-2.040
C	-0.893	6.214	-0.699
P	-2.391	5.663	0.311
C	-1.695	5.371	1.849
C	-7.819	0.935	4.612
P	-8.026	2.590	4.247
C	-8.353	3.271	5.982
C	-8.206	4.792	6.127
P	-6.492	5.528	6.388
C	-5.633	5.270	4.806
N	-0.154	2.413	2.661
B	1.191	2.414	3.385
N	-5.800	6.234	-1.147
B	-6.172	7.479	-1.657
H	-1.169	-3.361	6.183
H	0.148	-5.571	0.883
H	-1.362	-5.824	2.650
H	-2.812	-5.003	6.088
H	-4.966	-7.832	5.757
H	-4.588	-6.304	6.575
H	-7.063	-6.642	5.906
H	-6.582	-6.547	4.202
H	-2.491	3.533	-3.044
H	-7.058	-4.700	3.024
H	-7.196	-1.580	5.225
H	-7.768	0.632	5.665
H	-7.725	2.743	6.716
H	-9.399	3.000	6.203
H	-8.645	5.323	5.266
H	-8.779	5.131	7.005
H	-6.224	5.556	3.928
H	-4.313	5.656	2.533
H	-0.472	4.610	4.107
H	-1.609	3.371	7.396
H	0.114	1.579	8.091
H	1.436	2.507	7.369
H	2.256	0.412	6.173
H	2.199	0.183	7.933
H	1.752	-1.318	4.818
H	-1.007	7.294	-0.892
H	0.022	6.087	-0.103
H	-0.601	5.443	1.923
H	0.031	5.895	-2.638
H	-1.712	5.579	-2.628
H	-8.252	0.949	1.896
H	-8.531	0.087	-0.269
H	-9.024	-0.155	-2.478
H	-9.592	-1.706	-3.125
H	-7.202	-2.126	-4.046

H	-8.118	-0.816	-4.817
H	-4.965	-1.917	-3.633
H	0.120	0.839	-2.456
H	0.931	-1.352	-2.519
H	2.285	-3.150	-2.437
H	1.880	-4.623	-3.340
H	1.158	-5.736	-1.131
H	2.887	-5.359	-1.257
H	-2.692	-2.349	-3.187
H	-4.017	1.752	-3.238
H	-7.541	-3.257	1.270
H	1.653	-2.759	2.980
H	-3.102	5.784	6.237
H	1.738	1.349	3.510
H	1.843	3.414	3.209
H	-0.574	1.489	2.535
H	-0.150	2.891	1.755
H	-0.968	3.117	3.355
H	0.787	2.601	4.763
H	-3.876	4.236	6.579
H	-5.921	4.460	7.167
H	-4.905	6.055	-0.689
H	-6.398	5.414	-1.192
H	-5.403	8.400	-1.560
H	-7.250	7.599	-2.180

[P-cage-2H₂-TS-1^r][2 NH₂BH₂]

C	-2.953	-1.677	-2.002
C	-4.161	-0.963	-2.040
C	-4.115	0.441	-1.893
C	-2.903	1.119	-1.679
C	-1.707	0.363	-1.638
C	-1.710	-1.032	-1.808
C	-5.401	-1.699	-2.264
P	-6.992	-1.097	-2.166
C	-8.029	-2.595	-2.653
C	-9.066	-2.992	-1.583
P	-8.273	-3.852	-0.099
C	-8.635	-2.766	1.164
C	-8.237	-2.891	2.562
C	-8.451	-1.807	3.426
C	-8.035	-1.837	4.777
C	-7.409	-3.000	5.253
C	-7.185	-4.120	4.416
C	-7.612	-4.049	3.081
C	-6.518	-5.332	4.883
P	-5.739	-5.550	6.384
C	-5.158	-7.344	6.267
C	-3.641	-7.495	6.502
P	-2.617	-6.944	5.014
C	-1.664	-5.699	5.685
C	-0.674	-4.886	4.984
C	-0.137	-3.763	5.633
C	0.783	-2.905	4.988
C	1.183	-3.222	3.682
C	0.672	-4.349	2.997
C	-0.253	-5.168	3.662
C	1.285	-1.677	5.591
P	0.778	-0.970	7.057
C	1.793	0.622	7.069
C	0.896	1.867	7.174
P	-0.393	1.972	5.794
C	-1.400	3.337	6.349
C	-2.151	4.077	5.467
C	-3.448	4.747	5.893
C	-4.463	4.465	4.812
C	-4.091	5.073	3.479
C	-2.603	4.987	3.161

