Diboryne Nanostructures Stabilized by Multitopic N-Heterocyclic Carbenes: A Computational Study

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Supporting Information

DFT results and the structures and coordinates of diboryne nanomaterials

1 Preliminary Tests on the DFT Functionals

In this section, we show the DFT preliminary tests on selected energetic and structural properties of LBBL systems without periodic boundary conditions. Due to the lack of experimental data on such systems, the energetic parameters are compared to the average of the functionals. We have made calculations for seven functionals: B3LYP, PBE0, BHandHLYP, M06, M06-L, M06-HF and M06-2X, and for two distinct basis sets: 6-311G** and cc-pVTZ(-f). All calculations were performed with the Jaguar 7.9 program.[1] The results are summarized in Figure S1.

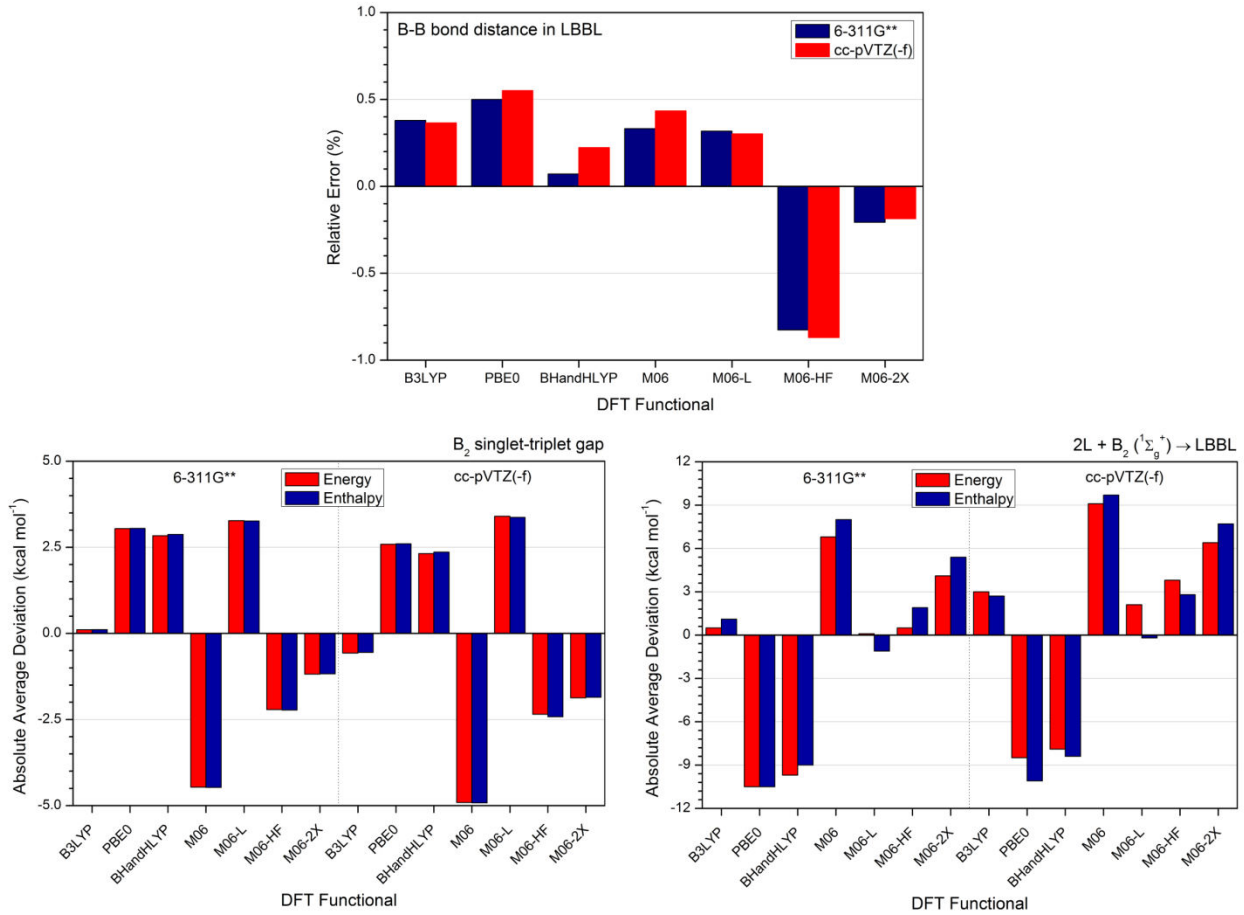


Figure S1. DFT Functionals.

Figure S1 (top panel) shows the relative error of the B-B bond length in the LBBL molecule (L = imidazolylidene, IY, **1**) in comparison to the experimental result obtained by Braunschweig and co-workers.[2] Among the functionals studied in this work, BHandHLYP has given the best result related to this geometrical property, followed by M06-2X. The functionals B3LYP, M06 and M06-L have also furnished satisfactory results, as the relative errors are smaller than 0.5%. Finally, PBE0 and M06-HF gave the worst results, although still acceptable, since in these cases the errors are smaller than 1%. These results are not critically dependent on the basis set.

Figure S1 (bottom left panel) shows the absolute average deviation of the DFT functionals with respect to the calculated singlet-triplet (S-T) gap of B_2. It is possible to see that B3LYP behaves quite close to the average value among the functionals. Furthermore, PBE0, BHandHLYP and M06-L values are

similar, around 2.5 kcal mol^{-1} above the average. The other M06 functionals give S-T gaps lower than the average, whose deviation from such reference value decreases in the following order: M06, M06-HF and M06-2X. The S-T gap calculated with the latter M06 functional is quite similar to the B3LYP result. Again, the choice of the basis set among the ones studied in this work does not influence significantly the result.

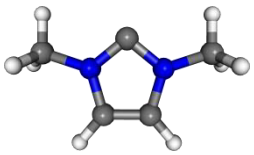
Finally, Figure S1 (bottom right panel) shows the absolute average deviation of the DFT functionals with respect to the calculated energy (and enthalpy) of formation of the LBBL species from isolated L and B_2 ($^1\Sigma_g^+$) units. Once more, the B3LYP functional stands as one of the functionals whose calculated energy is close to the average of the functionals studied herein. The PBE0 and BHandHLYP functionals have energy values around 10 kcal mol^{-1} smaller than the average, while the pure M06 functional is, among the M06 suite of functionals, the one in which the deviation from average is the largest.

From these preliminary tests, we have concluded that the B3LYP/6-311G** level of theory is a good choice for the calculations performed in this work.

2 Energy and structures of diboryne nanowires

2.1 Ligands

Ligand 1

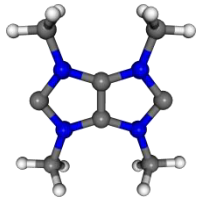


Total enthalpy, Htot (Utot + pV): -304.741191 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -304.779362 hartrees

XYZ Coordinates

C	0.0000000000	0.0000000000	0.9819613761
N	-1.0543761631	0.1305710867	0.1213775386
N	1.0543761631	-0.1305710867	0.1213775386
C	-0.6718347316	0.0836489178	-1.2144930759
C	0.6718347316	-0.0836489178	-1.2144930759
C	-2.4248325926	0.2992579174	0.5757349285
C	2.4248325926	-0.2992579174	0.5757349285
H	-2.4082486641	0.2999247676	1.6633877772
H	-3.0567634184	-0.5208170613	0.2235338196
H	-2.8404115543	1.2460634935	0.2195161977
H	2.4082486641	-0.2999247676	1.6633877772
H	3.0567634184	0.5208170613	0.2235338196
H	2.8404115543	-1.2460634935	0.2195161977
H	-1.3672944953	0.1681228898	-2.0333389390
H	1.3672944953	-0.1681228898	-2.0333389390

Ligand 2

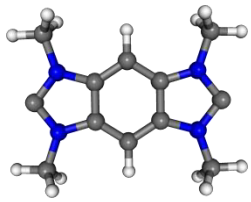


Total enthalpy, Htot (Utot + pV): -530.877719 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -530.928919 hartrees

XYZ Coordinates

N	-1.326819250	-1.088160351	0.000000000
C	-2.171768930	0.000000000	0.000000000
N	-1.326819250	1.088160351	0.000000000
C	0.000000000	0.675952158	0.000000000
C	0.000000000	-0.675952158	0.000000000
N	1.326819250	-1.088160351	0.000000000
C	2.171768930	0.000000000	0.000000000
N	1.326819250	1.088160351	0.000000000
C	-1.817918337	-2.455526720	0.000000000
C	1.817918337	-2.455526720	0.000000000
C	1.817918337	2.455526720	0.000000000
C	-1.817918337	2.455526720	0.000000000
H	-2.904426691	-2.401604237	0.000000000
H	-1.482767767	-2.994020299	0.890738244
H	-1.482767767	-2.994020299	-0.890738244
H	1.482767767	-2.994020299	-0.890738244
H	1.482767767	-2.994020299	0.890738244
H	2.904426691	-2.401604237	0.000000000
H	2.904426691	2.401604237	0.000000000
H	1.482767767	2.994020299	0.890738244
H	1.482767767	2.994020299	-0.890738244
H	-2.904426691	2.401604237	0.000000000
H	-1.482767767	2.994020299	-0.890738244
H	-1.482767767	2.994020299	0.890738244

Ligand 3



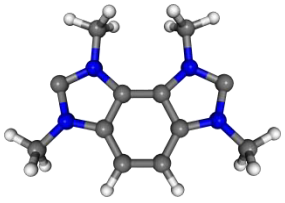
Total enthalpy, Htot (Utot + pV): -684.551935 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -684.606615 hartrees

XYZ Coordinates

C	0.000000000	3.366662731	0.000000000
N	0.000000000	2.519548387	-1.074734227
N	0.000000000	2.519548387	1.074734227
C	0.000000000	2.989204325	2.447544537
H	0.000000000	4.076508041	2.418474380
H	0.890167823	2.640196780	2.979950530
H	-0.890167823	2.640196780	2.979950530
H	0.000000000	4.076508041	-2.418474380
C	0.000000000	2.989204325	-2.447544537
H	0.890167823	2.640196780	-2.979950530
H	-0.890167823	2.640196780	-2.979950530
C	0.000000000	1.174920680	-0.705527603
C	0.000000000	1.174920680	0.705527603
H	0.000000000	0.000000000	2.536120646
C	0.000000000	0.000000000	1.453858891
C	0.000000000	0.000000000	-1.453858891
H	0.000000000	0.000000000	-2.536120646
C	0.000000000	-1.174920680	-0.705527603
C	0.000000000	-1.174920680	0.705527603
N	0.000000000	-2.519548387	1.074734227
N	0.000000000	-2.519548387	-1.074734227
C	0.000000000	-3.366662731	0.000000000
C	0.000000000	-2.989204325	2.447544537
H	0.890167823	-2.640196780	2.979950530
H	-0.890167823	-2.640196780	2.979950530
H	0.000000000	-4.076508041	2.418474380
C	0.000000000	-2.989204325	-2.447544537
H	0.890167823	-2.640196780	-2.979950530
H	-0.890167823	-2.640196780	-2.979950530
H	0.000000000	-4.076508041	-2.418474380

Ligand 4

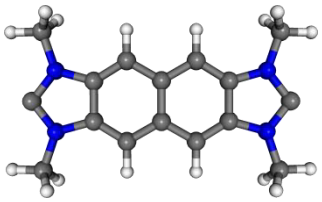


Total enthalpy, Htot (Utot + pV): -684.543405 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -684.598011 hartrees

XYZ Coordinates

C	0.704106377	0.000000000	0.350837713
C	-0.704106377	0.000000000	0.350837713
C	-1.355671437	0.000000000	-0.899837364
C	-0.693771610	0.000000000	-2.129571121
C	1.355671437	0.000000000	-0.899837364
C	0.693771610	0.000000000	-2.129571121
N	-1.739987460	0.000000000	1.295775023
C	-2.984318716	0.000000000	0.715299352
N	-2.720360295	0.000000000	-0.617695139
C	-1.627490979	0.000000000	2.744714184
C	-3.763808145	0.000000000	-1.627572338
H	-2.644570953	0.000000000	3.129358490
H	-1.107936234	-0.890873620	3.104298880
H	-1.107936234	0.890873620	3.104298880
H	-4.718160997	0.000000000	-1.106018557
H	-3.694438787	-0.889937472	-2.259971790
H	-3.694438787	0.889937472	-2.259971790
N	1.739987460	0.000000000	1.295775023
H	-1.249169004	0.000000000	-3.058750932
N	2.720360295	0.000000000	-0.617695139
H	1.249169004	0.000000000	-3.058750932
C	2.984318716	0.000000000	0.715299352
C	1.627490979	0.000000000	2.744714184
C	3.763808145	0.000000000	-1.627572338
H	2.644570953	0.000000000	3.129358490
H	1.107936234	0.890873620	3.104298880
H	1.107936234	-0.890873620	3.104298880
H	4.718160997	0.000000000	-1.106018557
H	3.694438787	-0.889937472	-2.259971790
H	3.694438787	0.889937472	-2.259971790

Ligand 5



Total enthalpy, Htot (Utot + pV): -838.177685 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -838.239914 hartrees

XYZ Coordinates

N	0.000000000	1.077307598	3.749036158
N	0.000000000	-1.077307598	3.749036158
C	0.000000000	0.000000000	4.592763017

C	0.000000000	0.709757991	2.402576112
C	0.000000000	-0.709757991	2.402576112
C	0.000000000	1.429019973	1.234466026
C	0.000000000	0.724466556	0.000000000
C	0.000000000	-0.724466556	0.000000000
C	0.000000000	-1.429019973	1.234466026
C	0.000000000	2.450096652	4.219000824
C	0.000000000	-2.450096652	4.219000824
C	0.000000000	1.429019973	-1.234466026
C	0.000000000	0.709757991	-2.402576112
C	0.000000000	-0.709757991	-2.402576112
C	0.000000000	-1.429019973	-1.234466026
N	0.000000000	1.077307598	-3.749036158
N	0.000000000	-1.077307598	-3.749036158
C	0.000000000	0.000000000	-4.592763017
C	0.000000000	2.450096652	-4.219000824
C	0.000000000	-2.450096652	-4.219000824
H	-0.889893178	2.981899839	3.868772382
H	0.000000000	2.421907138	5.306286627
H	0.889893178	2.981899839	3.868772382
H	-0.889893178	-2.981899839	3.868772382
H	0.000000000	-2.421907138	5.306286627
H	0.889893178	-2.981899839	3.868772382
H	0.000000000	2.421907138	-5.306286627
H	-0.889893178	2.981899839	-3.868772382
H	0.889893178	2.981899839	-3.868772382
H	0.000000000	-2.421907138	-5.306286627
H	-0.889893178	-2.981899839	-3.868772382
H	0.889893178	-2.981899839	-3.868772382
H	0.000000000	2.512786499	1.232473440
H	0.000000000	2.512786499	-1.232473440
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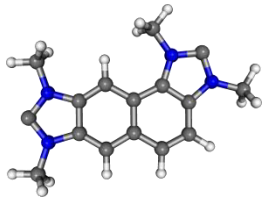
H	0.000000000	-2.512786499	1.232473440

Ligand 6

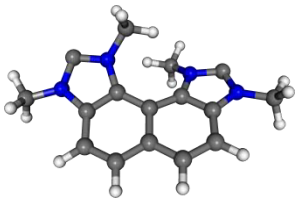


Total enthalpy, Htot (Utot + pV): -838.175997 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -838.237792 hartrees

XYZ Coordinates

C	1.985057376	0.615789693	0.000000000
C	0.671585983	1.025405154	0.000000000
C	-0.347008836	0.037883695	0.000000000
C	0.018590783	-1.363594055	0.000000000
C	2.342388264	-0.752757281	0.000000000
C	1.385950148	-1.737703999	0.000000000
C	-1.746890223	0.313274529	0.000000000
C	-2.687271726	-0.711207845	0.000000000
C	-2.325716646	-2.072244118	0.000000000
C	-0.989453943	-2.374217587	0.000000000
N	3.192994634	1.312126168	0.000000000
C	4.283388090	0.482247908	0.000000000
N	3.737907601	-0.771887394	0.000000000
N	-2.498432786	1.495384777	0.000000000
C	-3.850183180	1.262561615	0.000000000
N	-3.934797597	-0.099435989	0.000000000
C	-5.202023849	-0.809255063	0.000000000
C	-1.992700868	2.859195470	0.000000000
C	3.303632222	2.758949379	0.000000000
C	4.538628903	-1.982295320	0.000000000
H	4.363348402	3.003905271	0.000000000
H	2.831924520	3.186282998	-0.890142365
H	2.831924520	3.186282998	0.890142365
H	5.583736501	-1.680956065	0.000000000
H	4.333617412	-2.585022613	-0.889908914
H	4.333617412	-2.585022613	0.889908914
H	1.651247976	-2.788456716	0.000000000
H	0.427796888	2.076593019	0.000000000
H	-0.670616968	-3.410600443	0.000000000
H	-3.077567294	-2.851887100	0.000000000
H	-5.990846708	-0.060391107	0.000000000
H	-5.297986822	-1.437887223	0.890037669
H	-5.297986822	-1.437887223	-0.890037669
H	-2.862882969	3.511740176	0.000000000
H	-1.393422236	3.059389876	0.892179692
H	-1.393422236	3.059389876	-0.892179692

Ligand 7



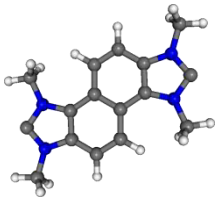
Total enthalpy, Htot (Utot + pV): -838.155066 hartrees

Total Gibbs free energy, Gtot (Htot - T*S): -838.216487 hartrees

XYZ Coordinates

C	-2.442749052	-0.042494377	0.568084575
C	-2.438705427	-0.222259114	1.963428398
C	-1.227353452	-0.134584765	2.605439483
C	0.000000000	0.000000000	1.895213817
C	0.000000000	0.000000000	0.451358628
C	-1.273789132	0.152708835	-0.162152345
C	1.273789132	-0.152708835	-0.162152345
C	2.442749052	0.042494377	0.568084575
C	2.438705427	0.222259114	1.963428398
C	1.227353452	0.134584765	2.605439483
N	3.492280668	-0.128664245	-0.330423597
C	3.067211078	-0.514794037	-1.566037587
N	1.696342810	-0.519424167	-1.451136003
C	4.897406030	0.015734357	0.010758473
C	0.926008162	-1.336869861	-2.393166309
H	-0.125338662	-1.064722210	-2.399252587
H	1.007052784	-2.391451248	-2.116903893
H	1.354439632	-1.200877579	-3.384349651
H	5.118036815	1.037228906	0.332785201
H	5.471604464	-0.215579747	-0.883468128
H	5.175907806	-0.676845500	0.810296030
H	-1.185749391	-0.183234584	3.687774895
N	-1.696342810	0.519424167	-1.451136003
N	-3.492280668	0.128664245	-0.330423597
H	-3.359419595	-0.362685854	2.515976621
C	-3.067211078	0.514794037	-1.566037587
C	-0.926008162	1.336869861	-2.393166309
C	-4.897406030	-0.015734357	0.010758473
H	-1.007052784	2.391451248	-2.116903893
H	0.125338662	1.064722210	-2.399252587
H	-1.354439632	1.200877579	-3.384349651
H	-5.175907806	0.676845500	0.810296030
H	-5.118036815	-1.037228906	0.332785201
H	-5.471604464	0.215579747	-0.883468128
H	1.185749391	0.183234584	3.687774895
H	3.359419595	0.362685854	2.515976621

Ligand 8

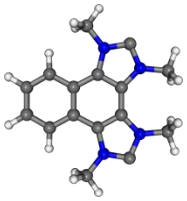


Total enthalpy, Htot (Utot + pV): -838.173307 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -838.233990 hartrees

XYZ Coordinates

C	-2.006423501	1.613188532	0.000000000
C	-1.878389882	0.244827954	0.000000000
C	-0.606390788	-0.395845694	0.000000000
C	0.606390788	0.395845694	0.000000000
C	0.432575625	1.809976819	0.000000000
C	-0.835701662	2.385345815	0.000000000
C	-0.432575625	-1.809976819	0.000000000
C	0.835701662	-2.385345815	0.000000000
C	2.006423501	-1.613188532	0.000000000
C	1.878389882	-0.244827954	0.000000000
N	-1.319280650	-2.895291255	0.000000000
C	-0.673056455	-4.106086824	0.000000000
N	0.646065914	-3.761524897	0.000000000
C	-2.774259724	-2.852999995	0.000000000
C	1.716793413	-4.742869409	0.000000000
N	-0.646065914	3.761524897	0.000000000
N	1.319280650	2.895291255	0.000000000
C	-1.716793413	4.742869409	0.000000000
C	2.774259724	2.852999995	0.000000000
H	-1.252256560	5.726405260	0.000000000
H	-2.343537500	4.636662910	-0.890137450
H	-2.343537500	4.636662910	0.890137450
H	3.111890454	3.886970356	0.000000000
H	3.155896099	2.349715342	-0.891933148
H	3.155896099	2.349715342	0.891933148
H	-2.985066821	2.077352494	0.000000000
H	-2.774824109	-0.355003055	0.000000000
H	2.774824109	0.355003055	0.000000000
H	2.985066821	-2.077352494	0.000000000
H	1.252256560	-5.726405260	0.000000000
H	2.343537500	-4.636662910	0.890137450
H	2.343537500	-4.636662910	-0.890137450
H	-3.111890454	-3.886970356	0.000000000
H	-3.155896099	-2.349715342	0.891933148
H	-3.155896099	-2.349715342	-0.891933148

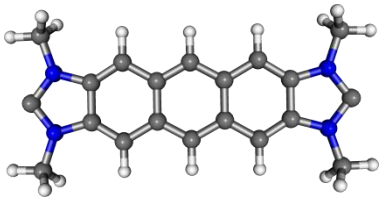
Ligand 9



Total enthalpy, Htot (Utot + pV): -838.158627 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -838.218993 hartrees

C	0.000000000	0.702013262	3.854663575
C	0.000000000	-0.702013262	3.854663575
C	0.000000000	-1.389839882	2.663492088
C	0.000000000	-0.719848721	1.413552018
C	0.000000000	0.719848721	1.413552018
C	0.000000000	1.389839882	2.663492088
C	0.000000000	1.384223736	0.148749407
C	0.000000000	0.711797993	-1.077829836
C	0.000000000	-0.711797993	-1.077829836
C	0.000000000	-1.384223736	0.148749407
N	0.000000000	-1.712930883	-2.056519693
C	0.000000000	-2.968893183	-1.515609716
N	0.000000000	1.712930883	-2.056519693
C	0.000000000	2.968893183	-1.515609716
N	0.000000000	2.748985948	-0.174151526
N	0.000000000	-2.748985948	-0.174151526
C	0.000000000	-3.890030645	0.731651562
C	0.000000000	-1.585001019	-3.505749837
C	0.000000000	1.585001019	-3.505749837
C	0.000000000	3.890030645	0.731651562
H	0.000000000	4.775682692	0.100644600
H	-0.892445893	3.897666554	1.361754503
H	0.892445893	3.897666554	1.361754503
H	0.000000000	-4.775682692	0.100644600
H	0.892445893	-3.897666554	1.361754503
H	-0.892445893	-3.897666554	1.361754503
H	-0.891626229	-1.067057434	-3.862490867
H	0.000000000	-2.600882857	-3.893238827
H	0.891626229	-1.067057434	-3.862490867
H	0.891626229	1.067057434	-3.862490867
H	0.000000000	2.600882857	-3.893238827
H	-0.891626229	1.067057434	-3.862490867
H	0.000000000	-2.467063893	2.694229900
H	0.000000000	2.467063893	2.694229900
H	0.000000000	1.247262389	4.791299453
H	0.000000000	-1.247262389	4.791299453

Ligand 10



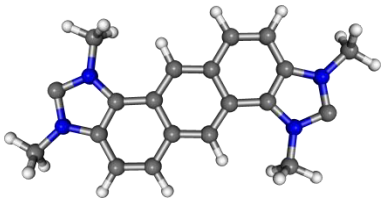
Total enthalpy, Htot (Utot + pV): -991.798644 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -991.867054 hartrees

XYZ Coordinates

C	3.627179535	-0.714058056	0.000000000
C	2.466713649	-1.435271957	0.000000000
C	1.226514124	-0.725761400	0.000000000
C	3.627179535	0.714058056	0.000000000
C	2.466713649	1.435271957	0.000000000
C	1.226514124	0.725761400	0.000000000
C	0.000000000	-1.397726086	0.000000000
C	-1.226514124	-0.725761400	0.000000000
C	-1.226514124	0.725761400	0.000000000
C	0.000000000	1.397726086	0.000000000
C	-2.466713649	-1.435271957	0.000000000
C	-3.627179535	-0.714058056	0.000000000
C	-3.627179535	0.714058056	0.000000000
C	-2.466713649	1.435271957	0.000000000
N	4.974823362	-1.078306654	0.000000000
C	5.817191652	0.000000000	0.000000000
N	4.974823362	1.078306654	0.000000000
N	-4.974823362	-1.078306654	0.000000000
C	-5.817191652	0.000000000	0.000000000
N	-4.974823362	1.078306654	0.000000000
C	5.445948802	-2.450739297	0.000000000
C	5.445948802	2.450739297	0.000000000
H	2.464381524	-2.518860343	0.000000000
H	2.464381524	2.518860343	0.000000000
H	0.000000000	2.483544555	0.000000000
H	0.000000000	-2.483544555	0.000000000
H	-2.464381524	2.518860343	0.000000000
H	-2.464381524	-2.518860343	0.000000000
C	-5.445948802	-2.450739297	0.000000000
C	-5.445948802	2.450739297	0.000000000
H	-6.533222442	-2.421888083	0.000000000
H	-5.095613719	-2.982533142	0.889848382
H	-5.095613719	-2.982533142	-0.889848382
H	-6.533222442	2.421888083	0.000000000
H	-5.095613719	2.982533142	0.889848382

H	-5.095613719	2.982533142	-0.889848382
H	6.533222442	-2.421888083	0.000000000
H	5.095613719	-2.982533142	-0.889848382
H	5.095613719	-2.982533142	0.889848382
H	6.533222442	2.421888083	0.000000000
H	5.095613719	2.982533142	-0.889848382
H	5.095613719	2.982533142	0.889848382

Ligand 11



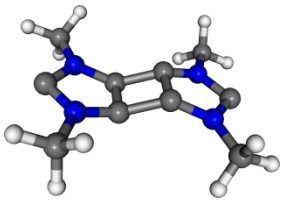
Total enthalpy, Htot (Utot + pV): -991.796586 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -991.863644 hartrees

XYZ Coordinates

C	2.886272104	-2.408945222	0.000000000
C	1.519794027	-2.412244569	0.000000000
C	0.759940676	-1.197546536	0.000000000
C	1.428617992	0.086975362	0.000000000
C	2.859362939	0.048805614	0.000000000
C	3.544645771	-1.157532240	0.000000000
C	-0.639024539	-1.240496309	0.000000000
C	-1.428617992	-0.086975362	0.000000000
C	-0.759940676	1.197546536	0.000000000
C	0.639024539	1.240496309	0.000000000
C	-2.859362939	-0.048805614	0.000000000
C	-3.544645771	1.157532240	0.000000000
C	-2.886272104	2.408945222	0.000000000
C	-1.519794027	2.412244569	0.000000000
N	-3.851789864	-1.033062002	0.000000000
C	-5.118761530	-0.506257385	0.000000000
N	-4.896456500	0.841029774	0.000000000
N	4.896456500	-0.841029774	0.000000000
C	5.118761530	0.506257385	0.000000000
N	3.851789864	1.033062002	0.000000000
C	5.974717445	-1.814859766	0.000000000
C	3.656188513	2.474712903	0.000000000
C	-3.656188513	-2.474712903	0.000000000
C	-5.974717445	1.814859766	0.000000000
H	0.979842109	-3.352378175	0.000000000
H	3.449229569	-3.334387645	0.000000000

H	1.105909316	2.215306115	0.000000000
H	-0.979842109	3.352378175	0.000000000
H	-3.449229569	3.334387645	0.000000000
H	-1.105909316	-2.215306115	0.000000000
H	-4.647531006	-2.922158429	0.000000000
H	-3.113661007	-2.799221624	-0.891711864
H	-3.113661007	-2.799221624	0.891711864
H	-6.909795708	1.259406079	0.000000000
H	-5.929007791	2.448724829	-0.890162018
H	-5.929007791	2.448724829	0.890162018
H	6.909795708	-1.259406079	0.000000000
H	5.929007791	-2.448724829	0.890162018
H	5.929007791	-2.448724829	-0.890162018
H	4.647531006	2.922158429	0.000000000
H	3.113661007	2.799221624	0.891711864
H	3.113661007	2.799221624	-0.891711864

Ligand 12



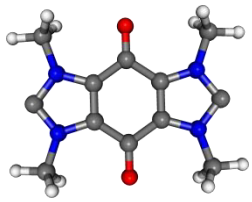
Total enthalpy, Htot (Utot + pV): -606.962328 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -607.017118 hartrees

XYZ Coordinates

C	0.671443396	-0.732868348	0.297648503
C	0.688863537	0.713335031	-0.266607410
C	-0.670221611	0.729763651	-0.265891642
C	-0.687864885	-0.716224405	0.297678351
N	1.109808190	2.000820851	0.007506760
C	0.034798664	2.867452583	0.073751664
N	-1.060343919	2.026426075	0.007792317
N	1.060428910	-2.029724328	0.019727091
C	-0.035809214	-2.869648967	-0.048219287
N	-1.109767576	-2.002228416	0.021357103
C	2.487127249	2.466356244	0.072484519
C	-2.425898799	2.524488819	0.075020528
C	2.425985309	-2.529034751	-0.046509887
C	-2.487194370	-2.466443877	-0.047208540
H	3.010032071	-1.930327754	-0.749387191
H	2.383362223	-3.560443783	-0.389511499
H	2.903060753	-2.493288654	0.936080806

H	3.051851263	1.868130349	0.791417680
H	2.468600298	3.505252399	0.394462320
H	2.968874186	2.398438027	-0.906036643
H	-2.381159141	3.566163672	0.384960762
H	-3.000708358	1.947907471	0.803514952
H	-2.914287222	2.456675839	-0.900108699
H	-2.468062810	-3.507418676	-0.362040385
H	-3.048231071	-1.872707021	-0.772687627
H	-2.973401893	-2.391357190	0.928456345

Ligand 13



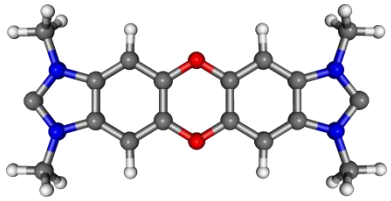
Total enthalpy, Htot (Utot + pV): -833.831557 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -833.892823 hartrees

XYZ Coordinates

C	-1.516563546	0.000000000	0.000000000
C	-0.687276346	0.000000000	1.218264236
C	-0.687276346	0.000000000	-1.218264236
C	0.687276346	0.000000000	-1.218264236
C	1.516563546	0.000000000	0.000000000
C	0.687276346	0.000000000	1.218264236
N	-1.073089702	0.000000000	-2.542835711
C	0.000000000	0.000000000	-3.398381510
N	1.073089702	0.000000000	-2.542835711
N	-1.073089702	0.000000000	2.542835711
C	0.000000000	0.000000000	3.398381510
N	1.073089702	0.000000000	2.542835711
O	2.738583935	0.000000000	0.000000000
C	-2.451691226	0.000000000	-3.027246491
C	2.451691226	0.000000000	-3.027246491
C	2.451691226	0.000000000	3.027246491
C	-2.451691226	0.000000000	3.027246491
H	-2.981245129	0.884473033	2.672150019
H	-2.399839026	0.000000000	4.113257487
H	-2.981245129	-0.884473033	2.672150019
H	-2.981245129	0.884473033	-2.672150019
H	-2.981245129	-0.884473033	-2.672150019
H	-2.399839026	0.000000000	-4.113257487
H	2.399839026	0.000000000	-4.113257487

H	2.981245129	-0.884473033	-2.672150019
H	2.981245129	0.884473033	-2.672150019
H	2.399839026	0.000000000	4.113257487
H	2.981245129	0.884473033	2.672150019
H	2.981245129	-0.884473033	2.672150019
O	-2.738583935	0.000000000	0.000000000

Ligand 14



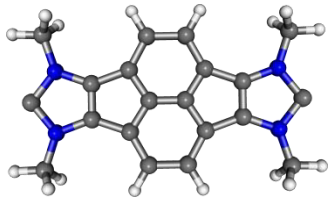
Total enthalpy, Htot (Utot + pV): -1064.843518 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1064.910091 hartrees