C	-1.743	4.248	4.089
C	-2.114	5.564	2.026
P	-3.029	6.700	0.921
C	-2.057	6.507	-0.685
C	-2.332	5.275	-1.555
P	-1.725	3.601	-0.920
C	-2.913	2.578	-1.596
C	-5.558	3.694	4.957
P	-6.056	2.815	6.497
C	-7.930	3.107	6.526
C	-8.735	1.823	6.817
P	-8.944	0.789	5.256
C	-8.207	-0.693	5.668
C	1.056	-4.651	1.621
P	2.200	-3.782	0.701
C	2.115	-4.638	-0.976
C	1.595	-3.680	-2.070
P	-0.276	-3.452	-2.010
C	-0.445	-1.763	-1.838
N	-0.533	2.336	2.603
B	0.874	2.356	3.181
N	-4.539	2.241	9.840
B	-4.807	2.943	11.016
N	-8.120	2.478	-1.777
B	-8.334	3.352	-2.845
H	-0.459	-3.532	6.651
H	0.534	-5.504	1.172
H	-0.658	-6.042	3.148
H	-1.811	-5.426	6.737
H	-3.408	-8.560	6.666
H	-3.322	-6.951	7.404
H	-5.700	-7.896	7.053
H	-5.456	-7.777	5.300
H	-3.807	3.043	-2.029
H	-6.510	-6.153	4.156
H	-7.088	-3.043	6.297
H	-7.799	-0.829	6.676
H	-8.280	1.230	7.625
H	-9.749	2.101	7.149
H	-8.244	3.552	5.569
H	-8.123	3.857	7.306
H	-6.192	3.527	4.077
H	-4.687	4.617	2.671
H	-0.680	4.523	4.009
H	-1.551	3.436	7.429
H	0.308	1.842	8.107
H	1.498	2.786	7.202
H	2.427	0.668	6.173
H	2.461	0.584	7.945
H	2.021	-1.143	4.977
H	-2.274	7.409	-1.278
H	-0.992	6.577	-0.411
H	-1.030	5.548	1.860
H	-1.809	5.402	-2.519
H	-3.405	5.199	-1.788
H	-8.933	-0.907	3.038
H	-9.189	-1.848	0.931
H	-9.650	-2.120	-1.251
H	-9.776	-3.710	-2.024
H	-7.368	-3.440	-2.900
H	-8.557	-2.314	-3.580
H	-5.261	-2.761	-2.498
H	-0.753	0.886	-1.533
H	0.450	-1.139	-1.747
H	2.103	-2.705	-2.018
H	1.816	-4.110	-3.061
H	1.499	-5.548	-0.917
H	3.141	-4.951	-1.228
H	-2.972	-2.759	-2.151

H	-5.039	1.018	-1.964
H	-7.446	-4.906	2.424
H	1.889	-2.564	3.170
H	-3.784	4.382	6.871
H	1.435	1.296	3.282
H	1.497	3.361	2.943
H	-0.954	1.407	2.522
H	-0.640	2.817	1.701
H	-1.288	3.044	3.352
H	0.598	2.553	4.621
H	-4.146	5.858	0.567
H	-4.368	6.147	3.491
H	-8.217	2.937	-3.968
H	-8.626	4.497	-2.612
H	-8.207	2.758	-0.805
H	-7.875	1.493	-1.892
H	-6.132	1.511	5.893
H	-3.294	5.841	5.959
H	-4.919	2.496	8.925
H	-3.950	1.414	9.811
H	-4.319	2.565	12.049
H	-5.522	3.911	10.965

NH₂BH₂

N	0.324	0.183	0.019
B	0.244	-0.244	1.347
H	1.097	0.104	2.120
H	-0.673	-0.947	1.674
H	-0.357	-0.068	-0.690
H	1.068	0.778	-0.331