XYZ Coordinates

O	0.000000000	-1.422049995	0.000000000
C	1.177682931	-0.702052740	0.000000000
C	1.177682931	0.702052740	0.000000000
O	0.000000000	1.422049995	0.000000000
C	-1.177682931	0.702052740	0.000000000
C	-1.177682931	-0.702052740	0.000000000
C	-2.364614342	-1.423571590	0.000000000
C	-3.553699515	-0.700554440	0.000000000
C	-3.553699515	0.700554440	0.000000000
C	-2.364614342	1.423571590	0.000000000
C	2.364614342	-1.423571590	0.000000000
C	3.553699515	-0.700554440	0.000000000
C	3.553699515	0.700554440	0.000000000
C	2.364614342	1.423571590	0.000000000
N	-4.894716328	-1.075508693	0.000000000
C	-5.742131884	0.000000000	0.000000000
N	-4.894716328	1.075508693	0.000000000
N	4.894716328	-1.075508693	0.000000000
C	5.742131884	0.000000000	0.000000000
N	4.894716328	1.075508693	0.000000000
C	-5.361603165	-2.450324881	0.000000000
C	-5.361603165	2.450324881	0.000000000
C	5.361603165	-2.450324881	0.000000000
C	5.361603165	2.450324881	0.000000000
H	5.010584116	-2.981363181	0.889340696
H	6.447710101	-2.423353431	0.000000000
H	5.010584116	-2.981363181	-0.889340696

H	6.447710101	2.423353431	0.000000000
H	5.010584116	2.981363181	0.889340696
H	5.010584116	2.981363181	-0.889340696
H	-5.010584116	-2.981363181	0.889340696
H	-5.010584116	-2.981363181	-0.889340696
H	-6.447710101	-2.423353431	0.000000000
H	-6.447710101	2.423353431	0.000000000
H	-5.010584116	2.981363181	-0.889340696
H	-5.010584116	2.981363181	0.889340696
H	2.326279087	2.505017858	0.000000000
H	-2.326279087	2.505017858	0.000000000
H	2.326279087	-2.505017858	0.000000000
H	-2.326279087	-2.505017858	0.000000000

Ligand 15



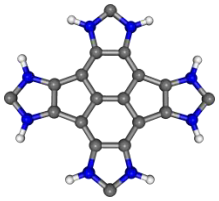
Total enthalpy, Htot (Utot + pV): -990.535211 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -990.593320 hartrees

XYZ Coordinates

C	2.395975816	-0.726740406	0.000000000
C	2.395975816	0.726740406	0.000000000
C	1.147460181	1.416433276	0.000000000
C	0.000000000	0.672315364	0.000000000
C	0.000000000	-0.672315364	0.000000000
C	1.147460181	-1.416433276	0.000000000
C	-1.147460181	-1.416433276	0.000000000
C	-2.395975816	-0.726740406	0.000000000
C	-2.395975816	0.726740406	0.000000000
C	-1.147460181	1.416433276	0.000000000
C	0.656117329	2.820838651	0.000000000
C	-0.656117329	2.820838651	0.000000000
C	0.656117329	-2.820838651	0.000000000
C	-0.656117329	-2.820838651	0.000000000
N	1.136501642	-4.153775339	0.000000000
C	0.000000000	-5.066814591	0.000000000
N	-1.136501642	-4.153775339	0.000000000
N	1.136501642	4.153775339	0.000000000
C	0.000000000	5.066814591	0.000000000
N	-1.136501642	4.153775339	0.000000000

C	2.503932202	4.613527333	0.000000000
C	-2.503932202	4.613527333	0.000000000
C	2.503932202	-4.613527333	0.000000000
C	-2.503932202	-4.613527333	0.000000000
H	2.539813693	-5.723818092	0.000000000
H	3.025249595	-4.242064395	0.905920000
H	3.025249595	-4.242064395	-0.905920000
H	-2.539813693	-5.723818092	0.000000000
H	-3.025249595	-4.242064395	-0.905920000
H	-3.025249595	-4.242064395	0.905920000
H	2.539813693	5.723818092	0.000000000
H	3.025249595	4.242064395	-0.905920000
H	3.025249595	4.242064395	0.905920000
H	-2.539813693	5.723818092	0.000000000
H	-3.025249595	4.242064395	0.905920000
H	-3.025249595	4.242064395	-0.905920000
H	-3.326135129	-1.275559080	0.000000000
H	-3.326135129	1.275559080	0.000000000
H	3.326135129	1.275559080	0.000000000
H	3.326135129	-1.275559080	0.000000000

Ligand 16



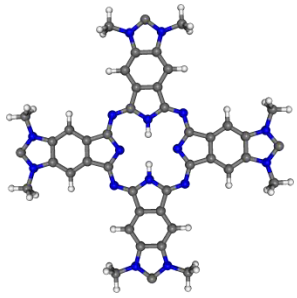
Total enthalpy, Htot (Utot + pV): -1128.550818 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1128.610979 hartrees

XYZ Coordinates

C	0.000000000	0.688904229	2.841709043
C	0.000000000	1.192897530	1.463615562
C	0.000000000	0.000000000	0.685089226
C	0.000000000	0.000000000	-0.685089226
C	0.000000000	-1.192897530	1.463615562
C	0.000000000	-0.688904229	2.841709043
C	0.000000000	1.192897530	-1.463615562
C	0.000000000	0.688904229	-2.841709043
C	0.000000000	-0.688904229	-2.841709043
C	0.000000000	-1.192897530	-1.463615562
N	0.000000000	1.066477283	-4.172751290
C	0.000000000	0.000000000	-5.042819482
N	0.000000000	-1.066477283	-4.172751290

C	0.000000000	2.363059295	0.726096048
C	0.000000000	2.363059295	-0.726096048
N	0.000000000	3.714521265	1.064410229
C	0.000000000	4.573687175	0.000000000
N	0.000000000	3.714521265	-1.064410229
C	0.000000000	-2.363059295	0.726096048
C	0.000000000	-2.363059295	-0.726096048
N	0.000000000	-3.714521265	1.064410229
C	0.000000000	-4.573687175	0.000000000
N	0.000000000	-3.714521265	-1.064410229
N	0.000000000	1.066477283	4.172751290
C	0.000000000	0.000000000	5.042819482
N	0.000000000	-1.066477283	4.172751290
H	0.000000000	2.010050253	4.521931179
H	0.000000000	-2.010050253	4.521931179
H	0.000000000	-4.062748569	2.008322435
H	0.000000000	-4.062748569	-2.008322435
H	0.000000000	-2.010050253	-4.521931179
H	0.000000000	2.010050253	-4.521931179
H	0.000000000	4.062748569	-2.008322435
H	0.000000000	4.062748569	2.008322435

Ligand 17



Total enthalpy, Htot (Utot + pV): -2572.957579 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2573.085360 hartrees

XYZ Coordinates

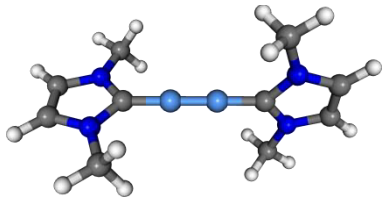
C	0.000000000	6.522891096	-0.707303048
C	0.000000000	6.522891096	0.707303048
C	0.000000000	5.346212790	-1.450880619
C	0.000000000	4.171893252	-0.705062967
C	0.000000000	4.171893252	0.705062967
C	0.000000000	5.346212790	1.450880619
C	0.000000000	2.760382066	1.096413104
N	0.000000000	1.952123961	0.000000000
C	0.000000000	2.760382066	-1.096413104
N	0.000000000	2.394499260	2.379545407

C	0.000000000	1.144463366	2.787899290
N	0.000000000	0.000000000	2.023717987
C	0.000000000	-1.144463366	2.787899290
C	0.000000000	-0.709699895	4.171974530
C	0.000000000	0.709699895	4.171974530
C	0.000000000	1.452403987	5.353495515
C	0.000000000	0.709743983	6.524551027
C	0.000000000	-0.709743983	6.524551027
C	0.000000000	-1.452403987	5.353495515
N	0.000000000	-2.394499260	2.379545407
C	0.000000000	-2.760382066	1.096413104
N	0.000000000	-1.952123961	0.000000000
C	0.000000000	-2.760382066	-1.096413104
C	0.000000000	-4.171893252	-0.705062967
C	0.000000000	-5.346212790	1.450880619
C	0.000000000	-6.522891096	0.707303048
C	0.000000000	-6.522891096	-0.707303048
C	0.000000000	-5.346212790	-1.450880619
C	0.000000000	-1.144463366	-2.787899290
N	0.000000000	0.000000000	-2.023717987
C	0.000000000	1.144463366	-2.787899290
C	0.000000000	0.709699895	-4.171974530
C	0.000000000	-0.709699895	-4.171974530
C	0.000000000	-1.452403987	-5.353495515
C	0.000000000	-0.709743983	-6.524551027
C	0.000000000	0.709743983	-6.524551027
C	0.000000000	1.452403987	-5.353495515
N	0.000000000	2.394499260	-2.379545407
N	0.000000000	-2.394499260	-2.379545407
C	0.000000000	-4.171893252	0.705062967
H	0.000000000	0.000000000	1.012049003
H	0.000000000	0.000000000	-1.012049003
N	0.000000000	7.864909591	-1.075451233
N	0.000000000	7.864909591	1.075451233
H	0.000000000	5.330785146	-2.533064456
H	0.000000000	5.330785146	2.533064456
H	0.000000000	2.534280960	5.336682952
N	0.000000000	1.076484190	7.866063769
N	0.000000000	-1.076484190	7.866063769
H	0.000000000	-2.534280960	5.336682952
H	0.000000000	-5.330785146	2.533064456
N	0.000000000	-7.864909591	1.075451233
N	0.000000000	-7.864909591	-1.075451233
H	0.000000000	-5.330785146	-2.533064456
H	0.000000000	-2.534280960	-5.336682952
N	0.000000000	-1.076484190	-7.866063769
N	0.000000000	1.076484190	-7.866063769
H	0.000000000	2.534280960	-5.336682952

C	0.000000000	0.000000000	-8.712964625
C	0.000000000	8.712890371	0.000000000
C	0.000000000	0.000000000	8.712964625
C	0.000000000	-8.712890371	0.000000000
C	0.000000000	2.450422470	-8.338348094
C	0.000000000	-2.450422470	-8.338348094
C	0.000000000	-8.336412383	-2.449027747
C	0.000000000	-8.336412383	2.449027747
C	0.000000000	-2.450422470	8.338348094
C	0.000000000	2.450422470	8.338348094
C	0.000000000	8.336412383	2.449027747
C	0.000000000	8.336412383	-2.449027747
H	0.000000000	9.423508959	-2.417731845
H	0.890041443	7.986842014	-2.980032049
H	-0.890041443	7.986842014	-2.980032049
H	0.000000000	9.423508959	2.417731845
H	-0.890041443	7.986842014	2.980032049
H	0.890041443	7.986842014	2.980032049
H	0.000000000	2.418559174	9.425349734
H	0.890252285	2.980853878	7.988877760
H	-0.890252285	2.980853878	7.988877760
H	0.000000000	-2.418559174	9.425349734
H	-0.890252285	-2.980853878	7.988877760
H	0.890252285	-2.980853878	7.988877760
H	0.000000000	-9.423508959	2.417731845
H	0.890041443	-7.986842014	2.980032049
H	-0.890041443	-7.986842014	2.980032049
H	0.000000000	-9.423508959	-2.417731845
H	-0.890041443	-7.986842014	-2.980032049
H	0.890041443	-7.986842014	-2.980032049
H	0.000000000	-2.418559174	-9.425349734
H	0.890252285	-2.980853878	-7.988877760
H	-0.890252285	-2.980853878	-7.988877760
H	0.000000000	2.418559174	-9.425349734
H	-0.890252285	2.980853878	-7.988877760
H	0.890252285	2.980853878	-7.988877760

2.2 LBBL Compounds

Compound 1BB1

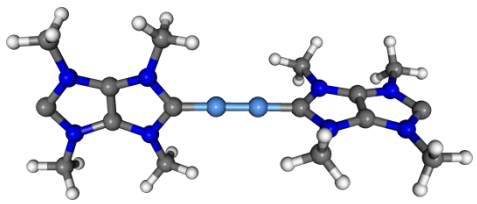


Total enthalpy, Htot (Utot + pV): -659.184922 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -659.250373 hartrees

XYZ Coordinates

B	0.000000000	0.000000000	-0.727244677
C	0.000000000	0.000000000	2.208120432
B	0.000000000	0.000000000	0.727244677
C	0.000000000	0.000000000	-2.208120432
N	-0.772492600	-0.772492600	-3.055768139
N	0.772492600	0.772492600	-3.055768139
C	-0.478533726	-0.478533726	-4.378479456
C	0.478533726	0.478533726	-4.378479456
N	0.772492600	-0.772492600	3.055768139
N	-0.772492600	0.772492600	3.055768139
C	0.478533726	-0.478533726	4.378479456
C	-0.478533726	0.478533726	4.378479456
C	1.738512889	-1.738512889	2.575918342
C	-1.738512889	-1.738512889	-2.575918342
C	-1.738512889	1.738512889	2.575918342
C	1.738512889	1.738512889	-2.575918342
H	1.243068345	-2.492759574	1.957964823
H	2.218102597	-2.218102597	3.429614303
H	2.492759574	-1.243068345	1.957964823
H	-1.243068345	2.492759574	1.957964823
H	-2.218102597	2.218102597	3.429614303
H	-2.492759574	1.243068345	1.957964823
H	1.243068345	2.492759574	-1.957964823
H	2.218102597	2.218102597	-3.429614303
H	2.492759574	1.243068345	-1.957964823
H	-1.243068345	-2.492759574	-1.957964823
H	-2.218102597	-2.218102597	-3.429614303
H	-2.492759574	-1.243068345	-1.957964823
H	0.971634710	-0.971634710	5.198145805
H	-0.971634710	0.971634710	5.198145805
H	-0.971634710	-0.971634710	-5.198145805
H	0.971634710	0.971634710	-5.198145805

Compound 2BB2

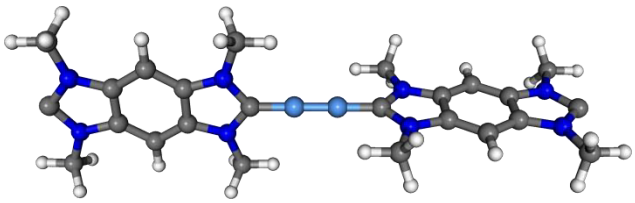


Total enthalpy, Htot (Utot + pV): -1111.458831 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1111.551833 hartrees
XYZ Coodinates

N	-2.222286027	2.861697976	0.194153551
C	-2.987980899	1.694968886	0.270326450
N	-2.095489992	0.627695294	0.132787806
C	-0.814307559	1.146075203	0.051767794
C	-0.893250900	2.497690965	0.071938208
N	0.368985787	2.987459764	-0.221384942
C	1.265076685	1.953214582	-0.392085758
N	0.497745852	0.816642906	-0.248987805
C	-2.785694216	4.193235122	0.309707093
C	0.771953336	4.382709174	-0.278427255
C	1.061106189	-0.518943098	-0.355140258
C	-2.496382834	-0.757094614	0.292990925
H	-3.768627131	4.096974266	0.775478378
H	-2.908776996	4.662937940	-0.670916127
H	-2.143954422	4.818337703	0.933970533
H	0.193640746	4.925919416	-1.030482239
H	1.824353931	4.395475320	-0.553141611
H	0.646476587	4.870825443	0.691964476
H	2.124819531	-0.397446888	-0.547541271
H	0.606595548	-1.073231950	-1.180885521
H	0.921395499	-1.079328357	0.573185186
H	-3.546949508	-0.832653835	0.007094811
H	-2.396128019	-1.085986523	1.332779006
H	-1.892211955	-1.396819725	-0.352448272
H	-7.010839442	0.719513561	-1.615234345
H	-7.892190761	1.443981090	4.211597397
H	-11.158582060	-0.171437241	-1.423968519
H	-10.404910783	0.688854623	4.461921438
C	-7.997551158	1.166730455	-1.489090046
C	-7.344405350	1.370278751	0.911442329
N	-8.315007307	1.159818063	-0.072951102
C	-7.372486127	1.879609481	3.357372904
N	-8.030114197	1.486296170	2.124961626
C	-9.561003183	1.284486992	0.520908668
C	-9.388798053	1.481254542	1.850706200
C	-11.558051258	0.728813162	-0.948691785
H	-8.738337699	0.583492993	-2.037054213
H	-6.347850209	1.507728177	3.323522098
N	-10.899912010	0.982999791	0.321943560
N	-10.623890127	1.298265933	2.454580734
C	-11.594553205	1.035024908	1.511597371
C	-10.934001051	1.438983216	3.867583100
H	-12.614105951	0.581448952	-0.732722888
H	-12.006268720	1.287426774	3.971579301
H	-7.965850086	2.187167693	-1.886101876

H	-7.341654772	2.969822458	3.464243507
H	-11.441349053	1.576261005	-1.629775576
H	-10.670916195	2.435996376	4.231257024
B	-4.449997947	1.601703984	0.486536808
B	-5.885551221	1.491645496	0.700631917

Compound 3BB3



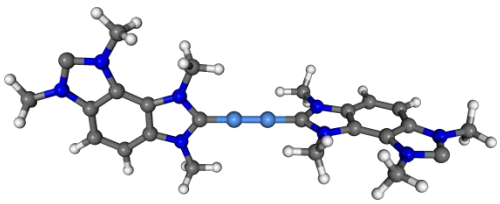
Total enthalpy, Htot (Utot + pV): -1418.820934 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1418.910827 hartrees

XYZ Coordinates

N	-0.759393283	-0.759393283	-8.070548274
C	0.000000000	0.000000000	-8.919795395
N	0.759393283	0.759393283	-8.070548274
C	0.496992993	0.496992993	-6.727245348
C	-0.496992993	-0.496992993	-6.727245348
C	-1.028300556	-1.028300556	-5.547514535
C	-0.500902049	-0.500902049	-4.374289319
C	0.500902049	0.500902049	-4.374289319
C	1.028300556	1.028300556	-5.547514535
N	-0.779447822	-0.779447822	-3.046553648
C	0.000000000	0.000000000	-2.206544913
N	0.779447822	0.779447822	-3.046553648
C	-1.730320792	-1.730320792	-8.538909838
C	-1.749837724	-1.749837724	-2.583301383
C	1.749837724	1.749837724	-2.583301383
C	1.730320792	1.730320792	-8.538909838
H	-1.793296502	-1.793296502	-5.546205999
H	1.793296502	1.793296502	-5.546205999
H	-1.710149738	-1.710149738	-9.626239819
H	-2.736237478	-1.477391074	-8.189758078
H	-1.477391074	-2.736237478	-8.189758078
H	1.710149738	1.710149738	-9.626239819
H	2.736237478	1.477391074	-8.189758078
H	1.477391074	2.736237478	-8.189758078
H	1.740897445	1.740897445	-1.493106204
H	1.491364821	2.752370548	-2.937674790
H	2.752370548	1.491364821	-2.937674790
H	-1.491364821	-2.752370548	-2.937674790

H	-2.752370548	-1.491364821	-2.937674790
H	-1.740897445	-1.740897445	-1.493106204
B	0.000000000	0.000000000	-0.729150266
B	0.000000000	0.000000000	0.729150266
C	0.000000000	0.000000000	2.206544913
N	0.779447822	-0.779447822	3.046553648
C	0.500902049	-0.500902049	4.374289319
C	-0.500902049	0.500902049	4.374289319
N	-0.779447822	0.779447822	3.046553648
C	-1.749837724	1.749837724	2.583301383
C	1.749837724	-1.749837724	2.583301383
H	-1.491364821	2.752370548	2.937674790
H	-2.752370548	1.491364821	2.937674790
H	-1.740897445	1.740897445	1.493106204
H	1.740897445	-1.740897445	1.493106204
H	1.491364821	-2.752370548	2.937674790
H	2.752370548	-1.491364821	2.937674790
C	-1.028300556	1.028300556	5.547514535
C	-0.496992993	0.496992993	6.727245348
C	0.496992993	-0.496992993	6.727245348
C	1.028300556	-1.028300556	5.547514535
N	-0.759393283	0.759393283	8.070548274
C	0.000000000	0.000000000	8.919795395
N	0.759393283	-0.759393283	8.070548274
C	-1.730320792	1.730320792	8.538909838
C	1.730320792	-1.730320792	8.538909838
H	-1.477391074	2.736237478	8.189758078
H	-1.710149738	1.710149738	9.626239819
H	-2.736237478	1.477391074	8.189758078
H	1.710149738	-1.710149738	9.626239819
H	2.736237478	-1.477391074	8.189758078
H	1.477391074	-2.736237478	8.189758078
H	-1.793296502	1.793296502	5.546205999
H	1.793296502	-1.793296502	5.546205999

Compound 4BB4



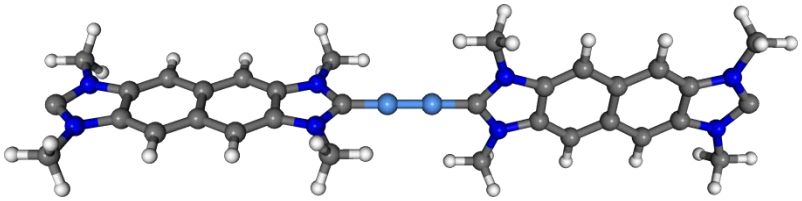
Total enthalpy, Htot (Utot + pV): -1418.798999 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1418.888016 hartrees

XYZ Coordinates

C	-4.389732447	-0.401939743	-0.014074074
C	-5.651393745	-0.825563287	-0.465527216
C	-6.789577848	-0.199051853	0.092953447
C	-6.738848215	0.804475120	1.055914063
C	-4.354933592	0.619635094	0.964951713
C	-5.488833835	1.224294693	1.503541843
N	-6.169437810	-1.758934267	-1.379786498
C	-7.540795412	-1.750392443	-1.422012715
N	-7.890013656	-0.796343253	-0.520367319
C	-5.438595338	-2.677812383	-2.235353517
C	-9.269664029	-0.445353536	-0.236728888
H	-6.187820151	-3.228765483	-2.798898381
H	-4.787526937	-2.144208266	-2.931402798
H	-4.842386516	-3.381317449	-1.649841416
H	-9.898589185	-1.074589856	-0.862357736
H	-9.459841547	0.606564151	-0.469757902
H	-9.508431065	-0.623245944	0.816038548
N	-3.061401246	-0.727151987	-0.279302940
H	-7.645083269	1.247989862	1.447292890
N	-3.021249621	0.866854357	1.245779684
H	-5.398630643	2.001287991	2.251249924
C	-2.205606373	0.052439950	0.492412654
C	-2.529700545	-1.714447965	-1.199523414
C	-2.535136414	1.846958489	2.195544968
H	-1.442825314	-1.684409082	-1.108124946
H	-2.878498294	-2.716962526	-0.944271200
H	-2.803694419	-1.480603888	-2.230431159
H	-1.445417894	1.814568496	2.181171100
H	-2.870796399	2.850579336	1.918000386
H	-2.889927205	1.615669941	3.204314277
B	-0.727465470	0.014424444	0.497341579
H	2.878498294	2.716962526	-0.944271200
H	4.842386516	3.381317449	-1.649841416
H	1.442825314	1.684409082	-1.108124946
C	2.529700545	1.714447965	-1.199523414
B	0.727465470	-0.014424444	0.497341579
C	2.205606373	-0.052439950	0.492412654
N	3.061401246	0.727151987	-0.279302940
C	5.438595338	2.677812383	-2.235353517
H	2.889927205	-1.615669941	3.204314277
H	6.187820151	3.228765483	-2.798898381
N	3.021249621	-0.866854357	1.245779684
C	4.389732447	0.401939743	-0.014074074
H	1.445417894	-1.814568496	2.181171100
C	2.535136414	-1.846958489	2.195544968
H	2.803694419	1.480603888	-2.230431159
N	6.169437810	1.758934267	-1.379786498

C	4.354933592	-0.619635094	0.964951713
C	5.651393745	0.825563287	-0.465527216
H	4.787526937	2.144208266	-2.931402798
C	7.540795412	1.750392443	-1.422012715
C	6.789577848	0.199051853	0.092953447
C	5.488833835	-1.224294693	1.503541843
N	7.890013656	0.796343253	-0.520367319
C	6.738848215	-0.804475120	1.055914063
H	9.508431065	0.623245944	0.816038548
H	5.398630643	-2.001287991	2.251249924
H	2.870796399	-2.850579336	1.918000386
C	9.269664029	0.445353536	-0.236728888
H	7.645083269	-1.247989862	1.447292890
H	9.898589185	1.074589856	-0.862357736
H	9.459841547	-0.606564151	-0.469757902

Compound 5BB5



Total enthalpy, Htot (Utot + pV): -1726.077881 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1726.180601 hartrees

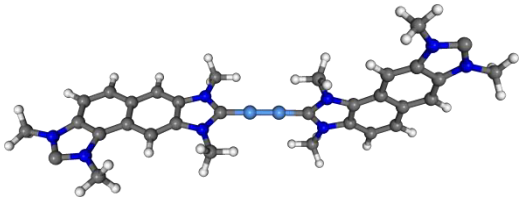
XYZ Coordinates

C	1.010986078	-1.010986078	5.538295424
C	0.503690102	-0.503690102	4.370277170
C	0.511751635	-0.511751635	6.777164084
C	-0.511751635	0.511751635	6.777164084
C	-1.010986078	1.010986078	5.538295424
C	-0.503690102	0.503690102	4.370277170
C	1.009181469	-1.009181469	8.008226753
C	0.500491779	-0.500491779	9.180027089
C	-0.500491779	0.500491779	9.180027089
C	-1.009181469	1.009181469	8.008226753
N	0.761309153	-0.761309153	10.526102090
C	0.000000000	0.000000000	11.370866428
N	-0.761309153	0.761309153	10.526102090
N	0.781080043	-0.781080043	3.042629713
C	0.000000000	0.000000000	2.205473576
N	-0.781080043	0.781080043	3.042629713
C	1.731909005	-1.731909005	10.995315455
C	-1.731909005	1.731909005	10.995315455

C	-1.752037354	1.752037354	2.580897812
C	1.752037354	-1.752037354	2.580897812
H	1.493058390	-2.753041048	2.937802654
H	2.753041048	-1.493058390	2.937802654
H	1.746995053	-1.746995053	1.491195935
H	1.478873695	-2.737176136	10.644880959
H	1.712295943	-1.712295943	12.082686491
H	2.737176136	-1.478873695	10.644880959
H	-1.712295943	1.712295943	12.082686491
H	-2.737176136	1.478873695	10.644880959
H	-1.478873695	2.737176136	10.644880959
H	-1.746995053	1.746995053	1.491195935
H	-1.493058390	2.753041048	2.937802654
H	-2.753041048	1.493058390	2.937802654
H	-2.753041048	-1.493058390	-2.937802654
H	1.493058390	2.753041048	-2.937802654
C	-1.752037354	-1.752037354	-2.580897812
C	0.000000000	0.000000000	-2.205473576
N	-0.781080043	-0.781080043	-3.042629713
H	-1.493058390	-2.753041048	-2.937802654
C	-0.503690102	-0.503690102	-4.370277170
N	0.781080043	0.781080043	-3.042629713
C	1.752037354	1.752037354	-2.580897812
C	-1.010986078	-1.010986078	-5.538295424
C	0.503690102	0.503690102	-4.370277170
H	1.746995053	1.746995053	-1.491195935
H	-1.712295943	-1.712295943	-12.082686491
C	-0.511751635	-0.511751635	-6.777164084
C	1.010986078	1.010986078	-5.538295424
C	-1.009181469	-1.009181469	-8.008226753
C	0.511751635	0.511751635	-6.777164084
H	1.478873695	2.737176136	-10.644880959
C	-0.500491779	-0.500491779	-9.180027089
C	1.009181469	1.009181469	-8.008226753
H	-1.746995053	-1.746995053	-1.491195935
C	-1.731909005	-1.731909005	-10.995315455
C	0.500491779	0.500491779	-9.180027089
H	-2.737176136	-1.478873695	-10.644880959
N	-0.761309153	-0.761309153	-10.526102090
C	0.000000000	0.000000000	-11.370866428
N	0.761309153	0.761309153	-10.526102090
C	1.731909005	1.731909005	-10.995315455
H	2.753041048	1.493058390	-2.937802654
H	1.712295943	1.712295943	-12.082686491
H	-1.478873695	-2.737176136	-10.644880959
H	2.737176136	1.478873695	-10.644880959
B	0.000000000	0.000000000	0.730876101
B	0.000000000	0.000000000	-0.730876101

H	1.775529210	-1.775529210	8.006401004
H	-1.775529210	1.775529210	8.006401004
H	1.776978252	-1.776978252	5.539087914
H	-1.776978252	1.776978252	5.539087914
H	-1.776978252	-1.776978252	-5.539087914
H	1.776978252	1.776978252	-5.539087914
H	-1.775529210	-1.775529210	-8.006401004
H	1.775529210	1.775529210	-8.006401004

Compound 6BB6



Total enthalpy, Htot (Utot + pV): -1726.069023 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1726.171167 hartrees

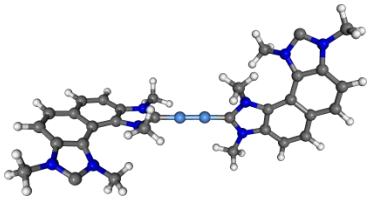
XYZ Coordinates

C	-5.832230524	2.097401543	-0.253572768
C	-4.519641058	2.464437390	-0.080169288
C	-3.528224094	1.446488254	-0.039679721
C	-3.926670128	0.058592686	-0.181323911
C	-6.221627255	0.742627011	-0.391532094
C	-5.296471619	-0.269057719	-0.357690336
C	-2.133793496	1.676772211	0.130637772
C	-1.222450583	0.621623903	0.153592350
C	-1.615114542	-0.720318326	0.017596704
C	-2.954412637	-0.979208681	-0.146574598
N	-7.015817528	2.830427814	-0.337182011
C	-8.118453657	2.037531797	-0.517687164
N	-7.608167318	0.769281280	-0.547381111
N	-1.384804719	2.840225021	0.294808600
C	-0.037521280	2.535759015	0.415776707
N	0.038988787	1.161306648	0.325310224
C	1.275529458	0.407624221	0.407595147
C	-1.852211420	4.214977565	0.346596844
C	-7.090409414	4.276915110	-0.245481941
C	-8.432278619	-0.412383789	-0.724032564
H	-8.137090486	4.555177936	-0.345848424
H	-6.712560583	4.626535336	0.720158071
H	-6.510834877	4.748882136	-1.044716711
H	-9.463235663	-0.079036590	-0.819227415
H	-8.343910911	-1.081027580	0.137579855

H	-8.141524895	-0.958550352	-1.626501613
H	-5.583722491	-1.308768904	-0.462878314
H	-4.254762999	3.505032879	0.020644656
H	-3.294915311	-2.002693866	-0.254922036
H	-0.886238082	-1.520671796	0.042029175
H	2.096656025	1.118462288	0.503364926
H	1.420356970	-0.190527588	-0.496414369
H	1.269056155	-0.252692470	1.279723878
H	-0.978754288	4.850195277	0.499285651
H	-2.335476870	4.499181993	-0.591214831
H	-2.544693610	4.360052451	1.179028504
C	5.057608770	6.752097511	0.462502959
C	6.017848657	7.535106001	-0.132461681
C	6.911059280	8.270108595	0.698022942
C	6.788183770	8.173774385	2.134853350
C	4.933373774	6.659605345	1.874907045
C	5.776634171	7.351120264	2.707061857
C	7.949244656	9.118725407	0.220957401
C	8.788412065	9.804242013	1.095808889
C	8.666567337	9.705662847	2.491950638
C	7.672639133	8.896116351	2.985383803
N	4.074432873	5.942174770	-0.072838504
C	3.329292885	5.340639268	0.934476470
N	3.878172907	5.800052864	2.123534856
N	8.390646242	9.480220041	-1.060130122
C	9.451967416	10.346664445	-1.030001055
N	9.673780648	10.527365409	0.304034854
C	10.725278990	11.386210757	0.819053843
C	7.845783045	9.038569958	-2.333826546
C	3.840556807	5.737419679	-1.487459160
C	3.405930126	5.419243115	3.438932361
H	3.002603951	5.047995134	-1.593674015
H	3.594325151	6.684149661	-1.977647549
H	4.725589743	5.306028534	-1.964781395
H	2.571588641	4.729121814	3.311336275
H	3.066205047	6.298478636	3.994732166
H	4.201489139	4.924161540	4.004056910
H	5.690749837	7.285125340	3.785091053
H	6.087895257	7.586233862	-1.207350471
H	7.545204137	8.793319782	4.057509769
H	9.330557827	10.247290253	3.154373275
H	11.243492223	11.811009897	-0.037866511
H	11.434101628	10.815386849	1.426297774
H	10.307710624	12.193386244	1.428236483
H	8.436494215	9.523845586	-3.107501055
H	7.928299686	7.954260049	-2.445816286
H	6.799180972	9.335207342	-2.441573556
B	2.198204007	4.410744076	0.770290909

B 1.085148326 3.484214876 0.601263419

Compound 7BB7



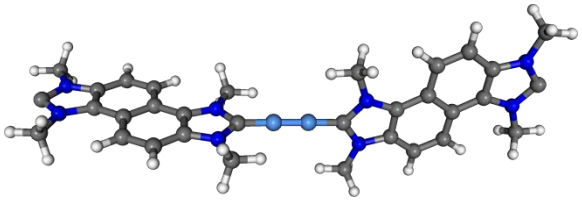
Total enthalpy, Htot (Utot + pV): -1726.028348 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1726.132655 hartrees

XYZ Coordinates

C	-7.387027161	0.128217223	1.443440380
C	-8.127562318	1.316325759	1.283657467
C	-7.682651650	2.211755323	0.344565942
C	-6.456482777	2.030631240	-0.359289057
C	-5.612587880	0.892318821	-0.060707444
C	-6.216087004	-0.125328531	0.736694765
C	-4.298219110	0.949140520	-0.587680205
C	-3.966763230	1.867473425	-1.586712511
C	-4.849550204	2.876506705	-2.000702136
C	-6.054020466	2.973187292	-1.339748739
N	-2.658638577	1.621875574	-1.957966938
C	-2.103675732	0.652812876	-1.139650815
N	-3.132771139	0.228184577	-0.299901178
C	-1.904152763	2.366427303	-2.945795964
C	-2.782598734	-0.326778540	1.008810944
H	-3.681315391	-0.571485068	1.567349618
H	-2.190604949	0.403492308	1.568701599
H	-2.177296088	-1.223644366	0.872731059
H	-2.504584589	2.507234236	-3.846952404
H	-1.010196404	1.791523568	-3.190512908
H	-1.597541638	3.342990903	-2.556904960
H	-8.262111835	3.102859003	0.130881692
N	-5.907887844	-1.470976903	1.001373088
N	-7.673552532	-1.035271412	2.150737802
H	-9.042111966	1.488206872	1.837415045
C	-6.805123024	-2.046870210	1.870163956
C	-5.121110965	-2.351828360	0.134746125
C	-8.806543949	-1.195092655	3.045979787
H	-5.741663265	-2.702672390	-0.694308903
H	-4.254284061	-1.845034974	-0.277763669
H	-4.809528134	-3.210406124	0.726443030
H	-9.747853496	-1.023956900	2.515807394

H	-8.741214609	-0.499402743	3.887192444
H	-8.781789252	-2.217199357	3.416879178
H	-6.727139695	3.791519894	-1.568327135
H	-4.566120894	3.592231221	-2.761741828
C	3.966763230	-1.867473425	-1.586712511
C	4.849550204	-2.876506705	-2.000702136
C	6.054020466	-2.973187292	-1.339748739
C	6.456482777	-2.030631240	-0.359289057
C	5.612587880	-0.892318821	-0.060707444
C	4.298219110	-0.949140520	-0.587680205
C	6.216087004	0.125328531	0.736694765
C	7.387027161	-0.128217223	1.443440380
C	8.127562318	-1.316325759	1.283657467
C	7.682651650	-2.211755323	0.344565942
N	7.673552532	1.035271412	2.150737802
C	6.805123024	2.046870210	1.870163956
N	5.907887844	1.470976903	1.001373088
C	8.806543949	1.195092655	3.045979787
C	5.121110965	2.351828360	0.134746125
H	4.254284061	1.845034974	-0.277763669
H	5.741663265	2.702672390	-0.694308903
H	4.809528134	3.210406124	0.726443030
H	8.741214609	0.499402743	3.887192444
H	8.781789252	2.217199357	3.416879178
H	9.747853496	1.023956900	2.515807394
H	6.727139695	-3.791519894	-1.568327135
N	3.132771139	-0.228184577	-0.299901178
N	2.658638577	-1.621875574	-1.957966938
H	4.566120894	-3.592231221	-2.761741828
C	2.103675732	-0.652812876	-1.139650815
C	2.782598734	0.326778540	1.008810944
C	1.904152763	-2.366427303	-2.945795964
H	2.190604949	-0.403492308	1.568701599
H	3.681315391	0.571485068	1.567349618
H	2.177296088	1.223644366	0.872731059
H	1.597541638	-3.342990903	-2.556904960
H	2.504584589	-2.507234236	-3.846952404
H	1.010196404	-1.791523568	-3.190512908
H	8.262111835	-3.102859003	0.130881692
H	9.042111966	-1.488206872	1.837415045
B	-0.700848806	0.206749657	-1.120418424
B	0.700848806	-0.206749657	-1.120418424

Compound 8BB8



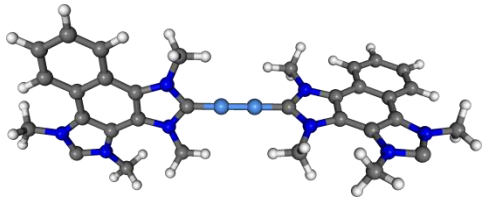
Total enthalpy, Htot (Utot + pV): -1726.059666 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1726.160797 hartrees

XYZ Coordinates

C	5.531341559	0.970184894	-1.703585536
C	6.740546703	0.480394652	-1.257376570
C	6.822717364	-0.529757646	-0.265209457
C	5.612119936	-1.082791817	0.315502219
C	4.384145494	-0.554292637	-0.169897597
C	4.361013517	0.442279116	-1.149445535
C	8.051529716	-1.064162408	0.224487507
C	8.076064738	-2.054755057	1.200545792
C	6.901712385	-2.584757683	1.759111221
C	5.698099470	-2.097519247	1.314397757
N	9.398870766	-0.811773879	-0.065357981
C	10.253980793	-1.589005840	0.674859743
N	9.414071620	-2.340642833	1.441697289
C	9.936025262	0.142926031	-1.023516081
C	9.888931399	-3.325278290	2.397792697
N	3.039296465	0.746325339	-1.410216306
C	2.206514640	-0.027620084	-0.627609391
N	3.052718840	-0.825796727	0.133733332
C	2.573472852	1.731982667	-2.365427727
C	2.512986953	-1.784276574	1.084259851
H	1.483761716	1.739932111	-2.331342088
H	2.950173807	2.725995084	-2.107512717
H	2.900731255	1.474017270	-3.376818656
H	1.425702750	-1.711096609	1.031332363
H	2.835519007	-1.550607570	2.101577911
H	2.813256691	-2.802277296	0.825482842
H	5.491094742	1.741662053	-2.462229027
H	7.645016722	0.884945647	-1.682715439
H	4.793938300	-2.501314563	1.740763134
H	6.940294274	-3.355622307	2.518954180
H	10.975768269	-3.316362613	2.355892768
H	9.523830805	-4.324574303	2.143646516
H	9.562438433	-3.075032393	3.411330076
H	11.018766239	0.055060261	-0.970439906
H	9.605314401	-0.086999417	-2.039511765

H	9.644726286	1.165290935	-0.769751914
H	-2.813256691	2.802277296	0.825482842
H	-9.523830805	4.324574303	2.143646516
C	-2.512986953	1.784276574	1.084259851
H	-2.900731255	-1.474017270	-3.376818656
C	-5.698099470	2.097519247	1.314397757
C	-6.901712385	2.584757683	1.759111221
H	-1.425702750	1.711096609	1.031332363
N	-3.052718840	0.825796727	0.133733332
C	-9.888931399	3.325278290	2.397792697
H	-9.605314401	0.086999417	-2.039511765
C	-2.206514640	0.027620084	-0.627609391
H	-4.793938300	2.501314563	1.740763134
H	-6.940294274	3.355622307	2.518954180
C	-5.612119936	1.082791817	0.315502219
C	-4.384145494	0.554292637	-0.169897597
C	-8.076064738	2.054755057	1.200545792
N	-9.414071620	2.340642833	1.441697289
N	-3.039296465	-0.746325339	-1.410216306
C	-4.361013517	-0.442279116	-1.149445535
C	-8.051529716	1.064162408	0.224487507
C	-6.822717364	0.529757646	-0.265209457
C	-10.253980793	1.589005840	0.674859743
C	-2.573472852	-1.731982667	-2.365427727
H	-10.975768269	3.316362613	2.355892768
C	-5.531341559	-0.970184894	-1.703585536
C	-6.740546703	-0.480394652	-1.257376570
N	-9.398870766	0.811773879	-0.065357981
H	-1.483761716	-1.739932111	-2.331342088
C	-9.936025262	-0.142926031	-1.023516081
H	-5.491094742	-1.741662053	-2.462229027
H	-7.645016722	-0.884945647	-1.682715439
H	-2.835519007	1.550607570	2.101577911
H	-11.018766239	-0.055060261	-0.970439906
H	-9.562438433	3.075032393	3.411330076
H	-2.950173807	-2.725995084	-2.107512717
H	-9.644726286	-1.165290935	-0.769751914
B	0.727783989	-0.010565638	-0.608272586
B	-0.727783989	0.010565638	-0.608272586

Compound 9BB9



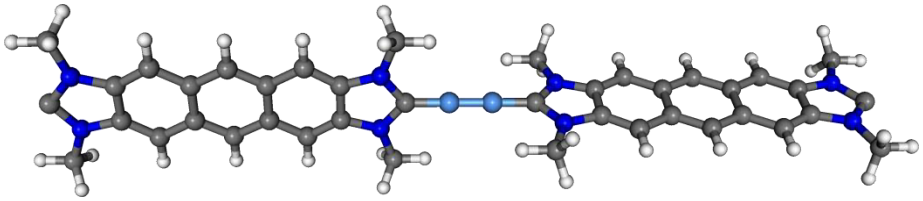
Total enthalpy, Htot (Utot + pV): -1726.025324 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1726.128098 hartrees

XYZ Coordinates

C	-7.742083469	-2.932248100	2.090190062
C	-6.475864946	-3.240517461	2.617626841
C	-5.359395836	-2.586608940	2.154438109
C	-5.439323627	-1.590473164	1.145227438
C	-6.738388210	-1.277341585	0.601127082
C	-7.863168335	-1.978249179	1.107984416
C	-6.808038633	-0.280784123	-0.415365915
C	-5.682792466	0.371944685	-0.934633150
C	-4.399329877	0.015684673	-0.444596001
C	-4.309830654	-0.904099861	0.609251993
N	-3.099691879	0.396515851	-0.762881657
C	-2.198581908	-0.220115209	0.090001250
N	-6.178072642	1.304018341	-1.857146595
C	-7.541402363	1.267163334	-1.949606278
N	-7.905390507	0.291242601	-1.076161528
N	-2.956885461	-1.003257349	0.934822556
C	-2.322899485	-1.750859042	2.008583583
C	-2.611522829	1.182472180	-1.882129629
C	-5.460757714	2.317286035	-2.616176959
C	-9.318666760	-0.015230869	-0.902503689
H	-9.857271586	0.658923450	-1.564400236
H	-9.539888122	-1.047499023	-1.184105178
H	-9.638140493	0.159106135	0.127484422
H	-1.276386446	-1.442675205	2.034026371
H	-2.789210103	-1.518025895	2.967670863
H	-2.365521900	-2.827278567	1.824764125
H	-3.088834166	0.862987867	-2.808747241
H	-1.537598053	1.000018117	-1.950062506
H	-2.770334441	2.251296139	-1.729177583
H	-4.840488601	2.934080267	-1.963634375
H	-6.223919687	2.939212539	-3.077649904
H	-4.842020274	1.877455508	-3.399772931
H	-4.401661324	-2.855220889	2.568592474
H	-8.844384528	-1.770718111	0.713368974
H	-8.623657739	-3.449203056	2.450960028

H	-6.375220237	-3.998432779	3.385788643
H	4.840488601	-2.934080267	-1.963634375
H	9.638140493	-0.159106135	0.127484422
H	2.770334441	-2.251296139	-1.729177583
H	2.789210103	1.518025895	2.967670863
C	5.460757714	-2.317286035	-2.616176959
C	7.541402363	-1.267163334	-1.949606278
C	9.318666760	0.015230869	-0.902503689
C	5.682792466	-0.371944685	-0.934633150
C	2.611522829	-1.182472180	-1.882129629
N	6.178072642	-1.304018341	-1.857146595
C	6.808038633	0.280784123	-0.415365915
N	7.905390507	-0.291242601	-1.076161528
C	4.399329877	-0.015684673	-0.444596001
C	6.738388210	1.277341585	0.601127082
C	7.863168335	1.978249179	1.107984416
C	4.309830654	0.904099861	0.609251993
C	2.198581908	0.220115209	0.090001250
N	3.099691879	-0.396515851	-0.762881657
C	5.439323627	1.590473164	1.145227438
C	7.742083469	2.932248100	2.090190062
C	5.359395836	2.586608940	2.154438109
C	6.475864946	3.240517461	2.617626841
C	2.322899485	1.750859042	2.008583583
N	2.956885461	1.003257349	0.934822556
H	6.223919687	-2.939212539	-3.077649904
H	9.857271586	-0.658923450	-1.564400236
H	1.537598053	-1.000018117	-1.950062506
H	8.844384528	1.770718111	0.713368974
H	8.623657739	3.449203056	2.450960028
H	1.276386446	1.442675205	2.034026371
H	4.401661324	2.855220889	2.568592474
H	6.375220237	3.998432779	3.385788643
H	4.842020274	-1.877455508	-3.399772931
H	9.539888122	1.047499023	-1.184105178
H	3.088834166	-0.862987867	-2.808747241
H	2.365521900	2.827278567	1.824764125
B	-0.724398759	-0.071680312	0.084659349
B	0.724398759	0.071680312	0.084659349

Compound 10BB10



Total enthalpy, Htot (Utot + pV): -2033.323716 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2033.437209 hartrees

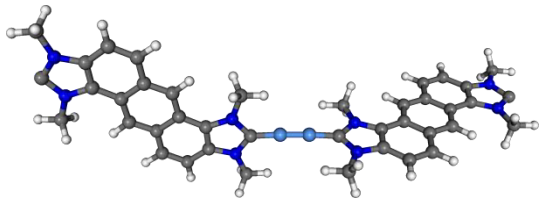
XYZ Coordinates

C	-0.504001459	0.504001459	-11.628128183
C	-1.013901026	1.013901026	-10.465101023
C	-0.512374627	0.512374627	-9.227330719
C	0.504001459	-0.504001459	-11.628128183
C	1.013901026	-1.013901026	-10.465101023
C	0.512374627	-0.512374627	-9.227330719
C	-0.987410999	0.987410999	-7.996457399
C	-0.513248101	0.513248101	-6.773107629
C	0.513248101	-0.513248101	-6.773107629
C	0.987410999	-0.987410999	-7.996457399
C	-1.015524487	1.015524487	-5.529761078
C	-0.506681463	0.506681463	-4.368381621
C	0.506681463	-0.506681463	-4.368381621
C	1.015524487	-1.015524487	-5.529761078
N	-0.762198661	0.762198661	-12.975937699
C	0.000000000	0.000000000	-13.818777763
N	0.762198661	-0.762198661	-12.975937699
N	-0.781556571	0.781556571	-3.039978206
C	0.000000000	0.000000000	-2.204888811
N	0.781556571	-0.781556571	-3.039978206
C	-1.732556499	1.732556499	-13.446175652
C	1.732556499	-1.732556499	-13.446175652
H	-1.780220234	1.780220234	-10.462661719
H	1.780220234	-1.780220234	-10.462661719
H	1.755239827	-1.755239827	-7.996922449
H	-1.755239827	1.755239827	-7.996922449
H	1.781429445	-1.781429445	-5.531058531
H	-1.781429445	1.781429445	-5.531058531
C	-1.752332246	1.752332246	-2.576978019
C	1.752332246	-1.752332246	-2.576978019
B	0.000000000	0.000000000	-0.731655091
C	-0.513248101	-0.513248101	6.773107629
C	0.506681463	0.506681463	4.368381621
C	0.513248101	0.513248101	6.773107629
C	0.000000000	0.000000000	2.204888811

C	0.000000000	0.000000000	13.818777763
C	-0.506681463	-0.506681463	4.368381621
C	1.015524487	1.015524487	5.529761078
C	-1.015524487	-1.015524487	5.529761078
C	-0.987410999	-0.987410999	7.996457399
C	0.512374627	0.512374627	9.227330719
C	1.013901026	1.013901026	10.465101023
B	0.000000000	0.000000000	0.731655091
C	0.504001459	0.504001459	11.628128183
C	0.987410999	0.987410999	7.996457399
C	-1.013901026	-1.013901026	10.465101023
C	-0.504001459	-0.504001459	11.628128183
C	-0.512374627	-0.512374627	9.227330719
N	-0.762198661	-0.762198661	12.975937699
N	-0.781556571	-0.781556571	3.039978206
N	0.781556571	0.781556571	3.039978206
N	0.762198661	0.762198661	12.975937699
C	1.732556499	1.732556499	13.446175652
H	1.781429445	1.781429445	5.531058531
C	1.752332246	1.752332246	2.576978019
C	-1.752332246	-1.752332246	2.576978019
H	-1.781429445	-1.781429445	5.531058531
H	1.755239827	1.755239827	7.996922449
C	-1.732556499	-1.732556499	13.446175652
H	1.780220234	1.780220234	10.462661719
H	-1.780220234	-1.780220234	10.462661719
H	-1.755239827	-1.755239827	7.996922449
H	-1.747845611	1.747845611	-1.487138953
H	-1.492902487	2.753091156	-2.934584219
H	-2.753091156	1.492902487	-2.934584219
H	1.747845611	-1.747845611	-1.487138953
H	2.753091156	-1.492902487	-2.934584219
H	1.492902487	-2.753091156	-2.934584219
H	-1.747845611	-1.747845611	1.487138953
H	-2.753091156	-1.492902487	2.934584219
H	-1.492902487	-2.753091156	2.934584219
H	1.747845611	1.747845611	1.487138953
H	1.492902487	2.753091156	2.934584219
H	2.753091156	1.492902487	2.934584219
H	-1.712603293	1.712603293	-14.533497933
H	-2.737817054	1.479504422	-13.095565500
H	-1.479504422	2.737817054	-13.095565500
H	1.712603293	-1.712603293	-14.533497933
H	1.479504422	-2.737817054	-13.095565500
H	2.737817054	-1.479504422	-13.095565500
H	1.712603293	1.712603293	14.533497933
H	1.479504422	2.737817054	13.095565500
H	2.737817054	1.479504422	13.095565500

H	-1.712603293	-1.712603293	14.533497933
H	-1.479504422	-2.737817054	13.095565500
H	-2.737817054	-1.479504422	13.095565500

Compound 11BB11



Total enthalpy, Htot (Utot + pV): -2033.305159 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2033.418319 hartrees

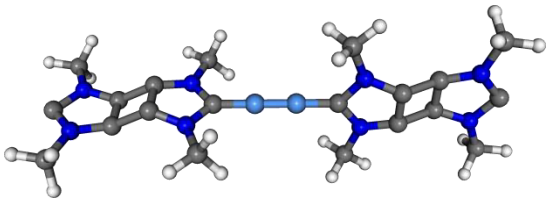
XYZ Coordinates

C	-9.222500045	-1.230994304	2.494679214
C	-7.921315813	-1.144794366	2.088200688
C	-7.506645604	-0.235727334	1.059832103
C	-8.472961074	0.630461758	0.412597174
C	-9.825594873	0.509073843	0.866661359
C	-10.169856307	-0.387955027	1.866399582
C	-6.165579874	-0.175714463	0.670954631
C	-5.705611533	0.692774161	-0.327329446
C	-6.673022167	1.558464778	-0.974861948
C	-8.016662686	1.496483316	-0.582332558
C	-4.355952680	0.810482543	-0.780656761
C	-4.014650808	1.707474271	-1.788705900
C	-4.960362774	2.547346943	-2.412166416
C	-6.264895742	2.462828192	-2.000879386
N	-3.178902223	0.167839619	-0.414449565
C	-2.112746907	0.635757285	-1.172795110
N	-2.657895049	1.588516897	-2.013581245
N	-11.537590612	-0.252223669	2.061861866
C	-12.093587459	0.685578544	1.240070744
N	-11.022232426	1.140263405	0.514066707
C	-12.315657154	-1.010653030	3.026078029
C	-11.202701224	2.171335600	-0.496287939
C	-2.992265256	-0.858888219	0.596507351
C	-1.893620813	2.337370200	-2.992250107
H	-7.167278762	-1.774865893	2.546250942
H	-9.522226806	-1.922252738	3.272922935
H	-8.709508148	2.155752210	-1.085959574
H	-7.018271288	3.093465842	-2.458694231
H	-4.660372230	3.236691880	-3.191512646
H	-5.474639657	-0.836271630	1.174600156

H	-1.929562971	-1.104842151	0.614392736
H	-3.291344561	-0.492750617	1.581455485
H	-3.561533778	-1.758349631	0.349162391
H	-0.865765315	1.974746301	-2.958237950
H	-1.906517864	3.406102812	-2.759685888
H	-2.299445932	2.181370328	-3.995766031
H	-13.347484226	-0.678180753	2.938696668
H	-12.260723495	-2.082583277	2.816235490
H	-11.960728567	-0.828945891	4.044462312
H	-12.260807508	2.423112642	-0.496570409
H	-10.917613853	1.806754139	-1.486541767
H	-10.618799153	3.063901546	-0.257086512
B	-0.697497673	0.207361001	-1.112585809
H	12.260723495	2.082583277	2.816235490
H	3.561533778	1.758349631	0.349162391
H	10.917613853	-1.806754139	-1.486541767
C	12.315657154	1.010653030	3.026078029
C	9.222500045	1.230994304	2.494679214
C	7.921315813	1.144794366	2.088200688
C	10.169856307	0.387955027	1.866399582
N	11.537590612	0.252223669	2.061861866
H	9.522226806	1.922252738	3.272922935
C	12.093587459	-0.685578544	1.240070744
H	13.347484226	0.678180753	2.938696668
C	7.506645604	0.235727334	1.059832103
C	9.825594873	-0.509073843	0.866661359
H	2.299445932	-2.181370328	-3.995766031
C	6.165579874	0.175714463	0.670954631
H	7.167278762	1.774865893	2.546250942
C	8.472961074	-0.630461758	0.412597174
C	2.992265256	0.858888219	0.596507351
N	11.022232426	-1.140263405	0.514066707
C	5.705611533	-0.692774161	-0.327329446
C	8.016662686	-1.496483316	-0.582332558
C	11.202701224	-2.171335600	-0.496287939
H	5.474639657	0.836271630	1.174600156
C	4.355952680	-0.810482543	-0.780656761
N	3.178902223	-0.167839619	-0.414449565
C	6.673022167	-1.558464778	-0.974861948
C	2.112746907	-0.635757285	-1.172795110
B	0.697497673	-0.207361001	-1.112585809
H	1.929562971	1.104842151	0.614392736
C	4.014650808	-1.707474271	-1.788705900
C	6.264895742	-2.462828192	-2.000879386
C	4.960362774	-2.547346943	-2.412166416
N	2.657895049	-1.588516897	-2.013581245
H	12.260807508	-2.423112642	-0.496570409
H	8.709508148	-2.155752210	-1.085959574

C	1.893620813	-2.337370200	-2.992250107
H	7.018271288	-3.093465842	-2.458694231
H	11.960728567	0.828945891	4.044462312
H	4.660372230	-3.236691880	-3.191512646
H	0.865765315	-1.974746301	-2.958237950
H	3.291344561	0.492750617	1.581455485
H	10.618799153	-3.063901546	-0.257086512
H	1.906517864	-3.406102812	-2.759685888

Compound 12BB12



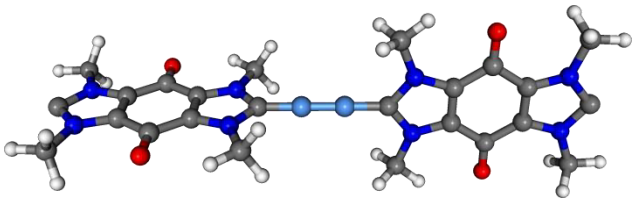
Total enthalpy, Htot (Utot + pV): -1263.637885 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1263.735661 hartrees

XYZ Coordinates

C	-2.822393932	1.934296592	-0.359402739
C	-1.403582930	2.084085211	0.244571850
C	-1.253636321	0.736839202	0.239475543
C	-2.670187228	0.576224260	-0.363805540
N	-0.156684305	2.634638181	0.012411388
C	0.812769850	1.649629844	-0.031238657
N	0.083578976	0.476093340	0.005802287
N	-4.123528786	2.220979994	-0.003855585
C	-4.837663774	1.017099651	0.072152825
N	-3.873586746	0.003619690	-0.016003355
C	0.171720939	4.051642240	-0.035097430
C	0.716363890	-0.832694411	-0.050607486
C	-4.779231346	3.514100465	0.008213240
C	-4.223839423	-1.403074035	-0.015532415
H	-4.020822523	4.291484086	0.102272850
H	-5.467177338	3.559624656	0.854335615
H	-5.356787852	3.667134533	-0.909799967
H	-0.457577636	4.558159422	-0.770962431
H	1.216660740	4.137214074	-0.325171843
H	0.026889166	4.519672025	0.941946426
H	1.758186301	-0.682542597	-0.324474792
H	0.224836893	-1.455734770	-0.801450049
H	0.664470917	-1.333201848	0.919274797
H	-4.884125404	-1.608332713	0.828797292
H	-3.310919276	-1.991748614	0.071555283

H	-4.753547644	-1.672386654	-0.935225891
H	-9.041120592	-0.490142819	-2.397625319
H	-15.641292964	-0.322003415	-1.823843788
C	-9.652998400	0.386523163	-2.159721422
H	-8.791975006	-0.468468189	2.969584552
H	-10.529670225	0.412774273	-2.806991467
N	-10.093452036	0.350549148	-0.778136530
C	-14.610137777	0.014003998	-1.908394070
C	-9.205627833	0.494702066	0.296323439
C	-11.305530863	-0.083694921	-0.286255423
H	-14.036016933	-0.706237184	-2.496575564
C	-12.766351299	0.425822199	-0.215883504
H	-13.761037083	-0.675672568	3.538547584
N	-14.066891608	0.107291988	-0.561526630
C	-11.242175718	-0.076196298	1.078817688
N	-9.989415978	0.360300974	1.450375305
C	-12.702756043	0.434035869	1.138214701
C	-14.864794799	0.019798610	0.564292349
C	-9.421929611	0.407652512	2.783753119
N	-13.964569709	0.122905244	1.608278920
H	-8.800179603	1.299631141	2.878884049
C	-14.378842082	0.047294444	3.000713293
H	-9.044466434	1.278301589	-2.319530081
H	-15.417501538	-0.275020801	3.017026553
H	-14.584059634	0.985684370	-2.407948414
H	-10.233977629	0.439388747	3.509880747
H	-14.293234047	1.022451382	3.486219287
B	-6.298492423	0.849231797	0.152779870
B	-7.746321485	0.676456618	0.225696991

Compound 13BB13



Total enthalpy, Htot (Utot + pV): -1717.372450 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1717.476616 hartree

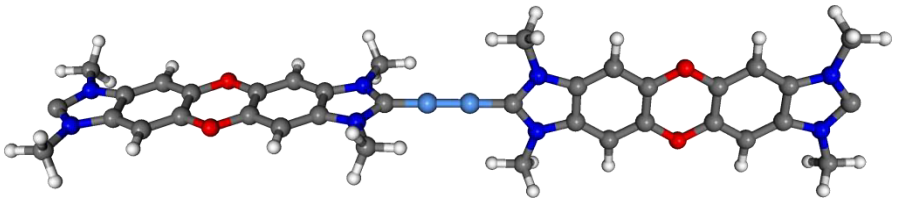
XYZ Coordinates

C	-5.666149402	0.492445800	1.081151413
C	-4.387836253	0.042785285	0.498442982
C	-6.818065208	-0.203987499	0.483958766
C	-6.717985966	-1.157181523	-0.496796838

C	-5.445281485	-1.610946808	-1.081871697
C	-4.287011696	-0.917102287	-0.487315066
N	-8.163686660	-0.066329942	0.754626993
C	-8.936895520	-0.897301709	-0.017459994
N	-8.006939961	-1.558131052	-0.780710037
N	-3.113598929	0.461870976	0.800218807
C	-2.191569985	-0.220966180	0.014458239
N	-2.952455190	-1.073827319	-0.777926650
O	-5.370128928	-2.462881092	-1.957238093
C	-8.747442226	0.843417145	1.737809651
C	-8.389405219	-2.564067351	-1.769016665
C	-2.341290697	-1.970913392	-1.750564764
C	-2.701713097	1.462226573	1.776797152
H	-3.583403573	1.851941291	2.275123075
H	-2.161395797	2.263147685	1.266055983
H	-2.021711476	1.001198266	2.497384333
H	-8.373117130	0.617532235	2.736691046
H	-9.824111266	0.698062450	1.694351802
H	-8.493243805	1.876766148	1.500165317
H	-9.473882164	-2.634983398	-1.736002917
H	-7.937778904	-3.526930504	-1.528547253
H	-8.057834405	-2.266999571	-2.764388702
H	-1.650325471	-2.642818391	-1.235485068
H	-1.767374929	-1.382325842	-2.470637950
H	-3.122929715	-2.533719508	-2.250523205
O	-5.770175832	1.341372469	1.956410795
H	9.824111266	-0.698062450	1.694351802
H	8.057834405	2.266999571	-2.764388702
H	2.161395797	-2.263147685	1.266055983
C	8.747442226	-0.843417145	1.737809651
C	8.936895520	0.897301709	-0.017459994
N	8.163686660	0.066329942	0.754626993
H	1.767374929	1.382325842	-2.470637950
C	6.818065208	0.203987499	0.483958766
C	8.389405219	2.564067351	-1.769016665
N	8.006939961	1.558131052	-0.780710037
H	8.493243805	-1.876766148	1.500165317
O	5.770175832	-1.341372469	1.956410795
C	5.666149402	-0.492445800	1.081151413
C	6.717985966	1.157181523	-0.496796838
H	9.473882164	2.634983398	-1.736002917
C	4.387836253	-0.042785285	0.498442982
C	5.445281485	1.610946808	-1.081871697
C	2.701713097	-1.462226573	1.776797152
C	4.287011696	0.917102287	-0.487315066
O	5.370128928	2.462881092	-1.957238093
N	3.113598929	-0.461870976	0.800218807
H	3.583403573	-1.851941291	2.275123075

C	2.191569985	0.220966180	0.014458239
N	2.952455190	1.073827319	-0.777926650
C	2.341290697	1.970913392	-1.750564764
H	8.373117130	-0.617532235	2.736691046
H	1.650325471	2.642818391	-1.235485068
H	7.937778904	3.526930504	-1.528547253
H	2.021711476	-1.001198266	2.497384333
H	3.122929715	2.533719508	-2.250523205
B	-0.726441034	-0.073243523	0.018814598
B	0.726441034	0.073243523	0.018814598

Compound 14BB14



Total enthalpy, Htot (Utot + pV): -2179.402907 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2179.513776 hartrees

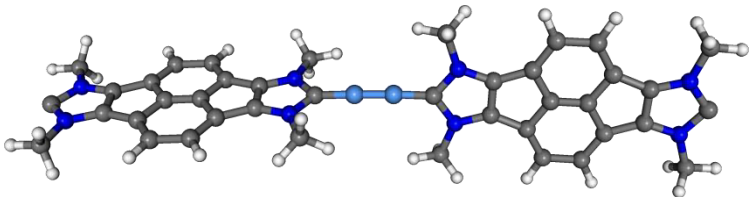
XYZ Coordinates

O	-3.305337899	0.711159790	1.473696811
C	-4.415984157	0.687041185	0.652277605
C	-4.298085367	0.684007250	-0.739161289
O	-3.065020829	0.704358760	-1.362166544
C	-1.954524277	0.767644118	-0.545061556
C	-2.073171316	0.771112925	0.854802114
C	-0.952390129	0.833227742	1.673093804
C	0.292295899	0.890651626	1.052871805
C	0.410563205	0.886949538	-0.342946862
C	-0.712040546	0.825842177	-1.163427638
C	-5.664671362	0.664094154	1.274555608
C	-6.786379815	0.638088347	0.456963226
C	-6.667620647	0.633996209	-0.945244902
C	-5.424353176	0.658577664	-1.562640420
N	1.595310226	0.959949298	1.539520409
C	2.529543686	1.000201788	0.539309540
N	1.776946738	0.954170845	-0.603699367
N	-8.138789269	0.615329364	0.744057763
C	-8.883550190	0.593322596	-0.426776866
N	-7.952402450	0.602832406	-1.455629248
C	1.943754570	0.987892062	2.948602929
C	2.357729329	0.974713667	-1.934135646
C	-8.713855230	0.615945223	2.074291250

C	-8.295273976	0.588415379	-2.863611763
H	-8.372023788	1.489432055	2.637071692
H	-8.436238885	-0.292621512	2.616938934
H	-9.798541785	0.655133163	1.971564802
H	-9.378455314	0.495444434	-2.945250997
H	-7.820523244	-0.261400957	-3.362427372
H	-7.976194388	1.515014381	-3.350169171
H	1.596112133	0.082132283	3.454239258
H	1.504020789	1.859906714	3.441677123
H	3.027956394	1.044491474	3.013171026
H	3.437388427	1.030666790	-1.815417952
H	2.008351998	1.844280246	-2.498703411
H	2.099065693	0.066442793	-2.486455759
H	-14.007192359	3.566810757	-1.563108991
H	-25.428374714	2.808898769	-1.843170636
C	-13.702042037	2.995999717	-0.681140238
H	-13.895986960	-2.431376477	-1.888903911
H	-14.124684573	3.463409043	0.213246774
N	-14.137895090	1.618116754	-0.791034486
C	-16.646256770	1.905985686	-0.965232564
C	-15.450858297	1.201878470	-0.913204838
C	-13.280829961	0.526547411	-0.783694308
C	-24.349152155	2.846856873	-1.713778031
C	-17.822661302	1.166661698	-1.094568324
O	-19.007965081	1.875128403	-1.138720316
H	-23.803460468	-2.515559274	-2.877508691
C	-21.355242683	1.852120893	-1.422409286
C	-20.164085343	1.144330568	-1.323106825
C	-15.427325155	-0.203080421	-0.987973881
H	-23.906211140	3.434350868	-2.523483655
N	-14.101081410	-0.585993022	-0.907164289
C	-22.524014654	1.118462475	-1.603819808
C	-17.799249302	-0.227492804	-1.171648642
N	-23.862108054	1.479459496	-1.740362331
C	-16.598566827	-0.936904908	-1.119613372
C	-20.140336408	-0.258117786	-1.403788990
C	-13.619086314	-1.952223079	-0.945165275
C	-24.685277431	0.397681675	-1.904358731
C	-22.500072578	-0.279699395	-1.686106830
O	-18.960121918	-0.965865630	-1.299313701
C	-21.306856237	-0.989454826	-1.587863415
N	-23.825397769	-0.667360004	-1.867262096
H	-12.532609430	-1.928138775	-0.858836338
C	-24.265423662	-2.044068765	-2.004988148
H	-12.614224620	2.999968506	-0.609205558
H	-25.345465031	-2.027755235	-2.132288621
H	-24.113888526	3.325971418	-0.758766148
H	-14.033859625	-2.529855762	-0.113833718

H	-24.013023731	-2.625172183	-1.113035022
B	-10.355231126	0.566137870	-0.550554517
B	-11.808569539	0.545517687	-0.668133912
H	-0.658871559	0.821650301	-2.244238866
H	-5.295498921	0.659302562	-2.636652793
H	-1.081812629	0.834783762	2.747463865
H	-5.718293982	0.666600809	2.354873676
H	-16.618039411	-2.016632537	-1.182126755
H	-16.701925369	2.984834147	-0.910089145
H	-21.250532092	-2.068532744	-1.646483416
H	-21.335563616	2.932032716	-1.355483325

Compound 15BB15



Total enthalpy, Htot (Utot + pV): -2030.778660 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2030.895396 hartrees

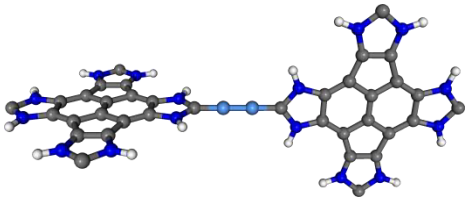
XYZ Coordinates

C	-2.126820121	2.404317232	0.040265640
C	-0.686296802	2.396516920	-0.095068351
C	0.020769870	1.208410232	-0.098953486
C	-0.737199824	0.006455998	0.038732963
C	-2.082131243	0.013562853	0.165881651
C	-2.837752340	1.222391399	0.169082881
C	-2.841619674	-1.186486762	0.304420280
C	-2.132905019	-2.375385783	0.298650136
C	-0.691981971	-2.383047047	0.160225066
C	0.018744013	-1.203287833	0.029837858
C	1.395122420	0.685582745	-0.204052593
C	1.394652185	-0.693928182	-0.131024552
C	-4.209815694	0.715658978	0.322998887
C	-4.212994145	-0.664193353	0.406119737
N	-5.512823291	1.143164264	0.398079959
C	-6.359329503	0.042974526	0.548197631
N	-5.518534398	-1.073221565	0.553391091
N	2.712215224	1.070004971	-0.356218384
C	3.564323220	-0.013717852	-0.384822719
N	2.712247506	-1.090045257	-0.242907034
C	3.185638538	2.442900977	-0.476875671
C	3.186924914	-2.467245501	-0.222727805

C	-5.992062067	2.513608666	0.375687256
C	-6.000108561	-2.440659303	0.656864093
H	-5.310679952	3.128136337	-0.215898163
H	-6.066526893	2.922843526	1.389276038
H	-6.988816335	2.519731588	-0.074899620
H	-7.047382210	-2.402745284	0.961307008
H	-5.417778150	-2.988005869	1.404671005
H	-5.930948778	-2.956003937	-0.307606697
H	2.746939653	2.926937340	-1.355934763
H	4.267930686	2.403088139	-0.584337649
H	2.930239284	3.024528069	0.416249657
H	4.268399921	-2.436910772	-0.337199010
H	2.746462709	-3.042844772	-1.046096191
H	2.935102957	-2.951229404	0.724789339
H	-21.466609861	1.167212672	-1.216031610
H	-11.234803153	-0.510889837	-2.085518256
H	-19.967406047	-0.344040786	4.036224494
C	-20.384385284	1.091324704	-1.283820385
C	-16.504595337	0.805223661	-1.336694333
C	-15.061984299	0.705768143	-1.381868818
N	-19.873060809	0.921670372	0.070268433
H	-20.120477986	0.232974249	-1.909380627
C	-20.697841545	0.880655694	1.170532401
H	-11.691270252	-0.688111566	3.907338190
C	-17.180593553	0.739203705	-0.136152920
C	-18.543452762	0.787239682	0.419666734
C	-11.202124793	0.469937086	-1.595705990
C	-14.318857510	0.542648222	-0.223930003
C	-18.505887005	0.653641827	1.792314777
C	-16.389278707	0.567660665	1.040455694
N	-19.815532241	0.713273271	2.219644740
C	-15.042374892	0.474455618	0.998370003
C	-12.930821095	0.404369371	0.244316267
H	-11.841731668	1.170753705	-2.140022195
N	-11.638859222	0.379821079	-0.216424210
C	-17.114172618	0.505227112	2.263534133
C	-20.255220868	0.617911492	3.602079744
C	-12.889067248	0.261437313	1.616549998
C	-10.759562851	0.201244141	0.853874997
C	-14.248701147	0.305495236	2.172645027
C	-16.369960349	0.343304640	3.418602846
C	-14.926987868	0.242762413	3.373629729
N	-11.569650061	0.124809901	1.985608082
H	-21.338895174	0.705616123	3.599672822
C	-11.042511210	-0.025657188	3.330159413
H	-19.982424644	2.002945734	-1.737574785
H	-10.045404492	-0.460095684	3.254419376
H	-10.169146716	0.828373120	-1.595593626

H	-19.821949114	1.424633866	4.203831070
H	-10.963009192	0.942854966	3.836170686
B	-7.833037411	0.070989359	0.675246714
B	-9.283443315	0.126226354	0.782523716
H	-2.632805112	-3.334569281	0.395487784
H	-0.194234029	-3.347917474	0.161882898
H	-2.623628057	3.369687378	0.039413020
H	-0.186038187	3.356095700	-0.193514886
H	-14.400852137	0.120488617	4.315501171
H	-16.841833497	0.289814078	4.392125914
H	-14.589086332	0.762128618	-2.354916145
H	-17.031231157	0.933469829	-2.278875311

Compound 16BB16



Total enthalpy, Htot (Utot + pV): -2306.828517 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2306.930036 hartrees

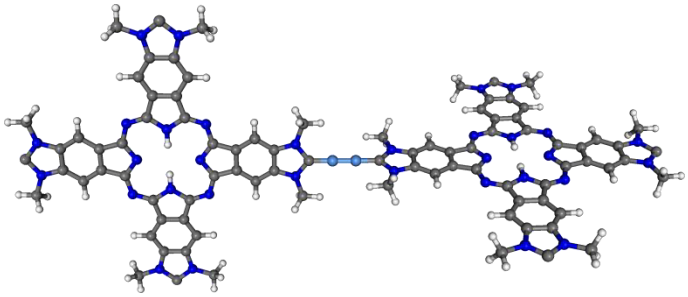
XYZ Coordinates

C	2.008743060	-2.008743060	-6.053329333
C	1.037645938	-1.037645938	-5.549539822
C	0.484107566	-0.484107566	-6.746070240
C	-0.484107566	0.484107566	-6.746070240
C	1.033433718	-1.033433718	-7.935210163
C	2.006113117	-2.006113117	-7.432507479
C	-1.037645938	1.037645938	-5.549539822
C	-2.008743060	2.008743060	-6.053329333
C	-2.006113117	2.006113117	-7.432507479
C	-1.033433718	1.033433718	-7.935210163
N	-2.952055402	2.952055402	-5.680310590
C	-3.564219986	3.564219986	-6.749410373
N	-2.947223067	2.947223067	-7.812871157
C	0.516544954	-0.516544954	-4.381703807
C	-0.516544954	0.516544954	-4.381703807
N	0.771707588	-0.771707588	-3.048089717
C	0.000000000	0.000000000	-2.201118734
N	-0.771707588	0.771707588	-3.048089717
C	0.510647292	-0.510647292	-9.110707868
C	-0.510647292	0.510647292	-9.110707868
N	0.751848220	-0.751848220	-10.461656722

C	0.000000000	0.000000000	-11.321930355
N	-0.751848220	0.751848220	-10.461656722
N	2.952055402	-2.952055402	-5.680310590
C	3.564219986	-3.564219986	-6.749410373
N	2.947223067	-2.947223067	-7.812871157
H	3.202204503	-3.202204503	-4.738727796
H	3.191388815	-3.191388815	-8.757836934
H	1.419808844	-1.419808844	-10.807599599
H	-1.419808844	1.419808844	-10.807599599
H	-3.191388815	3.191388815	-8.757836934
H	-3.202204503	3.202204503	-4.738727796
H	-1.437860442	1.437860442	-2.695878502
H	1.437860442	-1.437860442	-2.695878502
C	2.006113117	2.006113117	7.432507479
C	1.033433718	1.033433718	7.935210163
C	0.484107566	0.484107566	6.746070240
C	-0.484107566	-0.484107566	6.746070240
C	1.037645938	1.037645938	5.549539822
C	2.008743060	2.008743060	6.053329333
C	-1.033433718	-1.033433718	7.935210163
C	-2.006113117	-2.006113117	7.432507479
C	-2.008743060	-2.008743060	6.053329333
C	-1.037645938	-1.037645938	5.549539822
N	-2.947223067	-2.947223067	7.812871157
C	-3.564219986	-3.564219986	6.749410373
N	-2.952055402	-2.952055402	5.680310590
C	0.510647292	0.510647292	9.110707868
C	-0.510647292	-0.510647292	9.110707868
N	0.751848220	0.751848220	10.461656722
C	0.000000000	0.000000000	11.321930355
N	-0.751848220	-0.751848220	10.461656722
C	0.516544954	0.516544954	4.381703807
C	-0.516544954	-0.516544954	4.381703807
N	0.771707588	0.771707588	3.048089717
C	0.000000000	0.000000000	2.201118734
N	-0.771707588	-0.771707588	3.048089717
N	2.947223067	2.947223067	7.812871157
C	3.564219986	3.564219986	6.749410373
N	2.952055402	2.952055402	5.680310590
H	3.191388815	3.191388815	8.757836934
H	3.202204503	3.202204503	4.738727796
H	1.437860442	1.437860442	2.695878502
H	-1.437860442	-1.437860442	2.695878502
H	-3.202204503	-3.202204503	4.738727796
H	-3.191388815	-3.191388815	8.757836934
H	-1.419808844	-1.419808844	10.807599599
H	1.419808844	1.419808844	10.807599599
B	0.000000000	0.000000000	-0.733430436

B 0.000000000 0.000000000 0.733430436

Compound 17BB17



Total enthalpy, Htot (Utot + pV): -5195.634299 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -5195.866710 hartrees

XYZ Coordinates

C	0.211197003	-1.543404563	-9.337349543
C	-1.186200417	-1.326323402	-9.300837341
C	0.956664797	-1.783621314	-8.186753529
C	0.230648328	-1.794688324	-6.999877531
C	-1.162368091	-1.578267666	-6.963338360
C	-1.909819296	-1.338081312	-8.111784690
C	-1.536298399	-1.671707706	-5.550060225
N	-0.445325182	-1.926452306	-4.775151275
C	0.630533205	-2.007136808	-5.607086606
N	-2.801074301	-1.519574874	-5.153881032
C	-3.193606470	-1.598949267	-3.900886379
N	-2.429206456	-1.839103561	-2.782581012
C	-3.176231785	-1.856594673	-1.626340206
C	-4.548616053	-1.606895848	-2.025074339
C	-4.559108476	-1.446051348	-3.435190591
C	-5.733538507	-1.190472829	-4.145060386
C	-6.886472250	-1.105874235	-3.379338472
C	-6.876162126	-1.267077967	-1.969068121
C	-5.712297491	-1.520047269	-1.258929794
N	-2.761183600	-2.053108504	-0.394098195
C	-1.486477851	-2.275168344	-0.065633345
N	-0.411303528	-2.349337716	-0.901095099
C	0.682127869	-2.581922679	-0.120404891
C	0.310582563	-2.658108810	1.292419944
C	-1.809606606	-2.477371423	2.519103521
C	-1.059470211	-2.679801071	3.671499447
C	0.348199316	-2.864837586	3.636393872
C	1.067758653	-2.860343998	2.447478017
C	2.339163564	-2.673038799	-1.768011111
N	1.572485889	-2.440624158	-2.887385891
C	2.315936587	-2.439294747	-4.044850762

C	3.687297766	-2.697127586	-3.648295813
C	3.701858457	-2.841487156	-2.236492080
C	4.876979259	-3.098856205	-1.528661278
C	6.025839184	-3.203609562	-2.298214273
C	6.011117114	-3.059185157	-3.709987769
C	4.846816623	-2.803339948	-4.418059548
N	1.901330098	-2.244275468	-5.277580760
N	1.948404343	-2.734445140	-0.514004180
C	-1.082393648	-2.467860927	1.327269586
H	-1.428509216	-1.988936876	-2.804310037
H	0.572661277	-2.285970071	-2.860164382
N	0.562293818	-1.456756322	-10.681404066
N	-1.562151726	-1.126579611	-10.625851334
H	2.025883339	-1.951991556	-8.198949697
H	-2.978804386	-1.174056626	-8.068244720
H	-5.724405556	-1.070398334	-5.220450339
N	-8.216693127	-0.871424012	-3.711939709
N	-8.201141545	-1.116228181	-1.573332595
H	-5.687149437	-1.645446231	-0.184418452
H	-2.881980354	-2.334207048	2.531009856
N	-1.430118984	-2.739698310	5.001292530
N	0.755592897	-3.030127895	4.946203424
H	2.139923781	-2.998973452	2.406525599
H	4.871363857	-3.206404457	-0.452031142
N	7.355178496	-3.446940880	-1.968642801
N	7.332789776	-3.227992504	-4.109551831
H	4.818660081	-2.690579218	-5.493794561
C	8.180319322	-3.467281251	-3.061230265
C	-0.507871386	-1.201328776	-11.496419134
C	-9.046415655	-0.872134149	-2.622776266
C	-0.325076944	-2.951882218	5.811104178
C	7.784579756	-3.160501100	-5.488621021
C	7.835771580	-3.658401915	-0.614113684
C	2.123084651	-3.254850174	5.372752227
C	-2.782785742	-2.584567924	5.499468848
C	-8.658091528	-1.206038544	-0.197123372
C	-8.693155594	-0.648370415	-5.066233041
C	-2.923610864	-0.866087730	-11.059091544
C	1.915019345	-1.617629288	-11.185256204
H	1.874327430	-1.496606946	-12.265338941
H	2.581311462	-0.862352842	-10.758300522
H	2.304328058	-2.611073301	-10.943961176
H	-2.903010406	-0.755926002	-12.140885056
H	-3.582981022	-1.696192680	-10.789290468
H	-3.306961444	0.052817565	-10.606005412
H	-9.768465500	-0.496731317	-5.009601256
H	-8.222210802	0.237047681	-5.502587715
H	-8.479461637	-1.513569598	-5.700345009

H	-9.733591069	-1.045808404	-0.202714301
H	-8.438301800	-2.192289899	0.221402216
H	-8.178603628	-0.442344349	0.422015738
H	-2.745952216	-2.608049266	6.588635063
H	-3.200580363	-1.628707880	5.171157829
H	-3.421629458	-3.397510231	5.143161732
H	2.116482434	-3.434040492	6.447955195
H	2.540325235	-4.126577764	4.861082518
H	2.744422036	-2.380743486	5.158124557
H	8.909380904	-3.821253085	-0.674076764
H	7.633564315	-2.783546358	0.010562148
H	7.358298103	-4.533901577	-0.165003299
H	8.858588130	-3.330931582	-5.485508029
H	7.295178650	-3.927657818	-6.095417801
H	7.572144876	-2.177656489	-5.918906044
C	-0.137871391	-4.044146716	12.339195988
C	-0.244254143	-2.629741608	12.410068701
C	-0.049705640	-4.838845634	13.476029336
C	-0.071374777	-4.149669792	14.689893618
C	-0.185150071	-2.749556750	14.759746384
C	-0.271060869	-1.947597335	13.620585637
C	-0.181252653	-2.426027188	16.186431263
N	-0.060302197	-3.553996479	16.942865305
C	0.009682141	-4.605777431	16.077804365
N	-0.293484087	-1.165719374	16.612219263
C	-0.300435367	-0.818200559	17.880285165
N	-0.188127566	-1.631295390	18.985345206
C	-0.231402993	-0.926076584	20.165694925
C	-0.389668408	0.469073953	19.800756364
C	-0.431688856	0.536013713	18.383671945
C	-0.578091289	1.744756064	17.701379146
C	-0.679896554	2.872646218	18.501553693
C	-0.637814727	2.805691235	19.918691336
C	-0.492014109	1.607798334	20.601548648
N	-0.146900020	-1.389488650	21.393804394
C	0.000446226	-2.680758505	21.694496823
N	0.084462213	-3.732896843	20.833222524
C	0.228632445	-4.859555106	21.585336569
C	0.242056158	-4.534998573	23.013609200
C	0.060138128	-2.447367697	24.293014180
C	0.182679645	-3.239647393	25.430741991
C	0.331168493	-4.644621465	25.360543546
C	0.364495905	-5.329390113	24.149093240
C	0.333942519	-6.466200650	19.888864266
N	0.209347654	-5.655046692	18.784735719
C	0.234415526	-6.362770221	17.604278255
C	0.389414744	-7.758060010	17.969977738
C	0.451909382	-7.822166562	19.386420904

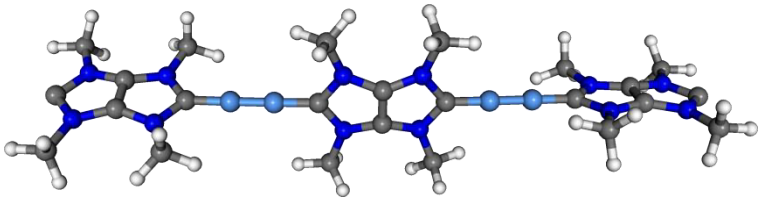
C	0.600843136	-9.030490956	20.069317079
C	0.683429822	-10.161000665	19.270441016
C	0.621391920	-10.096819816	17.853892272
C	0.473504139	-8.899232198	17.170412733
N	0.142158776	-5.899685449	16.377062669
N	0.345145589	-6.117775850	21.157078832
C	0.094218501	-3.134459597	23.083743429
H	-0.083990807	-2.636606712	18.933006653
H	0.108091473	-4.649112983	18.832559347
N	-0.136696206	-4.370757937	10.996399540
N	-0.310469690	-2.174678203	11.107222398
H	0.030699367	-5.917078155	13.436759113
H	-0.349452306	-0.870576951	13.689116383
H	-0.608593386	1.778806273	16.620255081
N	-0.832758676	4.222558419	18.202867517
N	-0.768907436	4.121087108	20.352045880
H	-0.458088577	1.539922621	21.680950778
H	-0.054370136	-1.371696201	24.330908418
N	0.194752330	-2.935424311	26.788819394
N	0.420806941	-5.071626932	26.682307254
H	0.476963050	-6.403599593	24.079704489
H	0.646700256	-9.062404398	21.149892050
N	0.831291440	-11.511551526	19.569958359
N	0.737176067	-11.414066085	17.421785741
H	0.424407321	-8.833375099	16.091442591
C	0.866949561	-12.304449507	18.454152967
C	-0.241822133	-3.231846387	10.213027698
C	-0.890466389	5.012593410	19.319942200
C	0.339799855	-4.042268491	27.581676540
C	0.723430805	-11.820609666	16.027062384
C	0.937705579	-12.042806261	20.918076746
C	0.583085464	-6.457748466	27.084209860
C	0.068040632	-1.592431029	27.326964751
C	-0.777865087	4.524575383	21.747801945
C	-0.923725639	4.756025945	16.854553803
C	-0.424183432	-0.783785348	10.713045510
C	-0.039353136	-5.715830672	10.463425900
H	0.094153855	-5.643271625	9.384116228
H	0.818580086	-6.231939277	10.901981732
H	-0.948791573	-6.285680423	10.674841053
H	-0.615720685	-0.750595271	9.640363032
H	-1.252822706	-0.310197599	11.245898187
H	0.500582231	-0.240488445	10.928781904
H	-1.037035628	5.834147342	16.940666810
H	-0.018110733	4.528573972	16.284916055
H	-1.787810197	4.339188110	16.329247164
H	-0.893889289	5.605561825	21.771101713
H	-1.609740435	4.056748315	22.281985352

H	0.159712446	4.247537607	22.238040639
H	0.112881204	-1.672660967	28.410633252
H	0.883063047	-0.953665205	26.974505899
H	-0.885700983	-1.144340523	27.033421891
H	0.621653251	-6.477013648	28.170986685
H	-0.259077966	-7.064160159	26.738197508
H	1.509742783	-6.874359774	26.678922089
H	1.042722701	-13.121899578	20.832850194
H	1.811855178	-11.630502489	21.430176337
H	0.041559881	-11.808117096	21.499690991
H	0.831547839	-12.902490561	16.004684198
H	-0.219165474	-11.538102252	15.549566303
H	1.550999416	-11.359779666	15.480112576
B	-0.273120164	-3.155844601	8.739669744
B	-0.301645029	-3.063982652	7.282647059

2.3 $L(BBL)_2$ Compounds

Compound $2(BB2)_2$

Total enthalpy, Htot (Utot + pV): -1692.044452 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1692.166718 hartrees



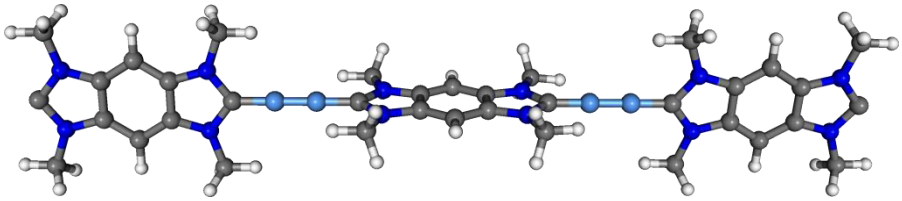
XYZ Coordinates

N	-3.430535981	1.228841411	0.009319460
C	-4.420082342	2.203438783	-0.149857974
N	-3.753932717	3.407843276	-0.397448212
C	-2.401311900	3.131501383	-0.516146935
C	-2.205613437	1.813232717	-0.271345400
N	-0.841155963	1.624496554	-0.113594742
C	-0.159357687	2.807457043	-0.304040620
N	-1.155112628	3.739144382	-0.505962946
C	-3.741589232	-0.184381288	0.118154967
C	-0.156601314	0.365827732	0.130009534
C	-0.865854654	5.141047869	-0.758318935
C	-4.451310874	4.623053377	-0.775354751
H	-4.698170896	-0.277790580	0.633597621
H	-2.965223996	-0.692174742	0.691318385
H	-3.834546368	-0.650421139	-0.868424812
H	-0.371668907	-0.358867379	-0.659918629

H	-0.446688798	-0.058176211	1.095281161
H	0.909138871	0.583679862	0.140009312
H	0.216094383	5.249975762	-0.727429406
H	-1.314417480	5.778446416	0.008518406
H	-1.233806526	5.448365603	-1.740993293
H	-5.451114195	4.581642873	-0.340758434
H	-4.548958255	4.705543064	-1.863878459
H	-3.920942885	5.495672985	-0.389034793
H	-12.036644144	1.685776106	3.111648069
H	-9.413335922	2.426713462	2.939214145
C	-12.682118162	1.131994435	2.428596964
C	-9.106380360	1.517512082	2.414273639
H	-9.459545615	0.641554357	2.964427467
H	-13.691097318	1.545023773	2.456651164
N	-12.189226597	1.263183367	1.068603491
N	-9.617190888	1.496862603	1.054652482
C	-10.882384788	1.134598211	0.633061262
H	-12.486613825	1.864031927	-3.129900896
H	-9.858799867	1.658055983	-3.246743715
C	-13.033894625	1.174893216	-0.043189025
C	-8.792395729	1.604959085	-0.070430220
C	-10.886295449	1.085828053	-0.726789214
N	-12.195176926	1.157704363	-1.163743360
N	-9.628728272	1.443515057	-1.179439642
C	-12.688660313	0.980434279	-2.518162563
C	-9.107321649	1.325460143	-2.529852153
H	-12.729975396	0.082035793	2.736368994
H	-13.768512587	0.832450816	-2.454641800
H	-8.016018329	1.494774398	2.356054702
H	-8.222369881	1.959247909	-2.600790689
H	-12.228843166	0.102852918	-2.980717696
H	-8.812604518	0.295231203	-2.755899705
B	-5.883957258	1.991990772	-0.113071841
B	-7.325569321	1.786291068	-0.089763141
H	-21.240673865	3.822543419	-0.231151596
H	-17.913343564	3.852737750	-0.605877643
C	-21.498062959	3.118967240	0.565104772
C	-17.890221147	3.338439004	0.360453152
H	-18.525455752	3.869155633	1.071712130
H	-22.578896805	3.005464396	0.612004705
N	-20.948136474	1.800807754	0.295399287
N	-18.325046211	1.959775803	0.237976251
C	-19.615153844	1.478990159	0.095747749
H	-21.044141870	-2.034072529	-1.329853584
H	-18.208878336	-2.018519574	-1.286429812
C	-21.745114032	0.684151307	0.155745188
C	-17.439516219	0.900001812	0.020641671
C	-19.555943958	0.147919786	-0.144701624

N	-20.851774991	-0.338342750	-0.086819223
N	-18.227729659	-0.235656010	-0.185233621
C	-21.280910324	-1.708462299	-0.313216684
C	-17.678884268	-1.551231667	-0.453448150
H	-21.134784268	3.508932997	1.519873349
H	-22.359279795	-1.727819584	-0.171829322
H	-16.861025455	3.328626597	0.722766366
H	-16.627447416	-1.420467375	-0.716523210
H	-20.808837435	-2.388927348	0.400363039
H	-17.742209213	-2.197790147	0.427023575
B	-14.507698470	1.061386486	-0.028474527
B	-15.960424548	0.975929543	-0.010533680

Compound 3(BB3)$_2$



Total enthalpy, Htot (Utot + pV): -2153.086331 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2153.221813 hartrees

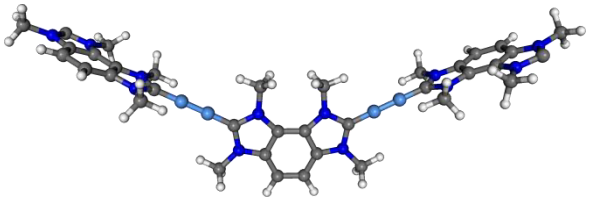
XYZ Coordinates

N	-2.380029798	1.151268308	0.198846502
C	-3.350954241	0.162388179	0.178493143
N	-2.652793893	-1.034907821	0.182951122
C	-1.287942200	-0.806612675	0.208972009
C	-1.113088932	0.594271295	0.212114627
C	0.148074540	1.191247465	0.229833787
C	1.223574522	0.302460846	0.248073322
C	1.048721724	-1.098289726	0.247360890
C	-0.212294294	-1.695376558	0.227736266
N	2.588313560	0.530727894	0.267772224
C	3.286425919	-0.666356021	0.282654012
N	2.315442668	-1.655036911	0.270134701
C	-2.668931036	2.570758869	0.193093213
C	3.216519911	1.835991654	0.273332819
C	2.603376609	-3.074696962	0.279501771
C	-3.281967057	-2.339660877	0.172623752
H	0.282153258	2.264314565	0.229084888
H	-0.346195378	-2.768469487	0.227757880
H	-3.749988338	2.694359111	0.263090275
H	-2.312959213	3.036853419	-0.730877774
H	-2.193187072	3.059560321	1.048415174

H	-4.359205811	-2.193011148	0.089597892
H	-3.063294604	-2.883928587	1.096503619
H	-2.930445024	-2.926133226	-0.681485747
H	3.686109643	-3.198393865	0.311050830
H	2.212596802	-3.553874037	-0.623273180
H	2.160089453	-3.550855666	1.159340781
H	2.927763327	2.399670272	1.165651603
H	2.931113340	2.403418927	-0.617687139
H	4.296882268	1.689564469	0.275412302
B	4.753374891	-0.848810741	0.306087469
B	6.200759384	-1.025454019	0.327459005
B	-4.817789947	0.346137488	0.157956685
B	-6.264025354	0.532148964	0.140636482
C	7.666496826	-1.207164839	0.348129802
N	8.474387129	-1.396886420	1.458897120
C	9.801097339	-1.528443717	1.085515655
C	9.834854187	-1.421318514	-0.326989647
N	8.527457226	-1.225298963	-0.738552158
C	8.102455546	-1.057244808	-2.112816248
C	7.981996439	-1.452497232	2.819743157
C	-7.729446506	0.715540978	0.124594515
N	-8.564723985	0.909177714	1.214188889
C	-9.881749149	1.039831472	0.807255534
C	-9.880209548	0.927434645	-0.605300377
N	-8.562786235	0.731209529	-0.983346622
C	-8.106957666	0.963901183	2.587226815
C	-8.103276349	0.558647412	-2.346003087
H	-7.023426395	0.842427312	2.585384824
H	-8.558691457	0.160479962	3.177182981
H	-8.361410768	1.927525877	3.039244907
H	-8.333392519	1.444389529	-2.946060159
H	-8.575226003	-0.316561394	-2.803120593
H	-7.023152408	0.412176052	-2.320538889
H	8.317687776	-1.956748009	-2.697779198
H	8.611061181	-0.202438842	-2.568870293
H	7.026906646	-0.878253099	-2.112517849
H	6.897067653	-1.348454187	2.789078595
H	8.405080516	-0.639604164	3.417862282
H	8.240233266	-2.410145066	3.282001673
C	11.016808662	-1.510869798	-1.053465549
C	12.169544356	-1.712188083	-0.287290412
C	12.136162533	-1.817171308	1.113812943
C	10.947702016	-1.728218474	1.845880050
N	13.511699331	-1.850364299	-0.637740679
C	14.328768913	-2.035215412	0.444863380
N	13.460706084	-2.010469487	1.502998211
C	-11.043744398	1.012239890	-1.361468959
C	-12.215355285	1.216588806	-0.625174550

C	-12.216880796	1.328575010	0.775833602
C	-11.047001587	1.242949092	1.537850388
N	-13.548459859	1.352142258	-1.009656209
C	-14.392396936	1.541627669	0.051446828
N	-13.550838252	1.522926489	1.131012153
C	-14.011117835	1.299006167	-2.383692886
C	-14.016286875	1.690691411	2.494834220
C	14.008426649	-1.805993335	-2.000154926
C	13.892177326	-2.170796434	2.878878897
H	13.565464552	-2.603925884	-2.604152201
H	15.086616136	-1.942638389	-1.956410653
H	13.783134949	-0.842349115	-2.467454652
H	14.971754692	-2.302861542	2.866495754
H	13.424213149	-3.048227896	3.335887127
H	13.641298196	-1.286615123	3.473018901
H	11.041215333	-1.431139279	-2.132069448
H	10.920817592	-1.808389213	2.924391586
H	-13.553813615	2.093564158	-2.981489423
H	-15.090172119	1.435047848	-2.367684154
H	-13.773687509	0.332648111	-2.839332258
H	-15.095454948	1.820854422	2.455116613
H	-13.561127792	2.571657647	2.958034730
H	-13.778773732	0.810489389	3.100331010
H	-11.046987045	1.328292829	2.616343146
H	-11.041301982	0.925930712	-2.439884408

Compound 4(BB4)$_2$



Total enthalpy, Htot (Utot + pV): -2153.052760 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2153.182703 hartrees

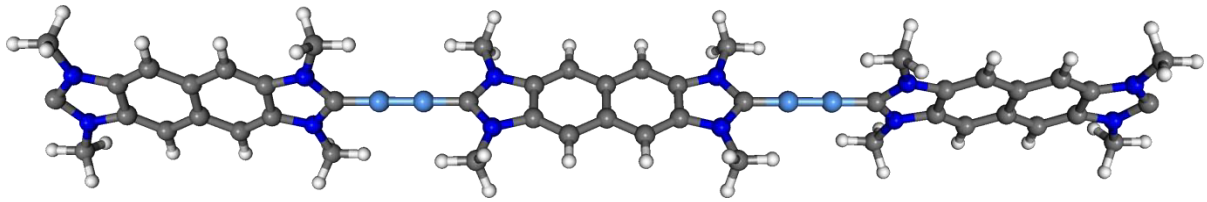
XYZ Coordinates

C	8.803927594	-1.367737333	-1.029676274
C	10.047886011	-1.002624008	-1.572301551
C	10.873586059	-2.037749157	-2.068913910
C	10.533608967	-3.387206179	-2.054061536
C	8.473235345	-2.743875632	-1.021009492
C	9.301267347	-3.749365390	-1.515821237
N	10.782540357	0.175862994	-1.789733499
C	11.997003308	-0.061553184	-2.382736356

N	12.025700291	-1.410330796	-2.540793990
C	10.404966953	1.541044971	-1.467147635
C	13.146465923	-2.111114283	-3.140470424
H	11.234242247	2.168403577	-1.785429592
H	9.501638266	1.843286860	-2.001803853
H	10.249816971	1.669922760	-0.393582076
H	13.889553541	-1.363380546	-3.408278425
H	12.832643144	-2.651380483	-4.038631863
H	13.583737923	-2.823139302	-2.434158757
N	7.721360595	-0.707355075	-0.453160604
H	11.207200978	-4.136418470	-2.449273216
N	7.218565027	-2.855679102	-0.444998974
H	8.992702965	-4.786035756	-1.482429651
C	6.734224649	-1.617279420	-0.086898729
C	7.537804193	0.712508563	-0.219627052
C	6.501957499	-4.097571763	-0.237872940
H	6.558894633	0.836044630	0.246314928
H	8.302015448	1.102546653	0.455824959
H	7.555886205	1.271035791	-1.157727307
H	5.555536159	-3.860266589	0.248730330
H	6.302686143	-4.592340027	-1.193213937
H	7.078612819	-4.771880924	0.402250183
B	5.437407476	-1.313427464	0.555003844
H	0.846540993	-1.132260518	-0.555158090
H	-1.270285559	-0.602679059	-0.562261453
H	2.548294530	-0.628714073	-0.596528247
C	1.560798329	-0.386034758	-0.201001668
B	4.163836569	-1.009793724	1.190892320
C	2.879888384	-0.699934774	1.856579001
N	1.666018860	-0.406105373	1.245191061
C	-1.560798329	0.386034758	-0.201001668
H	3.360428392	-1.731786764	4.854758079
H	-2.548294530	0.628714073	-0.596528247
N	2.641639422	-0.641297738	3.210871266
C	0.681407454	-0.165828269	2.205282845
H	4.584845183	-1.114736128	3.716981462
C	3.647497413	-0.885075415	4.224109802
H	1.270285559	0.602679059	-0.562261453
N	-1.666018860	0.406105373	1.245191061
C	1.318534499	-0.320154564	3.464212295
C	-0.681407454	0.165828269	2.205282845
H	-0.846540993	1.132260518	-0.555158090
C	-2.879888384	0.699934774	1.856579001
C	-1.318534499	0.320154564	3.464212295
C	0.678721310	-0.164715689	4.687069885
N	-2.641639422	0.641297738	3.210871266
C	-0.678721310	0.164715689	4.687069885
H	-3.783183115	-0.000481218	4.852122321

H	1.217462409	-0.295345300	5.615963973
H	3.783183115	0.000481218	4.852122321
C	-3.647497413	0.885075415	4.224109802
H	-1.217462409	0.295345300	5.615963973
H	-4.584845183	1.114736128	3.716981462
H	-3.360428392	1.731786764	4.854758079
B	-4.163836569	1.009793724	1.190892320
H	-8.302015448	-1.102546653	0.455824959
H	-10.249816971	-1.669922760	-0.393582076
H	-6.558894633	-0.836044630	0.246314928
C	-7.537804193	-0.712508563	-0.219627052
B	-5.437407476	1.313427464	0.555003844
C	-6.734224649	1.617279420	-0.086898729
N	-7.721360595	0.707355075	-0.453160604
C	-10.404966953	-1.541044971	-1.467147635
H	-7.078612819	4.771880924	0.402250183
H	-11.234242247	-2.168403577	-1.785429592
N	-7.218565027	2.855679102	-0.444998974
C	-8.803927594	1.367737333	-1.029676274
H	-5.555536159	3.860266589	0.248730330
C	-6.501957499	4.097571763	-0.237872940
H	-7.555886205	-1.271035791	-1.157727307
N	-10.782540357	-0.175862994	-1.789733499
C	-8.473235345	2.743875632	-1.021009492
C	-10.047886011	1.002624008	-1.572301551
H	-9.501638266	-1.843286860	-2.001803853
C	-11.997003308	0.061553184	-2.382736356
C	-10.873586059	2.037749157	-2.068913910
C	-9.301267347	3.749365390	-1.515821237
N	-12.025700291	1.410330796	-2.540793990
C	-10.533608967	3.387206179	-2.054061536
H	-13.583737923	2.823139302	-2.434158757
H	-8.992702965	4.786035756	-1.482429651
H	-6.302686143	4.592340027	-1.193213937
C	-13.146465923	2.111114283	-3.140470424
H	-11.207200978	4.136418470	-2.449273216
H	-13.889553541	1.363380546	-3.408278425
H	-12.832643144	2.651380483	-4.038631863

Compound 5(BB5)$_2$



Total enthalpy, Htot (Utot + pV): -2613.975820 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2614.124749 hartrees

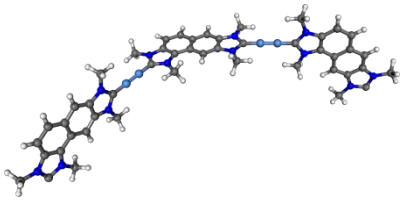
XYZ Coordinates

C	-4.540039057	-1.213750985	-2.820466455
C	-5.688757180	-0.587014116	-2.412028846
C	-3.332679024	-0.457911899	-2.888153406
C	-3.342990601	0.943279282	-2.524973031
C	-4.560860984	1.554841801	-2.105053615
C	-5.699163816	0.792594258	-2.055651163
C	-2.123377324	-1.066500485	-3.309490235
C	-0.982110142	-0.301181785	-3.362129192
C	-0.991930340	1.068716089	-3.005824742
C	-2.143371313	1.696146443	-2.591740372
N	0.337095804	-0.578726083	-3.724074752
C	1.155858564	0.513127473	-3.622180622
N	0.322204184	1.505150619	-3.181956033
N	-6.985738711	-1.043032446	-2.252728591
C	-7.814634537	-0.021696734	-1.813778225
N	-7.001370496	1.095429448	-1.697713126
C	0.805015881	-1.879236322	-4.164594019
C	0.771124117	2.861596750	-2.931137290
C	-7.462790541	2.397280761	-1.260964819
C	-7.429449772	-2.397180199	-2.513174044
H	-7.229958862	-2.671043300	-3.553476850
H	-8.502586102	-2.444813778	-2.328073456
H	-6.918288053	-3.103920563	-1.852619161
H	0.279389964	-2.196579682	-5.070501890
H	0.652445351	-2.633045806	-3.386052393
H	1.868016925	-1.787873764	-4.376345549
H	1.834560099	2.899240045	-3.156615614
H	0.610927253	3.138334082	-1.884541620
H	0.238329372	3.573111840	-3.569517826
H	-8.521308788	2.317402592	-1.013357234
H	-7.334026066	3.138804361	-2.055167287
H	-6.907817386	2.721208842	-0.375545727
H	-19.874211657	-0.321414696	3.654113103
H	-20.943067741	0.610490987	-2.181919262
C	-20.258764811	-1.155627650	3.059720179
H	-10.961199905	-0.588472707	1.285773130
C	-21.107510312	-0.772090800	0.733544939
N	-20.072271220	-0.905012958	1.645059536
H	-19.741933022	-2.073548942	3.354840873
C	-18.846427085	-0.769719620	1.015595774
C	-17.558590491	-0.822277538	1.490769914
N	-20.500153106	-0.549636141	-0.492011593
C	-19.121643915	-0.542884222	-0.360123679
C	-21.219002401	-0.348565555	-1.733743623

C	-16.483211591	-0.643306463	0.576847920
C	-15.134690224	-0.693235461	1.027475136
H	-13.414242966	1.082013571	-3.584101271
C	-18.111564801	-0.363795243	-1.273761611
C	-16.763289431	-0.407693618	-0.822047274
H	-22.286546804	-0.348990360	-1.513336238
C	-12.026654276	-0.697596229	1.488565977
C	-14.124740317	-0.510145409	0.114475098
H	-12.331351255	0.048711833	2.228197846
C	-15.688116891	-0.221234870	-1.734745859
N	-12.746181080	-0.500339971	0.246600632
C	-14.400311884	-0.274245652	-1.259731694
C	-12.139381525	-0.271499525	-0.977847553
N	-13.174514659	-0.136428591	-1.888816731
H	-21.326625652	-1.267191377	3.247985482
C	-12.987536318	0.114394035	-3.303390707
H	-11.917120463	0.121224643	-3.509286215
H	-20.998053183	-1.151786522	-2.443075366
H	-12.216131306	-1.697544709	1.890260107
H	-13.463978807	-0.672224420	-3.895847857
B	-9.259113648	-0.105729139	-1.531170945
B	-10.692058789	-0.188931531	-1.254890870
H	-35.225586117	0.901650832	3.556332526
H	-33.750829577	-4.384484265	2.166014489
C	-34.160734396	0.985863775	3.350939828
C	-34.421065277	-1.478104865	3.311976728
H	-24.852774200	1.501649487	1.503486593
N	-33.640313964	-0.359755182	3.199686717
H	-34.011414217	1.566970116	2.435689477
C	-32.304463727	-0.658052904	2.925963043
N	-33.545793049	-2.508732280	3.100728183
C	-31.186828980	0.120703291	2.737677137
C	-33.944930611	-3.903092429	3.129463716
C	-32.242596101	-2.070664350	2.859479960
H	-35.011752264	-3.931798956	3.339830949
C	-29.949300533	-0.517433412	2.469823494
C	-28.764536082	0.251196594	2.271981343
C	-31.062852491	-2.727743318	2.599754495
H	-26.156060358	-3.989191022	0.656271607
C	-29.886865586	-1.961829783	2.397654652
C	-27.588433179	-0.404003074	2.013500484
C	-25.911512107	1.450610922	1.757870092
N	-26.303911971	0.056215626	1.781349857
C	-28.642275586	-2.601973181	2.124122316
C	-27.527681173	-1.825668387	1.938949529
C	-25.434630486	-1.002550837	1.566080877
H	-26.490533052	1.996633236	1.007153849
H	-33.669789016	1.503120975	4.181040729

N	-26.209203976	-2.148181840	1.668237533
C	-25.696280790	-3.494614431	1.517206989
H	-33.405163139	-4.447209867	3.910649593
H	-24.619114612	-3.432573803	1.361918792
H	-26.069085683	1.912933963	2.736969640
H	-25.898637199	-4.082364067	2.417528089
B	-22.555330193	-0.850326173	1.010698240
B	-23.988783163	-0.926215514	1.287353711
H	-2.152878443	2.745159486	-2.319319287
H	-4.568354792	2.604208234	-1.835982074
H	-4.531277277	-2.262709130	-3.091099443
H	-2.117561095	-2.115653192	-3.581503597
H	-15.898740057	-0.040903049	-2.782028682
H	-18.320397163	-0.191399029	-2.322743928
H	-17.348263485	-0.994294113	2.539509081
H	-14.925697319	-0.873138509	2.075169327
H	-28.597045373	-3.682868827	2.066866711
H	-31.013974093	-3.809226463	2.547179231
H	-31.232057576	1.202363448	2.789831779
H	-28.811284249	1.331990606	2.329855574

Compound 6 $(BB6)_2$



Total enthalpy, Htot (Utot + pV): -2613.962378 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2614.103897 hartrees

XYZ Coordinates

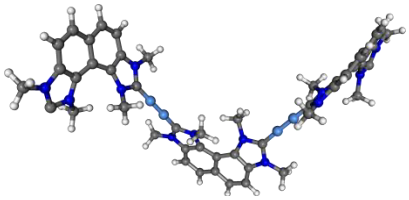
C	-5.516772617	0.012883887	0.793499770
C	-4.304791506	0.658059667	0.834374536
C	-3.113625372	-0.125401224	0.886913579
C	-3.212452551	-1.569979583	0.894944683
C	-5.614198138	-1.406425968	0.804079097
C	-4.493089569	-2.192813946	0.855113885
C	-1.795989180	0.404221581	0.923695519
C	-0.676380108	-0.430392371	0.951846505
C	-0.778523462	-1.828122072	0.961728548
C	-2.042904361	-2.372760471	0.935190006
N	-6.810543525	0.494556261	0.733213543
C	-7.725156655	-0.551913800	0.701163463
N	-6.962050672	-1.710354363	0.749946860
N	-1.303952237	1.710416283	0.931202095

C	0.080890076	1.705235601	0.949168868
N	0.446961992	0.377139980	0.962849659
C	1.819562574	-0.088806504	0.975556942
C	-2.049977732	2.957189428	0.928302297
C	-7.179903603	1.894827424	0.702006313
C	-7.514505840	-3.049316829	0.735790856
H	-8.267729114	1.955094575	0.660386760
H	-6.823664083	2.405997892	1.601604961
H	-6.757429358	2.385315364	-0.180286904
H	-8.600311508	-2.965441336	0.685226263
H	-7.235219121	-3.589668201	1.645328359
H	-7.153474622	-3.604535402	-0.135293882
H	-4.557567189	-3.274110736	0.860941047
H	-4.264423255	1.735489858	0.820325190
H	-2.162289782	-3.450251677	0.941420670
H	0.103913430	-2.454651900	0.989371991
H	2.471442276	0.781935646	0.901557502
H	2.004859582	-0.751318888	0.125435727
H	2.039515531	-0.624240980	1.903744060
H	-1.325766362	3.769645157	1.002559139
H	-2.617288751	3.074359213	0.001498972
H	-2.726194249	3.006238608	1.784664321
C	4.167168973	6.828939620	0.093992709
C	4.913081032	7.695652439	-0.668864119
C	5.667771407	8.708691267	-0.011043879
C	5.631977381	8.799098446	1.430930943
C	4.131225799	6.917112622	1.512118958
C	4.845146645	7.878826972	2.180246597
C	6.481074548	9.671992756	-0.671669593
C	7.192298816	10.635080577	0.039936552
C	7.154822338	10.718379263	1.441780941
C	6.378643340	9.803022072	2.110020206
N	3.352032077	5.770086791	-0.255311639
C	2.798638710	5.179542419	0.875744055
N	3.295604972	5.905853140	1.949775365
N	6.780689797	9.924488294	-2.018720722
C	7.633639445	10.984758425	-2.181886297
N	7.868643761	11.400119539	-0.903998019
C	8.734316533	12.521005023	-0.586201680
C	6.289638181	9.197865403	-3.178573434
C	3.098127967	5.322292244	-1.608993981
C	2.975356607	5.629024040	3.334730329
H	2.413233134	4.475343495	-1.559348263
H	2.641666904	6.122536389	-2.199467252
H	4.028422019	5.006730338	-2.091128584
H	2.308766733	4.766753859	3.360262338
H	2.474197502	6.486856046	3.793311914
H	3.883566922	5.400750906	3.900488427

H	4.823502227	7.953403763	3.260745644
H	4.921402325	7.604219986	-1.743463091
H	6.322835300	9.833845803	3.192583613
H	7.716082051	11.475140130	1.975797694
H	9.114081552	12.912286236	-1.527385882
H	9.572998624	12.202267279	0.039792160
H	8.181054848	13.306359925	-0.062728646
H	6.731286624	9.674095012	-4.051060799
H	6.595707925	8.148827112	-3.147921117
H	5.200287397	9.255279154	-3.250276272
B	1.883186858	4.027886867	0.918835375
B	0.984006048	2.880736051	0.946390219
C	-16.634285739	-0.074249511	-3.277994060
C	-15.424647332	-0.133944960	-2.628848435
C	-15.414212893	-0.114330731	-1.207564416
C	-16.670461166	-0.030693969	-0.486996130
C	-17.861295206	0.004996429	-2.574831256
C	-17.893857511	0.027599667	-1.204089824
C	-14.240848087	-0.169359615	-0.403007501
C	-14.313940879	-0.137115782	0.988969124
C	-15.533923782	-0.056113143	1.680418261
C	-16.686776360	-0.005272416	0.935171500
N	-16.983543061	-0.072740943	-4.628002786
C	-18.337178060	0.000967730	-4.825172574
N	-18.850206301	0.047212692	-3.558596049
N	-12.886032300	-0.256172117	-0.718372340
C	-12.120826571	-0.275024708	0.437328592
N	-13.022048803	-0.199119888	1.477854308
C	-12.647588474	-0.189918967	2.878725721
C	-12.266368924	-0.330181922	-2.030699432
C	-16.029624145	-0.141164575	-5.719388005
C	-20.272742874	0.131569598	-3.282668079
H	-16.596155145	-0.121684117	-6.647522231
H	-15.345456323	0.712380274	-5.693474049
H	-15.445510631	-1.065112886	-5.669643975
H	-20.789348126	0.148338613	-4.239562967
H	-20.507854491	1.043690152	-2.726086746
H	-20.608754254	-0.733137427	-2.702698788
H	-18.827011551	0.089556674	-0.656727377
H	-14.507029048	-0.192109095	-3.192814162
H	-17.646987632	0.057097888	1.434105922
H	-15.562214436	-0.035523466	2.762455208
H	-11.559297167	-0.215595854	2.935871098
H	-13.054663938	-1.064687519	3.393611804
H	-13.012215612	0.718070283	3.366903151
H	-11.190076349	-0.419155077	-1.877289185
H	-12.618973498	-1.207284218	-2.578191915
H	-12.467109065	0.574320612	-2.609942197

B	-10.644694731	-0.361073872	0.532926814
B	-9.192204885	-0.452773671	0.624821864

Compound 7(BB7)$_2$



Total enthalpy, Htot (Utot + pV): -2613.901031 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2614.047604 hartrees

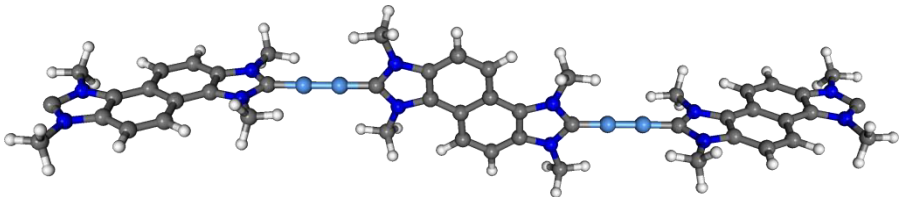
XYZ Coordinates

C	-2.705127274	0.666796075	-0.440303663
C	-3.085627675	0.397890165	0.889649956
C	-2.083432930	0.298930053	1.821165845
C	-0.704278039	0.335561580	1.462396031
C	-0.321571236	0.435726597	0.069361030
C	-1.374880061	0.771410848	-0.832392580
C	1.042761977	0.176375949	-0.211478260
C	1.993576330	0.160659169	0.811873960
C	1.637563348	0.229825635	2.167424815
C	0.293438666	0.258720772	2.467668986
N	3.231724285	-0.016554761	0.224498406
C	3.089393868	-0.234349341	-1.135745369
N	1.726397472	-0.100929858	-1.401148412
C	4.495698557	-0.116538465	0.926254342
C	1.167824007	-0.810315042	-2.553264372
H	0.099554049	-0.629798395	-2.627595268
H	1.350514568	-1.883942462	-2.446280594
H	1.665432612	-0.469064515	-3.461860385
H	4.572472040	0.675589360	1.674174108
H	5.296919666	-0.005381444	0.194745757
H	4.600589556	-1.090257039	1.416166209
H	-2.330688102	0.170742989	2.869160391
N	-1.414462210	1.256935291	-2.150780463
N	-3.466362924	1.011613933	-1.553080855
H	-4.128360975	0.330768885	1.174318879
C	-2.702281420	1.415336926	-2.606564342
C	-0.349541238	2.014763169	-2.812280270
C	-4.918767664	1.011038573	-1.587679854
H	-0.375159630	3.054846577	-2.476184023
H	0.632812594	1.608805625	-2.592568924
H	-0.537555236	1.988573663	-3.883846629
H	-5.325740655	1.681430306	-0.825030321

H	-5.313373871	0.004448074	-1.422795411
H	-5.217101488	1.361773699	-2.573108523
H	-0.025773113	0.224884604	3.503173932
H	2.387757644	0.193540684	2.947137672
C	7.939594609	-0.962854620	-5.529581824
C	8.775854616	-0.439416107	-6.530406558
C	9.377231340	-1.335219693	-7.382711407
C	9.265928993	-2.739803875	-7.209062630
C	8.533732077	-3.275542047	-6.075734879
C	7.750956344	-2.334392859	-5.352492891
C	8.697461220	-4.669006445	-5.844890400
C	9.251890628	-5.494020985	-6.824531755
C	9.822844795	-4.987000586	-8.004478428
C	9.868632676	-3.619893535	-8.145778812
N	9.193864876	-6.793065756	-6.358099787
C	8.711561885	-6.813837932	-5.061398578
N	8.398258907	-5.492249249	-4.752624391
C	9.693022415	-7.961805857	-7.055063574
C	8.373409544	-5.088450755	-3.347363595
H	8.168882243	-4.025523375	-3.264306497
H	9.340518773	-5.312070297	-2.887317899
H	7.606407783	-5.656560619	-2.819413185
H	9.264986456	-8.016950980	-8.058868125
H	9.398448752	-8.844110044	-6.486481031
H	10.784966579	-7.936583448	-7.128042685
H	9.964831626	-0.971115290	-8.217455308
N	6.728409436	-2.478132576	-4.406832470
N	7.115534385	-0.309809263	-4.633618699
H	8.888865802	0.628630919	-6.663803814
C	6.320683187	-1.222257590	-3.963624034
C	5.786927886	-3.593590033	-4.315800422
C	6.976304086	1.126129015	-4.499469470
H	4.855666381	-3.324139188	-4.822571360
H	6.209754497	-4.480541891	-4.777673510
H	5.557665752	-3.796246550	-3.268931746
H	6.380490487	1.544668423	-5.316881344
H	7.960761431	1.598144835	-4.489261165
H	6.466597056	1.328687366	-3.556901498
H	10.371568630	-3.184657549	-9.001515411
H	10.264014600	-5.645850125	-8.741270572
B	4.150361454	-0.586699011	-2.093492761
B	5.229322112	-0.923738595	-3.019724505
C	11.249352825	-13.736854761	1.475549740
C	10.322620255	-14.420592872	2.287959132
C	9.018737406	-14.452810830	1.862498500
C	8.572615168	-13.726549499	0.719768334
C	9.498281368	-12.882852649	-0.007194244
C	10.875623506	-13.061000417	0.318897816

C	8.912064419	-11.990081216	-0.937988365
C	7.589904365	-12.158045187	-1.355077981
C	6.729773808	-13.095308757	-0.762948436
C	7.220540484	-13.819901048	0.301126936
N	7.337135244	-11.207240795	-2.325140434
C	8.425756968	-10.362599710	-2.463973050
N	9.403679709	-10.860321920	-1.602171078
C	6.071717243	-11.016325981	-3.006044945
C	10.399876881	-9.931501579	-1.065349830
H	11.103016184	-10.456802331	-0.425729688
H	9.898705459	-9.147918729	-0.488801506
H	10.931040033	-9.459323914	-1.892644814
H	5.738832662	-11.953288900	-3.459539066
H	6.217795863	-10.268067853	-3.785394076
H	5.304532191	-10.658910822	-2.311449361
H	8.285423280	-15.032447531	2.412140559
N	12.081824948	-12.714002398	-0.313819994
N	12.639511159	-13.691048750	1.520110792
H	10.637712475	-14.948917315	3.179341853
C	13.180555632	-13.103574255	0.416164598
C	12.254381243	-12.480726570	-1.749706360
C	13.447253146	-14.260933785	2.584654103
H	12.283705695	-13.438146340	-2.277088733
H	11.446299905	-11.886707809	-2.164830648
H	13.206765261	-11.973624461	-1.891377398
H	13.259186499	-15.334109969	2.682924520
H	13.234076514	-13.774146074	3.540540296
H	14.489610487	-14.099860895	2.318805802
H	6.563311038	-14.491362513	0.841929355
H	5.701997101	-13.197070067	-1.087476885
B	8.603293049	-7.981982976	-4.168443467
B	8.520734745	-9.159978099	-3.308584773

Compound 8(BB8)$_2$



Total enthalpy, Htot (Utot + pV): -2613.945371 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2614.084954 hartrees

XYZ Coordinates

C	-11.218250872	-3.699483705	-1.331678643

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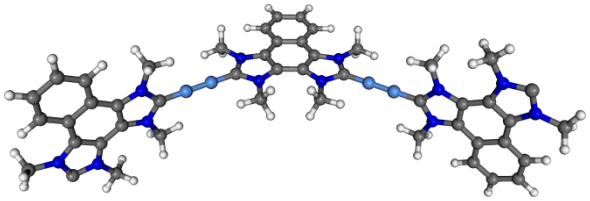
C	-12.916879292	-1.941831386	-1.223868270
C	-11.901831283	-0.910968582	-1.100634067
C	-10.550563837	-1.354718746	-1.111856254
C	-10.234446193	-2.712206797	-1.216830186
C	-14.270218000	-1.490358827	-1.222075864
C	-14.586761084	-0.141619227	-1.100626143
C	-13.600748626	0.849740044	-0.970774531
C	-12.285700724	0.456914168	-0.973122392
N	-15.506640223	-2.141767613	-1.324592334
C	-16.568148898	-1.273111572	-1.274610443
N	-15.972755139	-0.054704503	-1.136206596
C	-15.747087937	-3.569320802	-1.474142063
C	-16.725474212	1.183464214	-1.040303568
N	-8.858400548	-2.827845513	-1.186260428
C	-8.275114042	-1.580790955	-1.083056991
N	-9.334747261	-0.681515858	-1.034240212
C	-8.112882864	-4.067109368	-1.281403524
C	-9.090873576	0.748492004	-0.941548154
H	-7.065413277	-3.843484862	-1.076797156
H	-8.481641062	-4.787898710	-0.546805189
H	-8.196407659	-4.498537756	-2.283643396
H	-8.009566814	0.891918564	-0.969024232
H	-9.478151312	1.153720601	-0.003486834
H	-9.541887608	1.274671941	-1.785674541
H	-10.952124264	-4.745403873	-1.419460430
H	-13.300224670	-4.062887934	-1.426428509
H	-11.525671526	1.214522811	-0.869907166
H	-13.866102292	1.894961801	-0.870589782
H	-17.780072305	0.924417536	-1.102237193
H	-16.469104286	1.861004196	-1.859850005
H	-16.530485975	1.687003764	-0.089033480
H	-16.826172299	-3.694974085	-1.526717028
H	-15.294329558	-3.952973517	-2.391915125
H	-15.360827892	-4.128126052	-0.617890972
H	-3.015108783	-1.924511779	1.776069141
H	3.391486756	-0.812604494	3.860753510
C	-3.565781008	-1.061718085	1.395028018
H	-3.298688847	-0.954201166	-4.087279685
C	-0.452358814	-0.414792131	1.790891722
C	0.750515206	-0.275431727	2.446198271
H	-4.619163023	-1.327672774	1.295143691
N	-3.090497291	-0.689552470	0.072632504
C	3.682540346	0.155590104	3.445246971
H	3.475704283	0.226832452	-2.094308124
C	-3.957120846	-0.666324673	-1.014205886
H	-1.317555154	-0.695098224	2.369209439
H	0.823223539	-0.444187747	3.513103836

C	-0.580180001	-0.196249803	0.393102972
C	-1.803538929	-0.334493266	-0.322017705
C	1.873203644	0.094717281	1.695367135
N	3.181189557	0.291826337	2.092197673
N	-3.181189557	-0.291826337	-2.092197673
C	-1.873203644	-0.094717281	-1.695367135
C	1.803538929	0.334493266	0.322017705
C	0.580180001	0.196249803	-0.393102972
C	3.957120846	0.666324673	1.014205886
C	-3.682540346	-0.155590104	-3.445246971
H	4.770231934	0.221618896	3.407312882
C	-0.750515206	0.275431727	-2.446198271
C	0.452358814	0.414792131	-1.790891722
N	3.090497291	0.689552470	-0.072632504
H	-4.770231934	-0.221618896	-3.407312882
C	3.565781008	1.061718085	-1.395028018
H	-0.823223539	0.444187747	-3.513103836
H	1.317555154	0.695098224	-2.369209439
H	-3.475704283	-0.226832452	2.094308124
H	4.619163023	1.327672774	-1.295143691
H	3.298688847	0.954201166	4.087279685
H	-3.391486756	0.812604494	-3.860753510
H	3.015108783	1.924511779	-1.776069141
B	-6.829777846	-1.271098398	-1.041600556
B	-5.404204269	-0.975182372	-1.019146427
H	8.481641062	4.787898710	0.546805189
C	8.112882864	4.067109368	1.281403524
H	7.065413277	3.843484862	1.076797156
H	9.478151312	-1.153720601	0.003486834
C	8.275114042	1.580790955	1.083056991
N	8.858400548	2.827845513	1.186260428
C	10.234446193	2.712206797	1.216830186
N	9.334747261	0.681515858	1.034240212
C	9.090873576	-0.748492004	0.941548154
H	8.009566814	-0.891918564	0.969024232
C	11.218250872	3.699483705	1.331678643
C	10.550563837	1.354718746	1.111856254
H	10.952124264	4.745403873	1.419460430
H	15.360827892	4.128126052	0.617890972
C	12.539355598	3.304247126	1.335664251
C	11.901831283	0.910968582	1.100634067
H	8.196407659	4.498537756	2.283643396
C	12.916879292	1.941831386	1.223868270
C	12.285700724	-0.456914168	0.973122392
H	13.300224670	4.062887934	1.426428509
H	11.525671526	-1.214522811	0.869907166
C	14.270218000	1.490358827	1.222075864
C	13.600748626	-0.849740044	0.970774531

C	15.747087937	3.569320802	1.474142063
H	16.530485975	-1.687003764	0.089033480
C	14.586761084	0.141619227	1.100626143
N	15.506640223	2.141767613	1.324592334
H	9.541887608	-1.274671941	1.785674541
H	13.866102292	-1.894961801	0.870589782
C	16.568148898	1.273111572	1.274610443
N	15.972755139	0.054704503	1.136206596
H	16.826172299	3.694974085	1.526717028
C	16.725474212	-1.183464214	1.040303568
H	15.294329558	3.952973517	2.391915125
H	17.780072305	-0.924417536	1.102237193
H	16.469104286	-1.861004196	1.859850005
B	5.404204269	0.975182372	1.019146427
B	6.829777846	1.271098398	1.041600556

Compound 9(BB9)$_2$



Total enthalpy, Htot (Utot + pV): -2613.893339 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2614.033663 hartrees

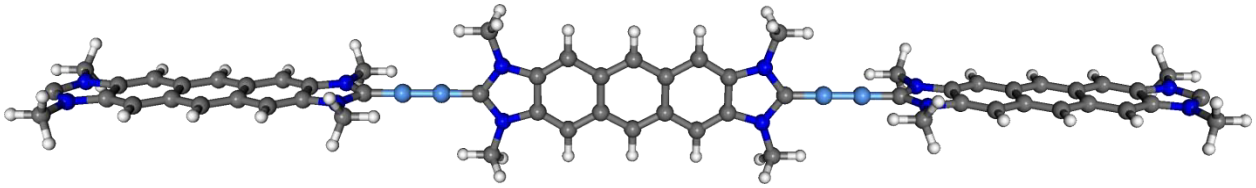
XYZ Coordinates

C	-11.865426737	-2.847915823	-3.076398114
C	-10.796282944	-3.544441181	-2.485891094
C	-9.764491056	-2.852406966	-1.899102596
C	-9.737060169	-1.432617932	-1.865651860
C	-10.833995118	-0.718135681	-2.471220587
C	-11.878133719	-1.473411162	-3.066174301
C	-10.798216768	0.705965168	-2.433442976
C	-9.761256969	1.439414661	-1.840791778
C	-8.684285268	0.735503879	-1.240101678
C	-8.693841235	-0.666788834	-1.267982973
N	-7.524481100	1.118115011	-0.573673561
C	-6.802921554	0.001261223	-0.186821577
N	-10.103001025	2.787419051	-2.021684055
C	-11.286120800	2.937722835	-2.689280305
N	-11.694506115	1.664210485	-2.929881880
N	-7.531302476	-1.085240332	-0.620127669
C	-7.044734557	-2.433883160	-0.376041567
C	-7.017383976	2.440741798	-0.254703747

C	-9.388544413	3.988177857	-1.616709417
C	-12.947888217	1.444991650	-3.638889966
H	-13.347509840	2.433003659	-3.855417418
H	-12.785479090	0.909135644	-4.576996791
H	-13.662741101	0.895180766	-3.022081601
H	-6.092570846	-2.335395066	0.147998723
H	-7.739167730	-2.994538899	0.253496310
H	-6.878750698	-2.966706964	-1.314851342
H	-6.813830569	3.015965683	-1.158702606
H	-6.081096090	2.293403077	0.286642599
H	-7.711210279	2.985498646	0.386897314
H	-9.280138030	4.045681206	-0.532763280
H	-9.996384296	4.822641538	-1.957646218
H	-8.405725220	4.047596416	-2.086920102
H	-8.960859229	-3.415601226	-1.455285229
H	-12.710276960	-0.965968516	-3.525771365
H	-12.680684930	-3.391078191	-3.540122150
H	-10.782502401	-4.628188847	-2.491329649
H	1.051133917	-0.893502424	-0.393300426
H	3.904759891	-0.869485341	4.861163644
H	-1.039445886	-0.894141704	-0.398685382
H	-3.889729670	-0.919529205	4.863976172
C	1.560664689	0.004822213	-0.042163671
C	2.947582921	0.016881456	1.972547713
C	3.891231284	0.025984515	4.235908267
C	0.708593308	0.004562095	2.399874643
C	-1.560664689	-0.004822213	-0.042163671
N	1.685262462	0.009745220	1.404441154
C	1.386099446	0.009393666	3.632272104
N	2.749329386	0.018084374	3.335218819
C	-0.708593308	-0.004562095	2.399874643
C	0.722484643	0.005218590	4.890233879
C	1.390500355	0.010322492	6.145488763
C	-1.386099446	-0.009393666	3.632272104
C	-2.947582921	-0.016881456	1.972547713
N	-1.685262462	-0.009745220	1.404441154
C	-0.722484643	-0.005218590	4.890233879
C	0.704036867	0.005291108	7.334713612
C	-1.390500355	-0.010322492	6.145488763
C	-0.704036867	-0.005291108	7.334713612
C	-3.891231284	-0.025984515	4.235908267
N	-2.749329386	-0.018084374	3.335218819
H	2.576677841	0.009710374	-0.441460322
H	4.785670004	0.034927322	3.610572974
H	-2.576677841	-0.009710374	-0.441460322
H	2.466913090	0.018514622	6.179487261
H	1.249351190	0.009278789	8.271504208
H	-4.785670004	-0.034927322	3.610572974

H	-2.466913090	-0.018514622	6.179487261
H	-1.249351190	-0.009278789	8.271504208
H	1.039445886	0.894141704	-0.398685382
H	3.889729670	0.919529205	4.863976172
H	-1.051133917	0.893502424	-0.393300426
H	-3.904759891	0.869485341	4.861163644
B	-5.512965209	-0.012890564	0.543481238
B	-4.244665244	-0.019313732	1.254568976
H	9.280138030	-4.045681206	-0.532763280
H	13.662741101	-0.895180766	-3.022081601
H	7.711210279	-2.985498646	0.386897314
H	7.739167730	2.994538899	0.253496310
C	9.388544413	-3.988177857	-1.616709417
C	11.286120800	-2.937722835	-2.689280305
C	12.947888217	-1.444991650	-3.638889966
C	9.761256969	-1.439414661	-1.840791778
C	7.017383976	-2.440741798	-0.254703747
N	10.103001025	-2.787419051	-2.021684055
C	10.798216768	-0.705965168	-2.433442976
N	11.694506115	-1.664210485	-2.929881880
C	8.684285268	-0.735503879	-1.240101678
C	10.833995118	0.718135681	-2.471220587
C	11.878133719	1.473411162	-3.066174301
C	8.693841235	0.666788834	-1.267982973
C	6.802921554	-0.001261223	-0.186821577
N	7.524481100	-1.118115011	-0.573673561
C	9.737060169	1.432617932	-1.865651860
C	11.865426737	2.847915823	-3.076398114
C	9.764491056	2.852406966	-1.899102596
C	10.796282944	3.544441181	-2.485891094
C	7.044734557	2.433883160	-0.376041567
N	7.531302476	1.085240332	-0.620127669
H	9.996384296	-4.822641538	-1.957646218
H	13.347509840	-2.433003659	-3.855417418
H	6.081096090	-2.293403077	0.286642599
H	12.710276960	0.965968516	-3.525771365
H	12.680684930	3.391078191	-3.540122150
H	6.092570846	2.335395066	0.147998723
H	8.960859229	3.415601226	-1.455285229
H	10.782502401	4.628188847	-2.491329649
H	8.405725220	-4.047596416	-2.086920102
H	12.785479090	-0.909135644	-4.576996791
H	6.813830569	-3.015965683	-1.158702606
H	6.878750698	2.966706964	-1.314851342
B	4.244665244	0.019313732	1.254568976
B	5.512965209	0.012890564	0.543481238

Compound 10(BB10)$_2$



Total enthalpy, Htot (Utot + pV): -3074.846901 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -3075.004958 hartrees

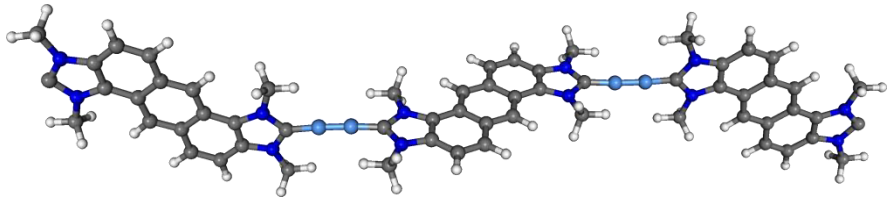
XYZ Coordinates

C	0.000000000	0.712742186	19.629939565
C	0.000000000	1.433835879	18.466873883
C	0.000000000	0.724609117	17.229235662
C	0.000000000	-0.712742186	19.629939565
C	0.000000000	-1.433835879	18.466873883
C	0.000000000	-0.724609117	17.229235662
C	0.000000000	1.396308699	15.998260126
C	0.000000000	0.725887056	14.774862133
C	0.000000000	-0.725887056	14.774862133
C	0.000000000	-1.396308699	15.998260126
C	0.000000000	1.436213850	13.531492660
C	0.000000000	0.716600325	12.369822362
C	0.000000000	-0.716600325	12.369822362
C	0.000000000	-1.436213850	13.531492660
N	0.000000000	1.078092771	20.977710767
C	0.000000000	0.000000000	21.820707776
N	0.000000000	-1.078092771	20.977710767
N	0.000000000	1.105245579	11.041726855
C	0.000000000	0.000000000	10.205740557
N	0.000000000	-1.105245579	11.041726855
C	0.000000000	2.450206078	21.448170078
C	0.000000000	-2.450206078	21.448170078
H	0.000000000	2.517574637	18.464488953
H	0.000000000	-2.517574637	18.464488953
H	0.000000000	-2.482162816	15.998744696
H	0.000000000	2.482162816	15.998744696
H	0.000000000	-2.519386044	13.532712399
H	0.000000000	2.519386044	13.532712399
C	0.000000000	2.478253312	10.579242208
C	0.000000000	-2.478253312	10.579242208
B	0.000000000	0.000000000	8.733057780
C	0.724553748	0.000000000	1.227455336
C	-0.715384273	0.000000000	3.631923903
C	-0.724553748	0.000000000	1.227455336
C	0.000000000	0.000000000	5.795342465
C	0.000000000	0.000000000	-5.795342465

C	0.715384273	0.000000000	3.631923903
C	-1.434832584	0.000000000	2.468461148
C	1.434832584	0.000000000	2.468461148
C	1.394964437	0.000000000	0.000000000
C	-0.724553748	0.000000000	-1.227455336
C	-1.434832584	0.000000000	-2.468461148
B	0.000000000	0.000000000	7.269755848
C	-0.715384273	0.000000000	-3.631923903
C	-1.394964437	0.000000000	0.000000000
C	1.434832584	0.000000000	-2.468461148
C	0.715384273	0.000000000	-3.631923903
C	0.724553748	0.000000000	-1.227455336
N	1.104962910	0.000000000	-4.960792751
N	1.104962910	0.000000000	4.960792751
N	-1.104962910	0.000000000	4.960792751
N	-1.104962910	0.000000000	-4.960792751
C	-2.477857836	0.000000000	-5.423056608
H	-2.518000239	0.000000000	2.466904952
C	-2.477857836	0.000000000	5.423056608
C	2.477857836	0.000000000	5.423056608
H	2.518000239	0.000000000	2.466904952
H	-2.480740274	0.000000000	0.000000000
C	2.477857836	0.000000000	-5.423056608
H	-2.518000239	0.000000000	-2.466904952
H	2.518000239	0.000000000	-2.466904952
H	2.480740274	0.000000000	0.000000000
H	0.000000000	2.471759914	9.489416113
H	-0.891093700	3.002560703	10.936904810
H	0.891093700	3.002560703	10.936904810
H	0.000000000	-2.471759914	9.489416113
H	-0.891093700	-3.002560703	10.936904810
H	0.891093700	-3.002560703	10.936904810
H	2.472180659	0.000000000	6.512825482
H	3.001814478	0.891119815	5.065315971
H	3.001814478	-0.891119815	5.065315971
H	-2.472180659	0.000000000	6.512825482
H	-3.001814478	0.891119815	5.065315971
H	-3.001814478	-0.891119815	5.065315971
H	0.000000000	2.421534055	22.535521898
H	0.889752308	2.982310561	21.097741219
H	-0.889752308	2.982310561	21.097741219
H	0.000000000	-2.421534055	22.535521898
H	0.889752308	-2.982310561	21.097741219
H	-0.889752308	-2.982310561	21.097741219
H	-2.472180659	0.000000000	-6.512825482
H	-3.001814478	0.891119815	-5.065315971
H	-3.001814478	-0.891119815	-5.065315971
H	2.472180659	0.000000000	-6.512825482

H	3.001814478	-0.891119815	-5.065315971
H	3.001814478	0.891119815	-5.065315971
H	0.891093700	-3.002560703	-10.936904810
H	-0.891093700	-3.002560703	-10.936904810
H	0.889752308	-2.982310561	-21.097741219
C	0.000000000	-2.478253312	-10.579242208
H	0.000000000	-2.471759914	-9.489416113
H	-0.889752308	-2.982310561	-21.097741219
C	0.000000000	-2.450206078	-21.448170078
H	0.000000000	-2.519386044	-13.532712399
H	0.000000000	-2.482162816	-15.998744696
H	0.000000000	-2.421534055	-22.535521898
H	0.000000000	-2.517574637	-18.464488953
C	0.000000000	-1.436213850	-13.531492660
C	0.000000000	-1.396308699	-15.998260126
C	0.000000000	-1.433835879	-18.466873883
N	0.000000000	-1.105245579	-11.041726855
N	0.000000000	-1.078092771	-20.977710767
C	0.000000000	-0.716600325	-12.369822362
C	0.000000000	-0.725887056	-14.774862133
C	0.000000000	-0.724609117	-17.229235662
C	0.000000000	-0.712742186	-19.629939565
B	0.000000000	0.000000000	-7.269755848
B	0.000000000	0.000000000	-8.733057780
C	0.000000000	0.000000000	-10.205740557
C	0.000000000	0.000000000	-21.820707776
C	0.000000000	0.716600325	-12.369822362
C	0.000000000	0.725887056	-14.774862133
C	0.000000000	0.724609117	-17.229235662
C	0.000000000	0.712742186	-19.629939565
N	0.000000000	1.105245579	-11.041726855
N	0.000000000	1.078092771	-20.977710767
C	0.000000000	1.436213850	-13.531492660
C	0.000000000	1.396308699	-15.998260126
C	0.000000000	1.433835879	-18.466873883
C	0.000000000	2.478253312	-10.579242208
C	0.000000000	2.450206078	-21.448170078
H	0.000000000	2.519386044	-13.532712399
H	0.000000000	2.471759914	-9.489416113
H	0.000000000	2.482162816	-15.998744696
H	0.000000000	2.517574637	-18.464488953
H	0.000000000	2.421534055	-22.535521898
H	0.891093700	3.002560703	-10.936904810
H	0.889752308	2.982310561	-21.097741219
H	-0.891093700	3.002560703	-10.936904810
H	-0.889752308	2.982310561	-21.097741219

Compound 11(BB11)$_2$



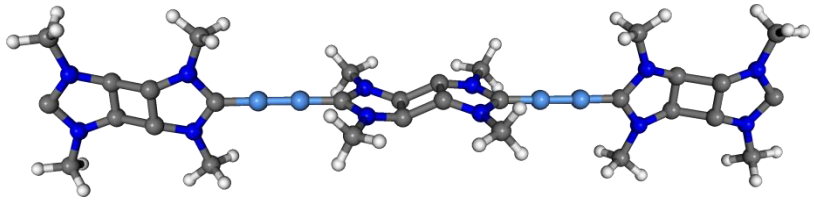
Total enthalpy, Htot (Utot + pV): -3074.813302 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -3074.970975 hartrees

C	15.908738325	-1.802876394	4.603472463
C	14.669089596	-1.541199773	4.092854215
C	14.404412667	-1.583295550	2.684347017
C	15.463116972	-1.909625338	1.748679857
C	16.746776711	-2.177974863	2.323559945
C	16.945513291	-2.122650357	3.694660403
C	13.122741185	-1.309576664	2.199133696
C	12.808937083	-1.335584694	0.834161477
C	13.869601829	-1.658573101	-0.101537121
C	15.153048902	-1.934318074	0.388204912
C	11.527396270	-1.069039143	0.261992292
C	11.334339602	-1.117148350	-1.115603511
C	12.370866287	-1.429820712	-2.019150376
C	13.613174262	-1.695063675	-1.505052552
N	10.296766946	-0.736893283	0.817311450
C	9.341407901	-0.573485528	-0.178431226
N	10.010794121	-0.815819940	-1.364093624
N	18.282232183	-2.430397396	3.910321348
C	18.955582796	-2.681601344	2.749390333
N	17.991531095	-2.520279784	1.787100322
C	18.919537346	-2.485388992	5.214673486
C	18.316917202	-2.705609353	0.381298827
C	9.963078363	-0.556594558	2.219666384
C	9.388187224	-0.753611244	-2.671935149
H	13.850221935	-1.292679244	4.758441336
H	16.094886986	-1.767393124	5.669979062
H	15.918149630	-2.171679820	-0.337420068
H	14.432973877	-1.940085435	-2.170456587
H	12.185652960	-1.459317985	-3.085646183
H	12.359526592	-1.070304207	2.925506996
H	8.900934988	-0.312400711	2.270090540
H	10.145696982	-1.474101138	2.784052043
H	10.538151641	0.264661188	2.654616717
H	8.343830804	-0.474545980	-2.527804400
H	9.437053269	-1.726495372	-3.169528179
H	9.879987965	-0.002594789	-3.296711558

H	19.961523671	-2.751111916	5.051659330
H	18.866583049	-1.515325536	5.717033040
H	18.447268622	-3.240690508	5.849196213
H	19.371971988	-2.966486380	0.339141592
H	18.148673402	-1.786861713	-0.186542901
H	17.726527269	-3.514772708	-0.056370338
B	7.914315972	-0.211497199	-0.025709097
H	-5.266678847	-3.698090264	-0.815802874
H	3.619865554	-2.126257791	-0.756710298
H	-3.606203486	2.068040324	-1.029494583
C	-5.447508488	-3.059519591	0.053664012
C	-2.319054250	-2.955702752	0.089615351
C	-0.978986724	-2.672449700	0.103579822
C	-3.224482754	-1.874799923	0.023976358
N	-4.604762181	-1.880836228	0.006783211
H	-2.677793427	-3.976677074	0.129943359
C	-5.090598621	-0.587764930	-0.047401273
H	-6.485549584	-2.725154219	0.046009307
C	-0.492066155	-1.330605070	0.051636391
C	-2.807012073	-0.548985303	-0.029025407
H	5.259997932	3.631410575	-0.966904682
C	0.884130007	-1.078257266	0.069276296
H	-0.256466288	-3.478749334	0.155816100
C	-1.417557423	-0.213625472	-0.019493067
C	4.075418838	-1.670828998	0.126099214
N	-3.962270220	0.223104722	-0.077288869
C	1.417557423	0.213625472	0.019493067
C	-0.884130007	1.078257266	-0.069276296
C	-4.075418838	1.670828998	-0.126099214
H	1.541192990	-1.934351680	0.124136000
C	2.807012073	0.548985303	0.029025407
N	3.962270220	-0.223104722	0.077288869
C	0.492066155	1.330605070	-0.051636391
C	5.090598621	0.587764930	0.047401273
B	6.510680219	0.167005807	0.048074557
H	5.139846624	-1.910548232	0.141289282
C	3.224482754	1.874799923	-0.023976358
C	0.978986724	2.672449700	-0.103579822
C	2.319054250	2.955702752	-0.089615351
N	4.604762181	1.880836228	-0.006783211
H	-5.139846624	1.910548232	-0.141289282
H	-1.541192990	1.934351680	-0.124136000
C	5.447508488	3.059519591	-0.053664012
H	0.256466288	3.478749334	-0.155816100
H	-5.259997932	-3.631410575	0.966904682
H	2.677793427	3.976677074	-0.129943359
H	6.485549584	2.725154219	-0.046009307
H	3.606203486	-2.068040324	1.029494583

H	-3.619865554	2.126257791	0.756710298
H	5.266678847	3.698090264	0.815802874
H	-16.094886986	1.767393124	-5.669979062
H	-13.850221935	1.292679244	-4.758441336
H	-18.447268622	3.240690508	-5.849196213
H	-18.866583049	1.515325536	-5.717033040
C	-18.919537346	2.485388992	-5.214673486
C	-15.908738325	1.802876394	-4.603472463
C	-14.669089596	1.541199773	-4.092854215
H	-19.961523671	2.751111916	-5.051659330
H	-10.145696982	1.474101138	-2.784052043
H	-8.900934988	0.312400711	-2.270090540
H	-10.538151641	-0.264661188	-2.654616717
C	-9.963078363	0.556594558	-2.219666384
H	-12.359526592	1.070304207	-2.925506996
C	-16.945513291	2.122650357	-3.694660403
N	-18.282232183	2.430397396	-3.910321348
C	-14.404412667	1.583295550	-2.684347017
C	-13.122741185	1.309576664	-2.199133696
C	-16.746776711	2.177974863	-2.323559945
N	-10.296766946	0.736893283	-0.817311450
C	-18.955582796	2.681601344	-2.749390333
C	-15.463116972	1.909625338	-1.748679857
B	-6.510680219	-0.167005807	-0.048074557
C	-12.808937083	1.335584694	-0.834161477
B	-7.914315972	0.211497199	0.025709097
C	-11.527396270	1.069039143	-0.261992292
C	-9.341407901	0.573485528	0.178431226
N	-17.991531095	2.520279784	-1.787100322
C	-15.153048902	1.934318074	-0.388204912
C	-13.869601829	1.658573101	0.101537121
C	-11.334339602	1.117148350	1.115603511
N	-10.010794121	0.815819940	1.364093624
C	-18.316917202	2.705609353	-0.381298827
H	-15.918149630	2.171679820	0.337420068
H	-17.726527269	3.514772708	0.056370338
C	-13.613174262	1.695063675	1.505052552
H	-19.371971988	2.966486380	-0.339141592
H	-18.148673402	1.786861713	0.186542901
C	-12.370866287	1.429820712	2.019150376
C	-9.388187224	0.753611244	2.671935149
H	-8.343830804	0.474545980	2.527804400
H	-14.432973877	1.940085435	2.170456587
H	-9.437053269	1.726495372	3.169528179
H	-9.879987965	0.002594789	3.296711558
H	-12.185652960	1.459317985	3.085646183

Compound 12(BB12)$_2$



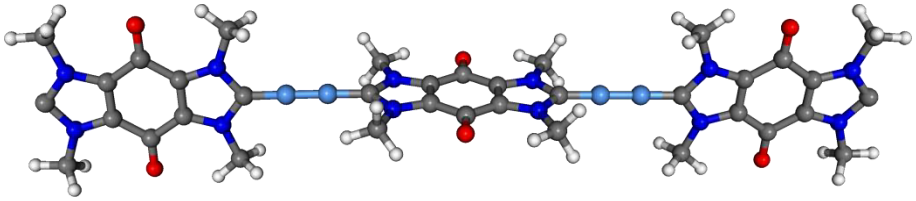
Total enthalpy, Htot (Utot + pV): -1920.316457 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1920.444985 hartrees

XYZ Coordinates

C	-2.818686702	1.933039030	-0.360810175
C	-1.389980561	2.088290901	0.217532098
C	-1.243872542	0.740469761	0.231701315
C	-2.671356966	0.574708631	-0.344871741
N	-0.145706886	2.630713249	-0.044907031
C	0.819770655	1.642172358	-0.092963495
N	0.087970290	0.471448323	-0.023201323
N	-4.112998218	2.231194553	0.008212034
C	-4.830569965	1.031987985	0.115109053
N	-3.871267499	0.013232429	0.033191469
C	0.186910700	4.045263842	-0.120949815
C	0.715454491	-0.840485983	-0.071995928
C	-4.764389778	3.526884560	0.002078150
C	-4.226407585	-1.392421844	0.065587943
H	-4.003297180	4.303067924	0.081677242
H	-5.450059721	3.588191153	0.848841451
H	-5.343916904	3.667904930	-0.916360515
H	-0.441043741	4.539457905	-0.866250604
H	1.231819016	4.121853619	-0.413602367
H	0.044336591	4.532272385	0.846880887
H	1.753656340	-0.697504503	-0.363476751
H	0.210590140	-1.471558985	-0.807396208
H	0.676594762	-1.328390810	0.905015375
H	-4.867061008	-1.581834444	0.928457670
H	-3.313502113	-1.982901888	0.142039005
H	-4.778341485	-1.675838604	-0.836734965
H	-9.032329851	-0.496362411	-2.347089415
H	-15.192827826	-0.915119807	-2.026049575
C	-9.622084839	0.396753796	-2.115454948
H	-8.805712706	-0.415734184	3.026621863
H	-10.490917143	0.446549304	-2.771800326
N	-10.077302312	0.373270432	-0.738787741
C	-14.556690262	-0.033193343	-1.934154288
C	-9.200740188	0.523218951	0.345153918
C	-11.294888336	-0.053787323	-0.254616884

H	-13.737788393	-0.088438774	-2.651332036
C	-12.753888929	0.453781567	-0.208097459
H	-13.512053338	-0.015555041	3.669895509
N	-14.002851302	0.017570821	-0.595109603
C	-11.245903114	-0.039773117	1.107470418
N	-9.996572349	0.398137341	1.492676268
C	-12.705783282	0.465686649	1.154030935
C	-14.798930673	-0.110486666	0.551209138
C	-9.441827606	0.453962328	2.831302871
N	-13.923527686	0.037342773	1.636297309
H	-8.829429829	1.351844997	2.930723943
C	-14.380709212	0.007100003	3.011998328
H	-8.987749256	1.271450557	-2.268285360
H	-14.990417671	-0.884317107	3.168663267
H	-15.169196062	0.851371046	-2.137842007
H	-10.261066310	0.481722724	3.549584597
H	-14.995804357	0.884313870	3.238252187
B	-6.291213837	0.871418562	0.213470399
B	-7.740302186	0.704258289	0.286333151
C	-22.753364687	-0.280214600	0.581496878
C	-21.333881739	-0.139136660	1.183727531
C	-21.196838400	-1.498765938	1.167618857
C	-22.617382557	-1.629015925	0.564776943
N	-20.124267126	0.422148490	0.836885658
C	-19.172079047	-0.602204370	0.742099957
N	-19.899985053	-1.798050302	0.810010870
N	-24.087134660	-0.007546851	0.821767769
C	-24.828218501	-1.174241730	0.851601943
N	-23.869322648	-2.168106024	0.794831395
C	-19.755823788	1.824706245	0.847821074
C	-19.259126755	-3.098595436	0.785933718
C	-24.705435303	1.307836134	0.891926787
C	-24.212830702	-3.581518888	0.829720672
H	-24.202614669	1.919740217	1.644707040
H	-25.747269171	1.166739438	1.170968671
H	-24.654055143	1.815497410	-0.074429137
H	-20.661627118	2.426050593	0.771758491
H	-19.098753118	2.030273849	0.001072536
H	-19.216369576	2.078639104	1.766356314
H	-18.570861849	-3.144134805	-0.059782727
H	-20.026182636	-3.866109341	0.684178281
H	-18.684186408	-3.267365278	1.702523252
H	-25.260619899	-3.658266439	1.111310688
H	-23.594919960	-4.100322203	1.566461117
H	-24.065597387	-4.043444245	-0.149538989
B	-16.259016852	-0.290425334	0.605737929
B	-17.709312468	-0.450593542	0.665659990

Compound 13(BB13)$_2$



Total enthalpy, Htot (Utot + pV): -2600.913243 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2601.060577 hartrees

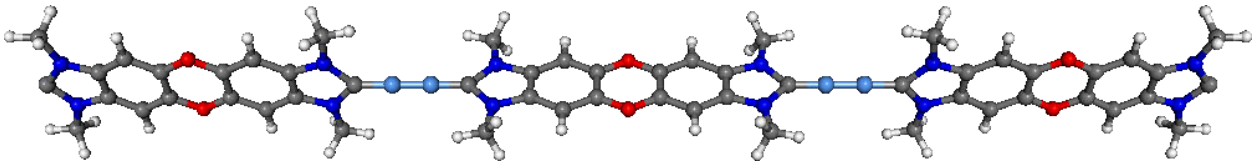
XYZ Coordinates

C	-3.306186270	-0.602302288	-0.676700567
C	-4.569658739	0.143214959	-0.519211393
C	-2.144093908	0.297731420	-0.762090245
C	-2.222539344	1.665636182	-0.699073457
C	-3.479504850	2.415437556	-0.539917533
C	-4.648901676	1.519094289	-0.458816808
N	-0.807520824	-0.007133823	-0.914322034
C	-0.019210786	1.116080581	-0.952086633
N	-0.930302043	2.133726390	-0.815734539
N	-5.848609833	-0.350029598	-0.412193913
C	-6.751476640	0.699101829	-0.288176406
N	-5.975058792	1.851352595	-0.313894224
O	-3.535865821	3.636382255	-0.483239528
C	-0.246478389	-1.351490573	-1.028957112
C	-0.526813300	3.538104237	-0.801888705
C	-6.566035668	3.180203228	-0.213603798
C	-6.282228754	-1.741706790	-0.426935112
H	-5.412407441	-2.380398252	-0.542121805
H	-6.983590000	-1.889869273	-1.251952473
H	-6.804680944	-1.965397280	0.506460629
H	-0.477422516	-1.938846333	-0.139831127
H	0.828857108	-1.230793548	-1.135370404
H	-0.659285828	-1.864757091	-1.897959835
H	0.554461805	3.551356447	-0.915489368
H	-0.816366443	4.009426283	0.137758503
H	-1.001884255	4.080083499	-1.620120508
H	-7.168011704	3.232850765	0.696797406
H	-7.227189021	3.348324658	-1.067609220
H	-5.771322994	3.919045044	-0.196323356
O	-3.222110003	-1.821788209	-0.732811832
H	-18.151639159	0.923861597	2.668663103
H	-10.839623892	1.389664098	2.578547514
C	-17.494402199	0.063555727	2.526888222
O	-14.489005805	0.261487980	2.778644919
C	-11.407100552	0.462477915	2.459900475

H	-16.646041459	0.110055953	3.201073956
C	-14.473695513	0.236671493	1.547834408
H	-16.767317791	0.017607965	-3.110139833
N	-17.002396453	0.062371944	1.150754170
H	-12.230208501	0.426532433	3.167228425
C	-15.711310069	0.136545312	0.718003101
H	-11.647904178	1.381754343	-2.883109917
C	-13.281479835	0.298781496	0.729004679
N	-11.948517248	0.394296612	1.110051221
C	-17.869237017	-0.021423326	0.062999471
C	-11.144160991	0.423923474	-0.011006680
C	-15.729249236	0.102271287	-0.663884088
C	-13.303786317	0.270473619	-0.650434556
N	-17.057625990	0.007156286	-1.053501809
C	-14.536639549	0.171790984	-1.481264411
N	-12.018488931	0.339173236	-1.093658705
C	-17.589912820	-0.065801146	-2.406252088
C	-11.557541903	0.370602284	-2.480504940
O	-14.506569164	0.155287386	-2.711095421
H	-18.309513185	0.743724814	-2.556198665
H	-18.078636481	-0.843621853	2.693412201
H	-10.508385949	0.075120896	-2.481146001
H	-10.725401155	-0.376625253	2.623604207
H	-18.114722095	-1.015382755	-2.544054006
H	-12.162831502	-0.302566051	-3.080717287
B	-8.216891717	0.609962635	-0.166274962
B	-9.671607055	0.521398018	-0.074791567
H	-28.522990358	2.172214443	-0.777477568
H	-22.179465506	2.247977878	-0.866295391
C	-28.830759258	1.673216895	0.141874982
O	-25.844864556	2.166850165	0.082695174
C	-22.768532922	2.111419568	0.044234701
H	-28.505728314	2.279082489	0.988175200
C	-25.744475100	0.949361602	0.154934294
H	-28.103580555	-3.765234314	-0.421026058
N	-28.249279564	0.334848433	0.217198850
H	-23.650438738	2.743720887	0.029076860
C	-26.901533472	0.041063057	0.221803433
H	-21.802374726	-2.960058490	-0.544101889
N	-23.186521864	0.718486701	0.140319094
C	-24.465292792	0.215149250	0.185108587
C	-29.027459342	-0.793443967	0.293527972
C	-22.266139227	-0.322134125	0.190535990
C	-26.805157923	-1.324542195	0.303717444
C	-24.368294763	-1.158542020	0.266953744
N	-28.098439283	-1.802567966	0.345874919
C	-25.531846277	-2.063244573	0.335490362
N	-23.031506516	-1.479805085	0.271049201

C	-28.485987717	-3.208603312	0.435038484
C	-22.422004993	-2.801804990	0.342212363
O	-25.459722151	-3.282478809	0.409976577
H	-29.573002743	-3.230632076	0.446858535
H	-29.910200740	1.543919855	0.160302690
H	-21.774565587	-2.851238171	1.221379812
H	-22.132395774	2.354701438	0.898998485
H	-28.086494760	-3.657997973	1.344632829
H	-23.206829242	-3.549054860	0.400534347
B	-19.340459354	-0.120678647	0.114766374
B	-20.797418150	-0.220381223	0.160619697

Compound 14(BB14)$_2$



Total enthalpy, Htot (Utot + pV): -3293.962304 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -3294.115936 hartrees

XYZ Structures

O	1.364796115	17.232320641	0.000000000
C	0.701725817	15.997744690	0.000000000
C	-0.701725817	15.997744690	0.000000000
O	-1.364796115	17.232320641	0.000000000
C	-0.707120638	18.455050181	0.000000000
C	0.707120638	18.455050181	0.000000000
C	1.412195444	19.706895257	0.000000000
C	0.675675829	20.913145461	0.000000000
C	-0.675675829	20.913145461	0.000000000
C	-1.412195444	19.706895257	0.000000000
C	1.388151749	14.691097629	0.000000000
C	0.666627344	13.380578513	0.000000000
C	-0.666627344	13.380578513	0.000000000
C	-1.388151749	14.691097629	0.000000000
N	1.132974251	22.254388660	0.000000000
C	0.000000000	23.164262098	0.000000000
N	-1.132974251	22.254388660	0.000000000
N	1.156556915	11.953389001	0.000000000
C	0.000000000	10.909372093	0.000000000
N	-1.156556915	11.953389001	0.000000000
C	2.506024327	22.699558694	0.000000000
C	-2.506024327	22.699558694	0.000000000
C	2.570336326	11.794710631	0.000000000

C	-2.570336326	11.794710631	0.000000000
H	2.823459439	10.721385312	0.000000000
H	2.976085757	12.268541821	0.909337453
H	2.976085757	12.268541821	-0.909337453
H	-2.823459439	10.721385312	0.000000000
H	-2.976085757	12.268541821	-0.909337453
H	-2.976085757	12.268541821	0.909337453
H	2.560999623	23.803986490	0.000000000
H	3.025886684	22.323554643	-0.901752840
H	3.025886684	22.323554643	0.901752840
H	-2.560999623	23.803986490	0.000000000
H	-3.025886684	22.323554643	0.901752840
H	-3.025886684	22.323554643	-0.901752840
H	-0.910390701	5.045131735	-2.944200617
H	0.910390701	5.045131735	2.944200617
H	-0.910390701	-5.045131735	-2.944200617
H	0.910390701	-5.045131735	2.944200617
C	0.000000000	5.532903963	-2.561910368
C	0.000000000	6.375222219	0.000000000
C	0.000000000	5.532903963	2.561910368
N	0.000000000	5.334965837	-1.154959052
C	0.000000000	3.899751635	-0.669714356
N	0.000000000	5.334965837	1.154959052
C	0.000000000	3.899751635	0.669714356
C	0.000000000	2.581168236	-1.391800719
C	0.000000000	2.581168236	1.391800719
C	0.000000000	1.258792003	-0.702817405
C	0.000000000	1.258792003	0.702817405
H	0.000000000	6.586700525	-2.855144990
C	0.000000000	-1.258792003	-0.702817405
O	0.000000000	0.000000000	-1.361783979
C	0.000000000	-1.258792003	0.702817405
O	0.000000000	0.000000000	1.361783979
C	0.000000000	-2.581168236	-1.391800719
C	0.000000000	-2.581168236	1.391800719
H	0.000000000	6.586700525	2.855144990
C	0.000000000	-3.899751635	-0.669714356
C	0.000000000	-3.899751635	0.669714356
C	0.000000000	-5.532903963	-2.561910368
C	0.000000000	-5.532903963	2.561910368
C	0.000000000	-6.375222219	0.000000000
N	0.000000000	-5.334965837	-1.154959052
N	0.000000000	-5.334965837	1.154959052
H	0.000000000	-6.586700525	2.855144990
H	0.000000000	-6.586700525	-2.855144990
H	0.910390701	5.045131735	-2.944200617
H	-0.910390701	5.045131735	2.944200617
H	0.910390701	-5.045131735	-2.944200617

H	-0.910390701	-5.045131735	2.944200617
B	0.000000000	9.409923793	0.000000000
B	0.000000000	7.874756898	0.000000000
H	-2.976085757	-12.268541821	0.909337453
H	2.976085757	-12.268541821	-0.909337453
H	3.025886684	-22.323554643	-0.901752840
H	-3.025886684	-22.323554643	0.901752840
C	2.570336326	-11.794710631	0.000000000
C	-2.570336326	-11.794710631	0.000000000
C	0.666627344	-13.380578513	0.000000000
C	-0.666627344	-13.380578513	0.000000000
C	1.388151749	-14.691097629	0.000000000
C	-1.388151749	-14.691097629	0.000000000
N	1.156556915	-11.953389001	0.000000000
C	0.000000000	-10.909372093	0.000000000
N	-1.156556915	-11.953389001	0.000000000
C	0.701725817	-15.997744690	0.000000000
C	-0.701725817	-15.997744690	0.000000000
H	2.823459439	-10.721385312	0.000000000
O	1.364796115	-17.232320641	0.000000000
C	0.707120638	-18.455050181	0.000000000
C	-0.707120638	-18.455050181	0.000000000
O	-1.364796115	-17.232320641	0.000000000
C	1.412195444	-19.706895257	0.000000000
C	-1.412195444	-19.706895257	0.000000000
H	-2.823459439	-10.721385312	0.000000000
C	0.675675829	-20.913145461	0.000000000
C	-0.675675829	-20.913145461	0.000000000
C	2.506024327	-22.699558694	0.000000000
C	-2.506024327	-22.699558694	0.000000000
C	0.000000000	-23.164262098	0.000000000
N	1.132974251	-22.254388660	0.000000000
N	-1.132974251	-22.254388660	0.000000000
H	-2.560999623	-23.803986490	0.000000000
H	2.560999623	-23.803986490	0.000000000
H	2.976085757	-12.268541821	0.909337453
H	-2.976085757	-12.268541821	-0.909337453
H	3.025886684	-22.323554643	0.901752840
H	-3.025886684	-22.323554643	-0.901752840
B	0.000000000	-7.874756898	0.000000000
B	0.000000000	-9.409923793	0.000000000
H	-2.488758773	-19.725669220	0.000000000
H	2.488758773	-19.725669220	0.000000000
H	-2.465621266	-14.680805662	0.000000000
H	2.465621266	-14.680805662	0.000000000
H	0.000000000	-2.592174408	2.470708704
H	0.000000000	-2.592174408	-2.470708704
H	0.000000000	2.592174408	2.470708704

H	0.000000000	2.592174408	-2.470708704
H	2.465621266	14.680805662	0.000000000
H	-2.465621266	14.680805662	0.000000000
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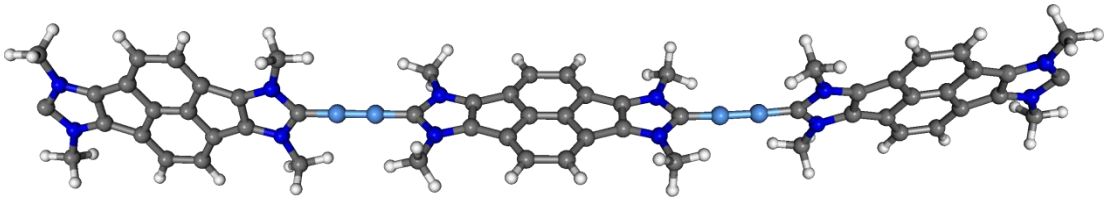
Compound 15(BB15)$_2$



Total enthalpy, Htot (Utot + pV): -3071.024885 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -3071.184713 hartrees

XYZ Structures

C	1.166110055	-0.289410697	1.082108368
C	2.576362600	-0.565709964	0.909102596
C	3.480377700	0.455618039	0.690598572
C	2.953072391	1.778507832	0.644149084
C	1.638521928	2.036294362	0.805957181
C	0.682780510	1.003738184	1.031854002
C	1.110361649	3.359331127	0.761952699
C	2.014677240	4.379797602	0.539907461
C	3.425058895	4.102989899	0.363679220
C	3.909012007	2.809852275	0.411615769
C	4.913249370	0.694844856	0.465223458
C	5.158613489	2.042668560	0.299963484
C	-0.567884400	1.768919507	1.136763084
C	-0.323094868	3.118829159	0.987359207
N	-1.918064792	1.606594672	1.330809809
C	-2.544746718	2.852750776	1.329172831
N	-1.522886081	3.777864878	1.111964718
N	6.112914585	0.034300959	0.361473791
C	7.132264941	0.951517473	0.104917179
N	6.505535228	2.198050436	0.072694980
C	6.338481264	-1.395842037	0.441151980
C	7.219596786	3.443275554	-0.134618070
C	-2.628851130	0.362460059	1.555041798
C	-1.751105075	5.206932566	1.012249550
H	-2.184837416	-0.426966906	0.946028530
H	-3.671185173	0.513983377	1.268273417
H	-2.596980380	0.073713322	2.610104312
H	-2.722935889	5.422197341	1.459989923

H	-1.764686388	5.531865157	-0.032548728
H	-0.968258663	5.744773177	1.550980055
H	5.631354263	-1.836544750	1.145542807
H	7.361417650	-1.558948669	0.785728156
H	6.224738972	-1.869257321	-0.538855565
H	8.181620160	3.205796470	-0.591708781
H	7.398535630	3.958203663	0.814222284
H	6.645385972	4.092479623	-0.798710825
H	-16.807081117	5.154119681	6.251806113
H	-6.494756593	5.022735558	4.658646666
H	-16.386969525	5.056596164	0.611122213
C	-15.737452876	5.039334331	6.090811843
C	-11.943339130	4.598643950	5.328651626
C	-10.529190273	4.435020624	5.069668680
N	-15.539159682	4.780502928	4.674173743
H	-15.222300180	5.955338744	6.392617458
C	-16.586782563	4.712203133	3.782661548
H	-7.950328053	4.146052122	-0.924974089
C	-12.870414606	4.500449658	4.310167588
C	-14.321279148	4.576112577	4.058545639
C	-6.717862080	3.969621183	4.461485243
C	-10.063750223	4.173051445	3.794635883
C	-14.590291164	4.368678585	2.722994006
C	-12.362409125	4.234551126	3.006077057
N	-15.960244459	4.455526423	2.583403331
C	-11.042484780	4.080150211	2.764164211
C	-8.818556209	3.934766720	3.050044532
H	-7.296461579	3.557386044	5.290017201
N	-7.460530807	3.814160777	3.225430747
C	-13.340822482	4.137986123	1.974982208
C	-16.694573399	4.300480027	1.338575881
C	-9.088623381	3.730444647	1.712515206
C	-6.851346096	3.547708869	1.998949743
C	-10.534605697	3.812741780	1.461082151
C	-12.875982629	3.880016307	0.700703325
C	-11.461891975	3.716979191	0.440729691
N	-7.895257165	3.494261238	1.073993348
H	-17.750351292	4.425697841	1.568444158
C	-7.700459942	3.253785919	-0.343435832
H	-15.365011622	4.205606419	6.692267702
H	-6.648696663	3.009150422	-0.498033523
H	-5.775876133	3.427642093	4.359279206
H	-16.528827345	3.307104003	0.912809011
H	-8.322769534	2.418349518	-0.674104568
B	-3.986778454	3.121553615	1.526954157
B	-5.406608302	3.347987033	1.747453673
H	1.697808538	5.415053541	0.488470403
H	4.083168320	4.947437087	0.194768475

H	0.508102649	-1.133450196	1.253434808
H	2.892427271	-1.601417888	0.954997631
H	-11.159226872	3.517482586	-0.580788143
H	-13.553542640	3.791818342	-0.140946648
H	-9.852059578	4.526876230	5.911006495
H	-12.245400751	4.800420022	6.350093246
H	16.675531533	-1.443806878	-4.998814518
H	19.278194211	-3.265161659	-5.295988831
H	14.386653446	-0.703475782	-4.544979576
H	19.865520406	-1.593404350	-5.116495131
H	12.081641050	0.555770952	-3.769701343
C	19.972862656	-2.618862790	-4.752616350
H	10.836180635	-0.693416517	-3.487978937
H	20.992315583	-2.959060622	-4.920429166
C	16.346600016	-1.437410407	-3.965849433
C	11.343999328	0.176757390	-3.061082608
C	14.994455402	-0.997998338	-3.697389021
H	10.595186230	0.943668153	-2.854874187
N	19.725220639	-2.685506985	-3.321775737
C	17.182636243	-1.835057646	-2.941592102
C	14.499728648	-0.961484846	-2.407520932
N	12.003115815	-0.160327530	-1.814373124
C	18.546158993	-2.338195005	-2.694429326
C	13.284467665	-0.627630170	-1.649268630
C	20.678826448	-3.117510536	-2.426972630
C	16.645798972	-1.789076700	-1.622762396
C	15.383587500	-1.378326035	-1.372063023
C	11.359634227	-0.109031591	-0.577987855
C	18.743874444	-2.552914674	-1.347520137
C	13.480475274	-0.849496331	-0.301418931
N	20.034530305	-3.021833078	-1.213286834
C	17.528150292	-2.210762937	-0.586602584
C	14.843261541	-1.340864344	-0.054531414
N	12.310632097	-0.537422985	0.349868131
C	17.031666490	-2.180888746	0.701469412
C	20.676576808	-3.382760696	0.039889405
C	15.679133349	-1.742931698	0.970627172
C	12.062904691	-0.601548473	1.777549377
H	20.133836631	-4.193692064	0.533190000
H	21.685646523	-3.712539551	-0.197136682
H	10.985504883	-0.527116953	1.932713292
H	12.427656238	-1.550594601	2.176957771
H	20.722229444	-2.522382729	0.713061636
H	17.637282501	-2.485086975	1.547643407
H	15.348349045	-1.742356431	2.002898469
H	12.553989356	0.225875308	2.298760817
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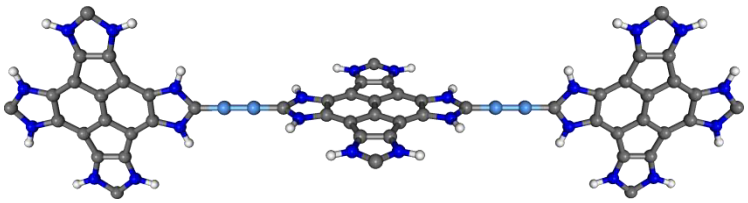
B	9.959818037	0.294609767	-0.322495314

Compound 16(BB16)$_2$



Total internal energy, Utot (SCFE + ZPE + U): -3485.106108 hartrees
Total enthalpy, Htot (Utot + pV): -3485.105164 hartrees

XYZ Coordinates

C	-2.837461133	0.000000000	0.690261690
C	-1.465924025	0.000000000	1.193013307
C	-0.684323414	0.000000000	0.000000000
C	0.684323414	0.000000000	0.000000000
C	-1.465924025	0.000000000	-1.193013307
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C	2.837461133	0.000000000	0.690261690
C	2.837461133	0.000000000	-0.690261690
C	1.465924025	0.000000000	-1.193013307
N	4.171314114	0.000000000	1.066171281
C	5.040013023	0.000000000	0.000000000
N	4.171314114	0.000000000	-1.066171281
C	-0.726810876	0.000000000	2.365970617
C	0.726810876	0.000000000	2.365970617
N	-1.089908060	0.000000000	3.700222921
C	0.000000000	0.000000000	4.546878202
N	1.089908060	0.000000000	3.700222921
C	-0.726810876	0.000000000	-2.365970617
C	0.726810876	0.000000000	-2.365970617
N	-1.089908060	0.000000000	-3.700222921
C	0.000000000	0.000000000	-4.546878202
N	1.089908060	0.000000000	-3.700222921
N	-4.171314114	0.000000000	1.066171281
C	-5.040013023	0.000000000	0.000000000
N	-4.171314114	0.000000000	-1.066171281
H	-4.522248227	0.000000000	2.008754504
H	-4.522248227	0.000000000	-2.008754504
H	-2.032161617	0.000000000	-4.052102763
H	2.032161617	0.000000000	-4.052102763
H	4.522248227	0.000000000	-2.008754504
H	4.522248227	0.000000000	2.008754504
H	2.032161617	0.000000000	4.052102763
H	-2.032161617	0.000000000	4.052102763
C	0.000000000	-2.837115486	14.182100678

C	0.000000000	-1.461614546	14.684721356
C	0.000000000	-0.684834889	13.495714656
C	0.000000000	0.684834889	13.495714656
C	0.000000000	-1.467716099	12.298911228
C	0.000000000	-2.840973094	12.802915574
C	0.000000000	1.461614546	14.684721356
C	0.000000000	2.837115486	14.182100678
C	0.000000000	2.840973094	12.802915574
C	0.000000000	1.467716099	12.298911228
N	0.000000000	4.168398881	14.562340741
C	0.000000000	5.041003174	13.499172137
N	0.000000000	4.175376805	12.430179574
C	0.000000000	-0.721897854	15.860484164
C	0.000000000	0.721897854	15.860484164
N	0.000000000	-1.063093355	17.211604867
C	0.000000000	0.000000000	18.072034726
N	0.000000000	1.063093355	17.211604867
C	0.000000000	-0.730888719	11.130596099
C	0.000000000	0.730888719	11.130596099
N	0.000000000	-1.091038839	9.797055460
C	0.000000000	0.000000000	8.949208685
N	0.000000000	1.091038839	9.797055460
N	0.000000000	-4.168398881	14.562340741
C	0.000000000	-5.041003174	13.499172137
N	0.000000000	-4.175376805	12.430179574
H	0.000000000	-4.513673955	15.507208567
H	0.000000000	-4.529030527	11.488611271
H	0.000000000	-2.032850051	9.443853307
H	0.000000000	2.032850051	9.443853307
H	0.000000000	4.529030527	11.488611271
H	0.000000000	4.513673955	15.507208567
H	0.000000000	2.007675853	17.557498088
H	0.000000000	-2.007675853	17.557498088
B	0.000000000	0.000000000	6.016508907
B	0.000000000	0.000000000	7.482568198
C	0.000000000	2.840973094	-12.802915574
C	0.000000000	1.467716099	-12.298911228
C	0.000000000	0.684834889	-13.495714656
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C	0.000000000	2.837115486	-14.182100678
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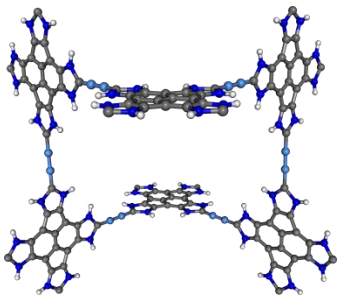
C	0.000000000	-2.840973094	-12.802915574
C	0.000000000	-2.837115486	-14.182100678
C	0.000000000	-1.461614546	-14.684721356
N	0.000000000	-4.175376805	-12.430179574
C	0.000000000	-5.041003174	-13.499172137
N	0.000000000	-4.168398881	-14.562340741

C	0.000000000	0.730888719	-11.130596099
C	0.000000000	-0.730888719	-11.130596099
N	0.000000000	1.091038839	-9.797055460
C	0.000000000	0.000000000	-8.949208685
N	0.000000000	-1.091038839	-9.797055460
C	0.000000000	0.721897854	-15.860484164
C	0.000000000	-0.721897854	-15.860484164
N	0.000000000	1.063093355	-17.211604867
C	0.000000000	0.000000000	-18.072034726
N	0.000000000	-1.063093355	-17.211604867
N	0.000000000	4.175376805	-12.430179574
C	0.000000000	5.041003174	-13.499172137
N	0.000000000	4.168398881	-14.562340741
H	0.000000000	4.529030527	-11.488611271
H	0.000000000	4.513673955	-15.507208567
H	0.000000000	2.007675853	-17.557498088
H	0.000000000	-2.007675853	-17.557498088
H	0.000000000	-4.513673955	-15.507208567
H	0.000000000	-4.529030527	-11.488611271
H	0.000000000	-2.032850051	-9.443853307
H	0.000000000	2.032850051	-9.443853307
B	0.000000000	0.000000000	-7.482568198
B	0.000000000	0.000000000	-6.016508907

3 Structures of diboryne nanorings

Compound 18



XYZ Structure

B	6.328257024	7.965127509	0.383435248
C	10.060037894	3.074184273	4.348310221
C	9.333943536	3.548878067	3.248136805
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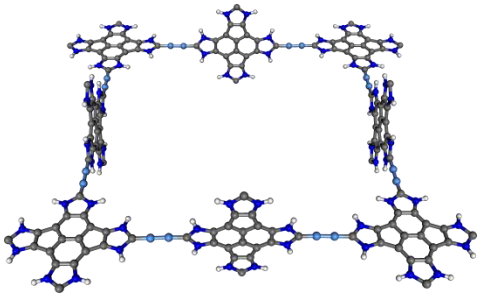
Compound 19



XYZ Structure

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N	12.939050000	0.000000000	-17.308660000
N	15.120595000	0.000000000	-9.872950000
N	12.941540000	0.000000000	-9.855295000
N	18.161035000	0.000000000	-14.689605000
N	18.199195000	0.000000000	-12.553430000
N	3.709900000	1.089160000	-13.733310000
N	1.067790000	4.175200000	-13.714445000
N	14.090540000	1.089580000	-3.712425000
N	14.088040000	4.176415000	-1.067860000
H	18.493700000	0.000000000	-15.647000000
H	18.575050000	0.000000000	-11.612720000
H	16.072760000	0.000000000	-9.525840000
H	11.997290000	0.000000000	-9.487200000
H	9.452740000	0.000000000	-11.567070000
H	9.532840000	0.000000000	-15.648580000
H	11.988305000	0.000000000	-17.658910000
H	16.016860000	0.000000000	-17.660270000
H	4.070610000	2.036100000	-13.742570000
H	2.016595000	4.530305000	-13.716760000
H	14.091050000	2.039110000	-4.066420000
H	14.087930000	4.532175000	-2.016580000
C	-14.090380000	-0.727480000	2.376090000
C	-2.375365000	-0.727310000	13.727590000
C	-14.093540000	-0.687670000	0.000000000
C	-14.091840000	-1.472740000	1.196170000
C	-1.196115000	-1.472230000	13.720990000
C	-14.089730000	-2.840510000	0.696290000
C	-0.696350000	-2.838970000	13.718920000
C	-14.086800000	-5.048960000	0.000000000
N	-14.090540000	-1.089580000	3.712425000
N	-3.709900000	-1.089160000	13.733310000
N	-14.088040000	-4.176415000	1.067860000
N	-1.067790000	-4.175200000	13.714445000
H	-14.091050000	-2.039110000	4.066420000
H	-4.070610000	-2.036100000	13.742570000
H	-14.087930000	-4.532175000	2.016580000
H	-2.016595000	-4.530305000	13.716760000
B	-14.055770000	0.000000000	7.529855000
B	-14.075220000	0.000000000	6.046385000
B	-6.042395000	0.000000000	13.721050000
B	-7.517770000	0.000000000	13.658010000
C	-14.086800000	5.048960000	0.000000000
C	-0.696350000	2.838970000	13.718920000
C	-14.089730000	2.840510000	0.696290000

C	-1.196115000	1.472230000	13.720990000
C	-14.091840000	1.472740000	1.196170000
C	-14.093540000	0.687670000	0.000000000
C	-2.375365000	0.727310000	13.727590000
C	-14.090380000	0.727480000	2.376090000
C	-14.039400000	0.000000000	9.009370000
C	-11.171550000	0.000000000	12.875510000
C	-14.086695000	0.000000000	4.564965000
C	-15.466840000	0.000000000	14.776955000
C	-14.694640000	0.000000000	13.577500000
C	-13.319900000	0.000000000	13.572420000
C	-14.002820000	0.000000000	18.176785000
C	-12.545020000	0.000000000	14.769670000
C	-13.283900000	0.000000000	15.959320000
C	-13.288530000	0.000000000	11.192590000
C	-14.722170000	0.000000000	15.960180000
C	-12.532040000	0.000000000	12.369170000
C	-14.749450000	0.000000000	11.204460000
C	-15.491600000	0.000000000	12.384650000
C	-19.052660000	0.000000000	13.637950000
C	-4.563720000	0.000000000	13.734470000
C	-16.835220000	0.000000000	14.292440000
C	-16.855570000	0.000000000	12.898930000
C	-11.186830000	0.000000000	14.276300000
C	-9.004110000	0.000000000	13.615090000
N	-1.067790000	4.175200000	13.714445000
N	-14.088040000	4.176415000	1.067860000
N	-3.709900000	1.089160000	13.733310000
N	-14.090540000	1.089580000	3.712425000
N	-9.839240000	0.000000000	12.503540000
N	-12.939050000	0.000000000	17.308660000
N	-9.877100000	0.000000000	14.695200000
N	-15.065150000	0.000000000	17.312170000
N	-15.120595000	0.000000000	9.872950000
N	-18.199195000	0.000000000	12.553430000
N	-18.161035000	0.000000000	14.689605000
N	-12.941540000	0.000000000	9.855295000
H	-2.016595000	4.530305000	13.716760000
H	-14.087930000	4.532175000	2.016580000
H	-4.070610000	2.036100000	13.742570000
H	-14.091050000	2.039110000	4.066420000
H	-16.072760000	0.000000000	9.525840000
H	-11.988305000	0.000000000	17.658910000
H	-18.493700000	0.000000000	15.647000000
H	-9.532840000	0.000000000	15.648580000
H	-18.575050000	0.000000000	11.612720000
H	-9.452740000	0.000000000	11.567070000
H	-16.016860000	0.000000000	17.660270000

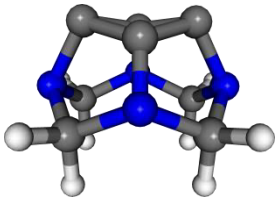
H	-11.997290000	0.000000000	9.487200000
C	14.086800000	-5.048960000	0.000000000
C	0.000000000	-0.687610000	13.720050000
C	14.090380000	-0.727480000	2.376090000
C	2.375365000	-0.727310000	13.727590000
C	14.093540000	-0.687670000	0.000000000
C	14.091840000	-1.472740000	1.196170000
C	1.196115000	-1.472230000	13.720990000
C	14.089730000	-2.840510000	0.696290000
C	0.696350000	-2.838970000	13.718920000
C	0.000000000	-5.047970000	13.713340000
N	14.090540000	-1.089580000	3.712425000
N	3.709900000	-1.089160000	13.733310000
N	14.088040000	-4.176415000	1.067860000
N	1.067790000	-4.175200000	13.714445000
H	14.091050000	-2.039110000	4.066420000
H	4.070610000	-2.036100000	13.742570000
H	14.087930000	-4.532175000	2.016580000
H	2.016595000	-4.530305000	13.716760000
B	6.042395000	0.000000000	13.721050000
B	14.075220000	0.000000000	6.046385000
B	14.055770000	0.000000000	7.529855000
B	7.517770000	0.000000000	13.658010000
C	0.000000000	5.047970000	13.713340000
C	14.086800000	5.048960000	0.000000000
C	0.696350000	2.838970000	13.718920000
C	14.089730000	2.840510000	0.696290000
C	1.196115000	1.472230000	13.720990000
C	14.091840000	1.472740000	1.196170000
C	14.093540000	0.687670000	0.000000000
C	2.375365000	0.727310000	13.727590000
C	14.090380000	0.727480000	2.376090000
C	0.000000000	0.687610000	13.720050000
C	15.466840000	0.000000000	14.776955000
C	14.694640000	0.000000000	13.577500000
C	16.835220000	0.000000000	14.292440000
C	4.563720000	0.000000000	13.734470000
C	14.039400000	0.000000000	9.009370000
C	13.288530000	0.000000000	11.192590000
C	13.319900000	0.000000000	13.572420000
C	14.749450000	0.000000000	11.204460000
C	13.283900000	0.000000000	15.959320000
C	14.722170000	0.000000000	15.960180000
C	14.002820000	0.000000000	18.176785000
C	19.052660000	0.000000000	13.637950000
C	15.491600000	0.000000000	12.384650000
C	16.855570000	0.000000000	12.898930000
C	12.532040000	0.000000000	12.369170000

C	12.545020000	0.000000000	14.769670000
C	9.004110000	0.000000000	13.615090000
C	11.171550000	0.000000000	12.875510000
C	11.186830000	0.000000000	14.276300000
C	14.086695000	0.000000000	4.564965000
N	1.067790000	4.175200000	13.714445000
N	14.088040000	4.176415000	1.067860000
N	3.709900000	1.089160000	13.733310000
N	14.090540000	1.089580000	3.712425000
N	9.877100000	0.000000000	14.695200000
N	15.120595000	0.000000000	9.872950000
N	12.941540000	0.000000000	9.855295000
N	12.939050000	0.000000000	17.308660000
N	9.839240000	0.000000000	12.503540000
N	15.065150000	0.000000000	17.312170000
N	18.199195000	0.000000000	12.553430000
N	18.161035000	0.000000000	14.689605000
H	2.016595000	4.530305000	13.716760000
H	14.087930000	4.532175000	2.016580000
H	4.070610000	2.036100000	13.742570000
H	14.091050000	2.039110000	4.066420000
H	18.493700000	0.000000000	15.647000000
H	16.072760000	0.000000000	9.525840000
H	11.997290000	0.000000000	9.487200000
H	9.452740000	0.000000000	11.567070000
H	18.575050000	0.000000000	11.612720000
H	16.016860000	0.000000000	17.660270000
H	9.532840000	0.000000000	15.648580000
H	11.988305000	0.000000000	17.658910000

4 Energy and structures of diboryne nanotents

4.1 $(CNC)_4(H_2)_n[B_2(NHC)]_m$

$(CNC)_4(H_2)_4$

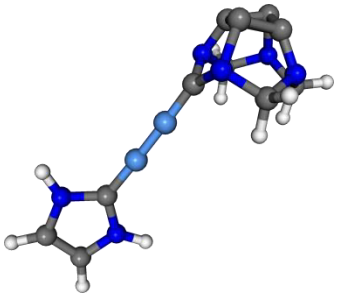


Total enthalpy, Htot (Utot + pV): -528.343770 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -528.383016 hartrees

XYZ Coordinates

C	0.000000000	-0.849509591	-1.001131335
C	-1.157991444	0.000000000	-1.229311240
C	0.000000000	0.849509591	-1.001131335
C	1.157991444	0.000000000	-1.229311240
N	1.845413600	0.000000000	0.120993466
C	1.350683048	1.236540318	0.756328116
N	0.000000000	1.542820264	0.157998616
C	-1.350683048	1.236540318	0.756328116
N	-1.845413600	0.000000000	0.120993466
C	-1.350683048	-1.236540318	0.756328116
N	0.000000000	-1.542820264	0.157998616
C	1.350683048	-1.236540318	0.756328116
H	1.302951483	-1.154125853	1.844190654
H	2.014127136	-2.060057180	0.490882630
H	2.014127136	2.060057180	0.490882630
H	1.302951483	1.154125853	1.844190654
H	-1.302951483	1.154125853	1.844190654
H	-2.014127136	2.060057180	0.490882630
H	-2.014127136	-2.060057180	0.490882630
H	-1.302951483	-1.154125853	1.844190654

$(CNC)_4(H_2)_3[B_2(NHC)]$



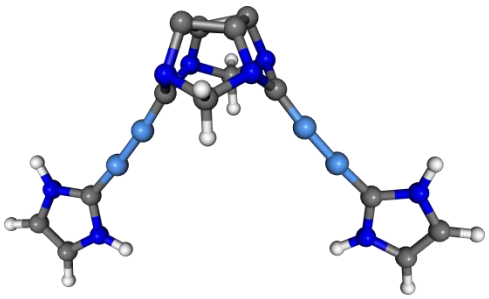
Total enthalpy, Htot (Utot + pV): -802.973873 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -803.031799 hartrees

XYZ Coordinates

C	0.080267174	0.900539467	4.036664576
C	-0.954021901	0.024758675	3.472820836
C	-0.457506419	-1.319393834	3.657970856
C	0.666472130	-0.384777461	3.794396790
N	1.564592261	-0.418086598	2.778646935
C	1.139806561	-1.635784644	1.975632518
N	-0.295763298	-1.816553527	2.239261237
C	-1.182022303	-0.930571078	1.448248192
N	-1.351051106	0.358035778	2.225751421
C	-0.665951668	1.688072495	1.978301035
N	0.538048917	1.688392102	2.843298552

C	1.600730034	0.922730599	2.228770070
B	2.500951364	1.382027887	1.202409755
B	3.450662783	1.843524814	0.172071064
C	4.427216605	2.336024477	-0.820652102
N	5.660841135	2.900483469	-0.578845125
C	6.299911771	3.246138852	-1.763290427
C	5.474109156	2.900538449	-2.773169787
N	4.336350817	2.347184724	-2.195498432
H	7.274161022	3.701371793	-1.779977607
H	5.590700570	2.996414066	-3.837947403
H	3.537446749	1.996923120	-2.695067548
H	6.024620346	3.040201527	0.348337269
H	-0.796176511	-0.748696211	0.443747294
H	-2.166997082	-1.393456779	1.380874836
H	1.364909811	-1.496179618	0.919512170
H	1.686102614	-2.492607045	2.368475665
H	-1.355389895	2.465082081	2.309533753
H	-0.401154641	1.829354203	0.932804153

$(CNC)_4(H_2)_2[B_2(NHC)]_2$



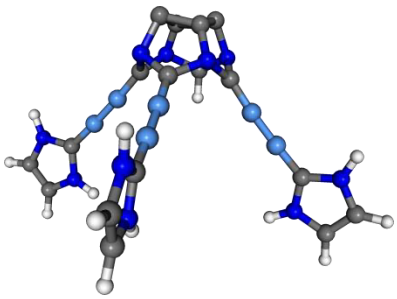
Total enthalpy, Htot (Utot + pV): -1077.602555 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1077.674809 hartrees

XYZ Coordinates

C	1.010222422	0.563870406	3.594109898
C	-0.441092348	0.730598602	3.381834053
C	-1.010222422	-0.563870406	3.594109898
C	0.441092348	-0.730598602	3.381834053
N	0.764039821	-1.320040784	2.204904974
C	-0.581727134	-1.818731621	1.677641884
N	-1.578685315	-0.884652967	2.246560527
C	-1.625203810	0.368325949	1.519686985
N	-0.764039821	1.320040784	2.204904974
C	0.581727134	1.818731621	1.677641884
N	1.578685315	0.884652967	2.246560527
C	1.625203810	-0.368325949	1.519686985
B	-2.420242422	0.639733370	0.351091468

B	-3.327361648	0.964760597	-0.769060228
B	2.420242422	-0.639733370	0.351091468
B	3.327361648	-0.964760597	-0.769060228
C	4.306765259	-1.294183266	-1.821627810
C	-4.306765259	1.294183266	-1.821627810
N	5.581169717	-1.794851426	-1.652334063
C	6.218886964	-1.978350717	-2.873153590
C	5.351595784	-1.596973392	-3.834015490
N	4.189298453	-1.182390824	-3.191204257
H	7.221670162	-2.360238559	-2.946734406
H	5.453864274	-1.583597865	-4.904486517
H	3.362694140	-0.832525943	-3.643358769
H	5.975018323	-1.988100505	-0.747419067
N	-5.581169717	1.794851426	-1.652334063
C	-6.218886964	1.978350717	-2.873153590
C	-5.351595784	1.596973392	-3.834015490
N	-4.189298453	1.182390824	-3.191204257
H	-3.362694140	0.832525943	-3.643358769
H	-5.453864274	1.583597865	-4.904486517
H	-7.221670162	2.360238559	-2.946734406
H	-5.975018323	1.988100505	-0.747419067
H	-0.737086377	-2.817827483	2.083247030
H	-0.600588331	-1.820582752	0.591673759
H	0.737086377	2.817827483	2.083247030
H	0.600588331	1.820582752	0.591673759

$(CNC)_4(H_2)[B_2(NHC)]_3$



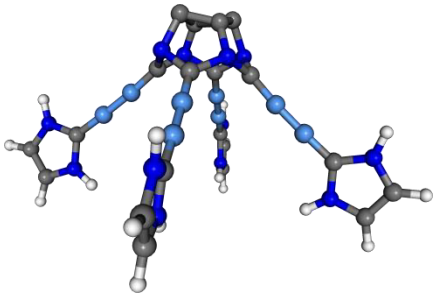
Total enthalpy, Htot (Utot + pV): -1352.215459 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1352.303361 hartrees

XYZ Coordinates

C	0.353445407	1.007206483	4.180992600
C	-0.781702909	0.099775113	3.952450359
C	-0.248416020	-1.224261967	4.094903127
C	0.870531724	-0.307458020	3.894801663
N	1.472253259	-0.441107874	2.686044290
C	0.855889246	-1.646177139	2.084644511

N	-0.440888812	-1.814538152	2.740695358
C	-1.432716398	-0.953457919	2.084862232
N	-1.453949068	0.315419927	2.796333477
C	-0.874176340	1.636473398	2.293544680
N	0.496299827	1.690663296	2.855695136
C	1.433703546	0.901600580	2.088680465
B	1.443479908	-2.509626442	1.110524698
B	2.101706560	-3.476955255	0.196206225
B	-2.273696085	-1.289386752	0.968989525
B	-3.237582725	-1.599243989	-0.109932576
B	2.194370775	1.376001196	0.966778307
B	3.016992850	1.944342636	-0.125403110
C	3.871182694	2.526740661	-1.173180106
C	-4.224701559	-1.944318703	-1.146609802
C	2.766093538	-4.473721857	-0.656641079
N	5.137546864	3.061285846	-1.035001849
C	5.625303893	3.527442063	-2.250368803
C	4.674057306	3.290008768	-3.177006498
N	3.609521856	2.679192779	-2.521076773
H	6.596131392	3.980623942	-2.344852905
H	4.657876996	3.496969801	-4.232282892
H	2.741133604	2.402172073	-2.943860745
H	5.621647840	3.096149887	-0.154620871
N	-5.475658682	-2.504371623	-0.975135898
C	-6.122471358	-2.681034239	-2.192672484
C	-5.287908574	-2.233791381	-3.153735424
N	-4.134377084	-1.787810942	-2.516087898
H	-3.330429578	-1.389041090	-2.968030505
H	-5.408501582	-2.192459752	-4.221654646
H	-7.108437663	-3.104752013	-2.264254649
H	-5.842885714	-2.751607695	-0.072531938
N	3.566989362	-5.528650875	-0.263629950
C	4.011403258	-6.260067059	-1.359735146
C	3.498854283	-5.675394976	-2.461699777
N	2.743265319	-4.587915784	-2.033114544
H	3.778533970	-5.726243051	0.699017206
H	4.646774281	-7.121630392	-1.256158758
H	3.602123984	-5.930108388	-3.501444791
H	2.230166515	-3.959973357	-2.626221171
H	-1.477289837	2.436081963	2.722409553
H	-0.869117252	1.676667028	1.208177887

$(CNC)_4$ $[B_2(NHC)]_4$



Total enthalpy, Htot (Utot + pV): -1626.828724 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1626.932575 hartrees

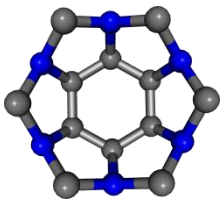
XYZ Coordinates

C	0.575684311	1.002300682	3.952537760
C	-0.736999606	0.423479364	3.736836024
C	-0.575684311	-1.002300682	3.952537760
C	0.736999606	-0.423479364	3.736836024
N	1.299181133	-0.746161830	2.544943348
C	0.383729368	-1.733845787	1.943972294
N	-0.905680431	-1.576423676	2.619766705
C	-1.694453932	-0.542894089	1.946403092
N	-1.299181133	0.746161830	2.544943348
C	-0.383729368	1.733845787	1.943972294
N	0.905680431	1.576423676	2.619766705
C	1.694453932	0.542894089	1.946403092
B	0.705806704	-2.698886137	0.936980930
B	1.061958741	-3.768596654	-0.027267206
B	-2.697865921	-0.750688186	0.946982276
B	-3.806552544	-0.979696996	-0.012229450
B	-0.705806704	2.698886137	0.936980930
B	-1.061958741	3.768596654	-0.027267206
B	2.697865921	0.750688186	0.946982276
B	3.806552544	0.979696996	-0.012229450
C	4.933881200	1.205939243	-0.927882635
C	-1.413338778	4.859466472	-0.947375838
C	-4.933881200	-1.205939243	-0.927882635
C	1.413338778	-4.859466472	-0.947375838
N	-1.925935661	6.105976701	-0.638857420
C	-2.121863306	6.869642381	-1.784187772
C	-1.739184420	6.115654267	-2.834985767
N	-1.311058646	4.893072548	-2.326063565
H	-2.115644565	6.400307238	0.303288441
H	-2.513600517	7.870665738	-1.747615332
H	-1.734179538	6.334679327	-3.887952275
H	-0.952344430	4.125316239	-2.865433434
N	6.268808866	1.380950524	-0.612939742

C	7.037173155	1.571663032	-1.755990655
C	6.199233473	1.519325583	-2.811531707
N	4.921075301	1.296827105	-2.307714874
H	8.100735078	1.726443037	-1.714489929
H	6.393794936	1.619082655	-3.864584189
H	4.081158025	1.213547621	-2.852379671
H	6.613376227	1.368144979	0.331187189
N	-6.268808866	-1.380950524	-0.612939742
C	-7.037173155	-1.571663032	-1.755990655
C	-6.199233473	-1.519325583	-2.811531707
N	-4.921075301	-1.296827105	-2.307714874
H	-4.081158025	-1.213547621	-2.852379671
H	-6.393794936	-1.619082655	-3.864584189
H	-8.100735078	-1.726443037	-1.714489929
H	-6.613376227	-1.368144979	0.331187189
N	1.925935661	-6.105976701	-0.638857420
C	2.121863306	-6.869642381	-1.784187772
C	1.739184420	-6.115654267	-2.834985767
N	1.311058646	-4.893072548	-2.326063565
H	2.115644565	-6.400307238	0.303288441
H	2.513600517	-7.870665738	-1.747615332
H	1.734179538	-6.334679327	-3.887952275
H	0.952344430	-4.125316239	-2.865433434

4.2 $(CNC)_6[B_2(NHC)]_m$

$(CNC)_6$



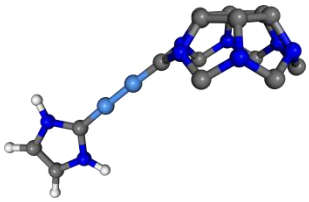
Total enthalpy, Htot (Utot + pV): -785.188189 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -785.229811 hartrees

XYZ Coordinates

C	1.386472444	0.000000000	1.042210465
C	0.693236222	-1.200720358	1.042210465
C	-0.693236222	-1.200720358	1.042210465
C	-1.386472444	0.000000000	1.042210465
C	-0.693236222	1.200720358	1.042210465
C	0.693236222	1.200720358	1.042210465
N	2.202289479	0.000000000	-0.133744373
C	2.065593210	1.192570796	-0.886141103

N	1.101144740	1.907238636	-0.133744373
C	0.000000000	2.385141591	-0.886141103
N	-1.101144740	1.907238636	-0.133744373
C	-2.065593210	1.192570796	-0.886141103
N	-2.202289479	0.000000000	-0.133744373
C	-2.065593210	-1.192570796	-0.886141103
N	-1.101144740	-1.907238636	-0.133744373
C	0.000000000	-2.385141591	-0.886141103
N	1.101144740	-1.907238636	-0.133744373
C	2.065593210	-1.192570796	-0.886141103

$(CNC)_6[B_2(NHC)]_1$



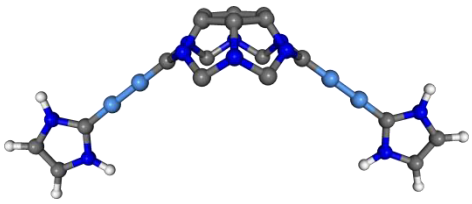
Total enthalpy, Htot (Utot + pV): -1061.101496 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1061.164378 hartrees

XYZ Coordinates

C	0.395933295	-3.645960018	-0.691676614
C	-0.373952643	-2.719195958	-1.386409076
C	-1.141214412	-1.795111290	-0.695496645
C	-1.141214412	-1.795111290	0.695496645
C	-0.373952643	-2.719195958	1.386409076
C	0.395933295	-3.645960018	0.691676614
N	1.747513118	-3.432966098	-1.102034999
C	2.630768223	-3.317474658	0.000000000
N	1.747513118	-3.432966098	1.102034999
C	1.857465054	-2.384783489	2.054310156
N	0.522869131	-1.961121301	2.194507002
C	0.309906280	-0.547957576	2.031843836
N	-0.741320695	-0.501563006	1.143324412
C	-0.843535061	0.417313813	0.000000000
N	-0.741320695	-0.501563006	-1.143324412
C	0.309906280	-0.547957576	-2.031843836
N	0.522869131	-1.961121301	-2.194507002
C	1.857465054	-2.384783489	-2.054310156
B	-0.938786004	1.834240630	0.000000000
B	-0.998102550	3.318131433	0.000000000
C	-1.008705489	4.798012869	0.000000000
N	0.077173741	5.637065597	0.000000000
C	-0.320123603	6.968759133	0.000000000

C	-1.669384166	6.978241579	0.000000000
N	-2.084003723	5.650202267	0.000000000
H	-3.040275875	5.337720416	0.000000000
H	-2.366558305	7.796934249	0.000000000
H	0.387770597	7.778260304	0.000000000
H	1.029206061	5.309831055	0.000000000

$(CNC)_6[B_2(NHC)]_2$



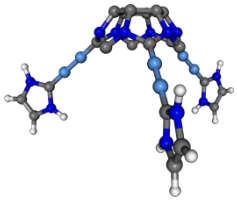
Total enthalpy, Htot (Utot + pV): -1337.006247 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1337.084173 hartrees

XYZ Coordinates

C	-0.693992349	-1.205530040	2.563762437
C	-1.386310836	0.000000000	2.564227957
C	-0.693992349	1.205530040	2.563762437
C	0.693992349	1.205530040	2.563762437
C	1.386310836	0.000000000	2.564227957
C	0.693992349	-1.205530040	2.563762437
N	-1.143330280	-1.936327191	1.427076258
C	0.000000000	-2.691125063	0.906645583
N	1.143330280	-1.936327191	1.427076258
C	2.018713602	-1.205416019	0.643542894
N	2.185149119	0.000000000	1.388049688
C	2.018713602	1.205416019	0.643542894
N	1.143330280	1.936327191	1.427076258
C	0.000000000	2.691125063	0.906645583
N	-1.143330280	1.936327191	1.427076258
C	-2.018713602	1.205416019	0.643542894
N	-2.185149119	0.000000000	1.388049688
C	-2.018713602	-1.205416019	0.643542894
B	0.000000000	-3.833192188	0.057699747
B	0.000000000	-5.023074430	-0.829435684
B	0.000000000	3.833192188	0.057699747
B	0.000000000	5.023074430	-0.829435684
C	0.000000000	6.190618820	-1.732994552
C	0.000000000	-6.190618820	-1.732994552
N	0.000000000	6.186194575	-3.108582146
C	0.000000000	7.481237091	-3.614046671
C	0.000000000	8.318688828	-2.556516933

N	0.000000000	7.527946640	-1.411722172
H	0.000000000	7.869084687	-0.465770217
H	0.000000000	9.393070519	-2.511926168
H	0.000000000	7.685000036	-4.669900036
H	0.000000000	5.342436156	-3.656500079
N	0.000000000	-6.186194575	-3.108582146
C	0.000000000	-7.481237091	-3.614046671
C	0.000000000	-8.318688828	-2.556516933
N	0.000000000	-7.527946640	-1.411722172
H	0.000000000	-5.342436156	-3.656500079
H	0.000000000	-7.685000036	-4.669900036
H	0.000000000	-9.393070519	-2.511926168
H	0.000000000	-7.869084687	-0.465770217

$(CNC)_6[B_2(NHC)]_3$



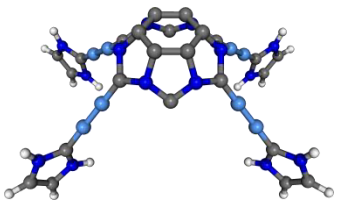
Total enthalpy, Htot (Utot + pV): -1612.897082 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1612.994500 hartrees

XYZ Coordinates

C	0.006036331	-3.030169848	-1.392347520
C	-1.208097617	-3.029421337	-0.691159071
C	-1.208097617	-3.029421337	0.691159071
C	0.006036331	-3.030169848	1.392347520
C	1.202933105	-3.030348414	0.700927270
C	1.202933105	-3.030348414	-0.700927270
N	0.029230677	-1.894395313	-2.240094760
C	1.178108209	-1.121799980	-2.038514336
N	1.925898834	-1.894695900	-1.144209678
C	2.640834245	-1.341282163	0.000000000
N	1.925898834	-1.894695900	1.144209678
C	1.178108209	-1.121799980	2.038514336
N	0.029230677	-1.894395313	2.240094760
C	-1.318719890	-1.339840981	2.286561137
N	-1.952616518	-1.892904123	1.095252842
C	-2.352245567	-1.119863165	0.000000000
N	-1.952616518	-1.892904123	-1.095252842
C	-1.318719890	-1.339840981	-2.286561137
B	3.734657364	-0.422412063	0.000000000
B	4.881613186	0.515710463	0.000000000

B	-1.865546420	-0.421169452	3.234155188
B	-2.439620031	0.516505298	4.227571862
B	-1.865546420	-0.421169452	-3.234155188
B	-2.439620031	0.516505298	-4.227571862
C	-3.003817670	1.467108842	-5.201894973
C	-3.003817670	1.467108842	5.201894973
C	6.006868705	1.467103331	0.000000000
N	-2.966503734	2.844560993	-5.154319053
C	-3.607489960	3.403586000	-6.254047433
C	-4.058294072	2.382311714	-7.011223301
N	-3.689542011	1.204760940	-6.368784034
H	-3.683297514	4.466868746	-6.395555480
H	-4.602169104	2.384589850	-7.938872096
H	-3.888232329	0.273985936	-6.692358807
H	-2.524130552	3.354625541	-4.409248275
N	-2.966503734	2.844560993	5.154319053
C	-3.607489960	3.403586000	6.254047433
C	-4.058294072	2.382311714	7.011223301
N	-3.689542011	1.204760940	6.368784034
H	-3.888232329	0.273985936	6.692358807
H	-4.602169104	2.384589850	7.938872096
H	-3.683297514	4.466868746	6.395555480
H	-2.524130552	3.354625541	4.409248275
N	5.945933356	2.844512873	0.000000000
N	7.360513157	1.205857061	0.000000000
C	8.100371190	2.383959819	0.000000000
C	7.218431720	3.404557371	0.000000000
H	7.740760073	0.275313691	0.000000000
H	9.175699478	2.387158359	0.000000000
H	7.378138845	4.467981532	0.000000000
H	5.078986592	3.353837566	0.000000000

$(CNC)_6[B_2(NHC)]_4$



Total enthalpy, Htot (Utot + pV): -1888.778307 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1888.887897 hartrees

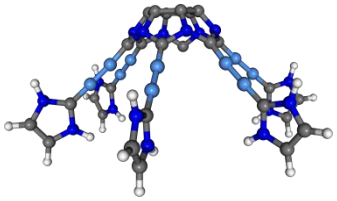
XYZ Coordinates

C	0.000000000	1.402647175	3.373100483
C	1.198150352	0.696512438	3.370757292

C	1.198150352	-0.696512438	3.370757292
C	0.000000000	-1.402647175	3.373100483
C	-1.198150352	-0.696512438	3.370757292
C	-1.198150352	0.696512438	3.370757292
N	0.000000000	2.336753894	2.320776972
C	-1.291885319	2.285751935	1.676981445
N	-1.928768637	1.094755165	2.226477819
C	-2.316318554	0.000000000	1.448514274
N	-1.928768637	-1.094755165	2.226477819
C	-1.291885319	-2.285751935	1.676981445
N	0.000000000	-2.336753894	2.320776972
C	1.291885319	-2.285751935	1.676981445
N	1.928768637	-1.094755165	2.226477819
C	2.316318554	0.000000000	1.448514274
N	1.928768637	1.094755165	2.226477819
C	1.291885319	2.285751935	1.676981445
B	-1.828401924	3.170447975	0.680451000
B	-2.443879990	4.095444144	-0.295132538
B	-1.828401924	-3.170447975	0.680451000
B	-2.443879990	-4.095444144	-0.295132538
B	1.828401924	-3.170447975	0.680451000
B	2.443879990	-4.095444144	-0.295132538
B	1.828401924	3.170447975	0.680451000
B	2.443879990	4.095444144	-0.295132538
C	3.087907803	4.997149157	-1.262932106
C	3.087907803	-4.997149157	-1.262932106
C	-3.087907803	-4.997149157	-1.262932106
C	-3.087907803	4.997149157	-1.262932106
N	3.079368367	4.915142448	-2.642190672
C	3.817560644	5.945521471	-3.214173731
C	4.297399428	6.698040212	-2.202274066
N	3.850716715	6.122579415	-1.017918396
H	3.931876347	6.050208030	-4.278455462
H	4.908704048	7.582781703	-2.217322761
H	4.045462478	6.459100890	-0.091119203
H	2.626344263	4.168367465	-3.139275393
N	3.079368367	-4.915142448	-2.642190672
C	3.817560644	-5.945521471	-3.214173731
C	4.297399428	-6.698040212	-2.202274066
N	3.850716715	-6.122579415	-1.017918396
H	4.045462478	-6.459100890	-0.091119203
H	4.908704048	-7.582781703	-2.217322761
H	3.931876347	-6.050208030	-4.278455462
H	2.626344263	-4.168367465	-3.139275393
N	-3.079368367	-4.915142448	-2.642190672
C	-3.817560644	-5.945521471	-3.214173731
C	-4.297399428	-6.698040212	-2.202274066
N	-3.850716715	-6.122579415	-1.017918396

H	-2.626344263	-4.168367465	-3.139275393
H	-3.931876347	-6.050208030	-4.278455462
H	-4.908704048	-7.582781703	-2.217322761
H	-4.045462478	-6.459100890	-0.091119203
N	-3.079368367	4.915142448	-2.642190672
C	-3.817560644	5.945521471	-3.214173731
C	-4.297399428	6.698040212	-2.202274066
N	-3.850716715	6.122579415	-1.017918396
H	-2.626344263	4.168367465	-3.139275393
H	-3.931876347	6.050208030	-4.278455462
H	-4.908704048	7.582781703	-2.217322761
H	-4.045462478	6.459100890	-0.091119203

$(CNC)_6[B_2(NHC)]_5$



Total enthalpy, Htot (Utot + pV): -2164.656345 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2164.778710 hartrees

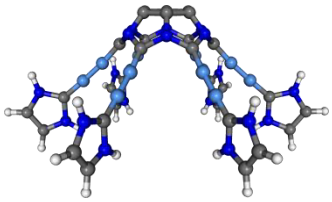
XYZ Coordinates

C	3.320725894	1.531501059	1.398435046
C	3.026616996	2.700637950	0.694702966
C	3.026616996	2.700637950	-0.694702966
C	3.320725894	1.531501059	-1.398435046
C	3.606464768	0.367952476	-0.697489230
C	3.606464768	0.367952476	0.697489230
N	2.294716894	1.263489836	2.317417460
C	1.986855922	-0.148196930	2.250136347
N	2.765986931	-0.655614112	1.147172422
C	2.283890563	-1.387417397	0.000000000
N	2.765986931	-0.655614112	-1.147172422
C	1.986855922	-0.148196930	-2.250136347
N	2.294716894	1.263489836	-2.317417460
C	1.359957767	2.360559153	-2.280400064
N	1.735494755	3.119895916	-1.094240860
C	0.883591061	3.304270911	0.000000000
N	1.735494755	3.119895916	1.094240860
C	1.359957767	2.360559153	2.280400064
B	1.085508413	-0.883883369	3.106065820
B	0.232943413	-1.619013727	4.060567377
B	1.471646658	-2.581925129	0.000000000

B	0.723058690	-3.853561775	0.000000000
B	1.085508413	-0.883883369	-3.106065820
B	0.232943413	-1.619013727	-4.060567377
B	0.273012548	2.651666064	-3.174653218
B	-0.794360152	3.067000516	-4.111044897
B	0.273012548	2.651666064	3.174653218
B	-0.794360152	3.067000516	4.111044897
C	-1.848228320	3.520441037	5.030428598
C	-1.848228320	3.520441037	-5.030428598
C	-0.599427718	-2.339824398	-5.033977054
C	0.004858081	-5.135174787	0.000000000
C	-0.599427718	-2.339824398	5.033977054
N	-3.204216018	3.252521306	4.979747228
C	-3.882902277	3.879220256	6.019793276
C	-2.963380657	4.543405617	6.750027644
N	-1.728020503	4.321750525	6.151373467
H	-4.947477010	3.793647911	6.147407442
H	-3.075086462	5.145369690	7.634526813
H	-0.847444025	4.689159113	6.466919448
H	-3.625114934	2.724412457	4.235666870
N	-3.204216018	3.252521306	-4.979747228
C	-3.882902277	3.879220256	-6.019793276
C	-2.963380657	4.543405617	-6.750027644
N	-1.728020503	4.321750525	-6.151373467
H	-0.847444025	4.689159113	-6.466919448
H	-3.075086462	5.145369690	-7.634526813
H	-4.947477010	3.793647911	-6.147407442
H	-3.625114934	2.724412457	-4.235666870
N	-1.959794266	-2.592596618	-4.985016867
C	-2.385715987	-3.299097665	-6.104623206
C	-1.299402734	-3.508352059	-6.877509089
N	-0.216583853	-2.928811695	-6.226908056
H	-2.541226495	-2.273420301	-4.230552224
H	-3.411597030	-3.588540646	-6.249186524
H	-1.201143518	-4.014261342	-7.821775701
H	0.731656901	-2.913934132	-6.559429374
N	-1.959794266	-2.592596618	4.985016867
C	-2.385715987	-3.299097665	6.104623206
C	-1.299402734	-3.508352059	6.877509089
N	-0.216583853	-2.928811695	6.226908056
H	-2.541226495	-2.273420301	4.230552224
H	-3.411597030	-3.588540646	6.249186524
H	-1.201143518	-4.014261342	7.821775701
H	0.731656901	-2.913934132	6.559429374
N	-1.361519619	-5.359773880	0.000000000
N	0.530338032	-6.416336833	0.000000000
C	-0.473840965	-7.377039669	0.000000000
C	-1.652549949	-6.719824211	0.000000000

H	1.519009952	-6.596990618	0.000000000
H	-0.262387522	-8.431862839	0.000000000
H	-2.660739519	-7.094853100	0.000000000
H	-2.031628728	-4.611511363	0.000000000

$(CNC)_6[B_2(NHC)]_6$



Total enthalpy, Htot (Utot + pV): -2440.534337 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2440.668974 hartrees

XYZ Coordinates

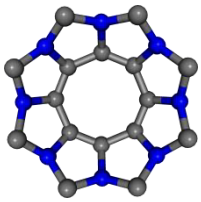
C	0.000000000	1.392301065	3.744602378
C	1.205768092	0.696150533	3.744602378
C	1.205768092	-0.696150533	3.744602378
C	0.000000000	-1.392301065	3.744602378
C	-1.205768092	-0.696150533	3.744602378
C	-1.205768092	0.696150533	3.744602378
N	0.000000000	2.291917838	2.673662630
C	-1.292279373	2.238293532	2.034033434
N	-1.984859071	1.145958919	2.673662630
C	-2.584558746	0.000000000	2.034033434
N	-1.984859071	-1.145958919	2.673662630
C	-1.292279373	-2.238293532	2.034033434
N	0.000000000	-2.291917838	2.673662630
C	1.292279373	-2.238293532	2.034033434
N	1.984859071	-1.145958919	2.673662630
C	2.584558746	0.000000000	2.034033434
N	1.984859071	1.145958919	2.673662630
C	1.292279373	2.238293532	2.034033434
B	-1.783614813	3.089311477	0.973337615
B	-2.333819489	4.042293930	-0.010300500
B	-3.567229626	0.000000000	0.973337615
B	-4.667638978	0.000000000	-0.010300500
B	-1.783614813	-3.089311477	0.973337615
B	-2.333819489	-4.042293930	-0.010300500
B	1.783614813	-3.089311477	0.973337615
B	2.333819489	-4.042293930	-0.010300500
B	3.567229626	0.000000000	0.973337615
B	4.667638978	0.000000000	-0.010300500
B	1.783614813	3.089311477	0.973337615

B	2.333819489	4.042293930	-0.010300500
C	2.898434985	5.020236656	-0.948686583
C	5.796869970	0.000000000	-0.948686583
C	2.898434985	-5.020236656	-0.948686583
C	-2.898434985	-5.020236656	-0.948686583
C	-5.796869970	0.000000000	-0.948686583
C	-2.898434985	5.020236656	-0.948686583
N	5.773880869	0.000000000	-2.334088018
C	7.060403927	0.000000000	-2.863261563
C	7.917309622	0.000000000	-1.820792446
N	7.152296779	0.000000000	-0.661293071
H	4.917908140	0.000000000	-2.859552269
H	7.249558244	0.000000000	-3.922138275
H	8.992689497	0.000000000	-1.801448460
H	7.506391252	0.000000000	0.278935924
N	2.886940435	5.000327511	-2.334088018
C	3.530201964	6.114489162	-2.863261563
C	3.958654811	6.856591262	-1.820792446
N	3.576148390	6.194070706	-0.661293071
H	3.624779122	6.278301606	-3.922138275
H	4.496344748	7.787897552	-1.801448460
H	3.753195626	6.500725515	0.278935924
H	2.458954070	4.259033383	-2.859552269
N	2.886940435	-5.000327511	-2.334088018
C	3.530201964	-6.114489162	-2.863261563
C	3.958654811	-6.856591262	-1.820792446
N	3.576148390	-6.194070706	-0.661293071
H	3.753195626	-6.500725515	0.278935924
H	4.496344748	-7.787897552	-1.801448460
H	3.624779122	-6.278301606	-3.922138275
H	2.458954070	-4.259033383	-2.859552269
N	-2.886940435	-5.000327511	-2.334088018
C	-3.530201964	-6.114489162	-2.863261563
C	-3.958654811	-6.856591262	-1.820792446
N	-3.576148390	-6.194070706	-0.661293071
H	-2.458954070	-4.259033383	-2.859552269
H	-3.624779122	-6.278301606	-3.922138275
H	-4.496344748	-7.787897552	-1.801448460
H	-3.753195626	-6.500725515	0.278935924
N	-2.886940435	5.000327511	-2.334088018
C	-3.530201964	6.114489162	-2.863261563
C	-3.958654811	6.856591262	-1.820792446
N	-3.576148390	6.194070706	-0.661293071
H	-2.458954070	4.259033383	-2.859552269
H	-3.624779122	6.278301606	-3.922138275
H	-4.496344748	7.787897552	-1.801448460
H	-3.753195626	6.500725515	0.278935924
N	-5.773880869	0.000000000	-2.334088018

N	-7.152296779	0.000000000	-0.661293071
C	-7.917309622	0.000000000	-1.820792446
C	-7.060403927	0.000000000	-2.863261563
H	-7.506391252	0.000000000	0.278935924
H	-8.992689497	0.000000000	-1.801448460
H	-7.249558244	0.000000000	-3.922138275
H	-4.917908140	0.000000000	-2.859552269

4.3 $(CNC)_8[B_2(NHC)]_m$

$(CNC)_8$

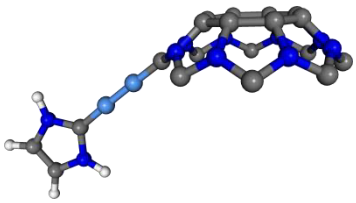


Total enthalpy, Htot (Utot + pV): -1047.052062 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1047.102007 hartrees

XYZ Coordinates

C	1.678478175	0.666166355	0.886198432
C	0.666176226	1.678374350	0.886062332
C	-0.666176226	1.678374350	0.886062332
C	-1.678478175	0.666166355	0.886198432
C	-1.678478175	-0.666166355	0.886198432
C	-0.666176226	-1.678374350	0.886062332
C	0.666176226	-1.678374350	0.886062332
C	1.678478175	-0.666166355	0.886198432
N	2.625663596	1.079562780	-0.111786411
C	3.252070082	0.000000000	-0.757016136
N	2.625663596	-1.079562780	-0.111786411
C	2.280087668	-2.279974944	-0.754186291
N	1.079560424	-2.625505859	-0.111886132
C	0.000000000	-3.251931901	-0.757115614
N	-1.079560424	-2.625505859	-0.111886132
C	-2.280087668	-2.279974944	-0.754186291
N	-2.625663596	-1.079562780	-0.111786411
C	-3.252070082	0.000000000	-0.757016136
N	-2.625663596	1.079562780	-0.111786411
C	-2.280087668	2.279974944	-0.754186291
N	-1.079560424	2.625505859	-0.111886132
C	0.000000000	3.251931901	-0.757115614
N	1.079560424	2.625505859	-0.111886132
C	2.280087668	2.279974944	-0.754186291

$(CNC)_8[B_2(NHC)]$

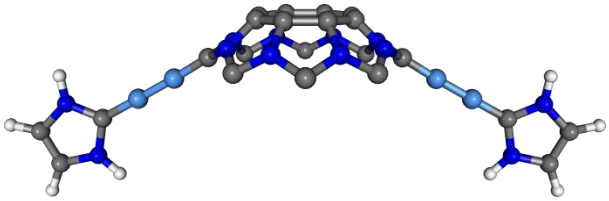


Total enthalpy, Htot (Utot + pV): -1322.972761 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1323.044364 hartrees

XYZ Coordinates

C	-1.624458426	-0.066247475	0.717071996
C	-1.624458426	-0.066247475	-0.717071996
C	-1.630137804	-1.017083821	-1.669170485
C	-1.536691310	-2.437132520	-1.644726619
C	-1.503209060	-3.391963520	-0.712825113
C	-1.503209060	-3.391963520	0.712825113
C	-1.536691310	-2.437132520	1.644726619
C	-1.630137804	-1.017083821	1.669170485
N	-0.725691360	0.935991049	1.128700923
C	-0.086889188	0.655281632	2.324623467
N	-0.675873817	-0.590953751	2.641613652
C	0.030742864	-1.645334322	3.241440466
N	-0.530898789	-2.771844036	2.616111105
C	0.174423517	-3.941784464	2.298500676
N	-0.450760998	-4.299150873	1.091869618
C	0.220791875	-4.868686127	0.000000000
N	-0.450760998	-4.299150873	-1.091869618
C	0.174423517	-3.941784464	-2.298500676
N	-0.530898789	-2.771844036	-2.616111105
C	0.030742864	-1.645334322	-3.241440466
N	-0.675873817	-0.590953751	-2.641613652
C	-0.086889188	0.655281632	-2.324623467
N	-0.725691360	0.935991049	-1.128700923
C	-0.281372809	1.718799546	0.000000000
B	0.491761980	2.921210590	0.000000000
B	1.314014247	4.156870233	0.000000000
C	2.166574965	5.368597071	0.000000000
N	1.782742010	6.684016052	0.000000000
C	2.889111155	7.526645098	0.000000000
C	3.983764027	6.737580044	0.000000000
N	3.535951009	5.422279863	0.000000000
H	2.794340635	8.597662336	0.000000000
H	5.029725309	6.986941095	0.000000000
H	4.123348310	4.604612801	0.000000000
H	0.822056492	6.983330763	0.000000000

$(CNC)_8[B_2(NHC)]_2$



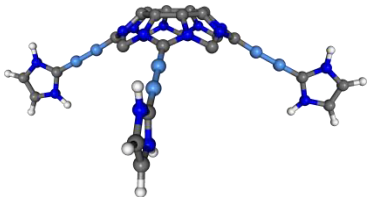
Total enthalpy, Htot (Utot + pV): -1598.880794 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1598.967375 hartrees

XYZ Coordinates

C	0.715374171	1.668292195	1.920560202
C	-0.715374171	1.668292195	1.920560202
C	-1.655394751	0.711688122	1.948857620
C	-1.655394751	-0.711688122	1.948857620
C	-0.715374171	-1.668292195	1.920560202
C	0.715374171	-1.668292195	1.920560202
C	1.655394751	-0.711688122	1.948857620
C	1.655394751	0.711688122	1.948857620
N	1.131677765	2.634330868	0.974008955
C	2.315638002	2.317554826	0.340970901
N	2.633286616	1.094366598	0.983501310
C	3.240451463	0.000000000	0.347421434
N	2.633286616	-1.094366598	0.983501310
C	2.315638002	-2.317554826	0.340970901
N	1.131677765	-2.634330868	0.974008955
C	0.000000000	-3.413484699	0.522304727
N	-1.131677765	-2.634330868	0.974008955
C	-2.315638002	-2.317554826	0.340970901
N	-2.633286616	-1.094366598	0.983501310
C	-3.240451463	0.000000000	0.347421434
N	-2.633286616	1.094366598	0.983501310
C	-2.315638002	2.317554826	0.340970901
N	-1.131677765	2.634330868	0.974008955
C	0.000000000	3.413484699	0.522304727
B	0.000000000	-4.632074006	-0.224991670
B	0.000000000	-5.925668903	-0.949138033
B	0.000000000	4.632074006	-0.224991670
B	0.000000000	5.925668903	-0.949138033
C	0.000000000	7.220260084	-1.662296411
C	0.000000000	-7.220260084	-1.662296411
N	0.000000000	8.486160462	-1.127812192
C	0.000000000	9.452292066	-2.128139981
C	0.000000000	8.797697401	-3.307877318
N	0.000000000	7.437981340	-3.018558965
H	0.000000000	10.505113162	-1.909335146

H	0.000000000	9.169664523	-4.316792259
H	0.000000000	6.694745169	-3.696788028
H	0.000000000	8.668643165	-0.138658680
N	0.000000000	-8.486160462	-1.127812192
N	0.000000000	-7.437981340	-3.018558965
C	0.000000000	-8.797697401	-3.307877318
C	0.000000000	-9.452292066	-2.128139981
H	0.000000000	-6.694745169	-3.696788028
H	0.000000000	-9.169664523	-4.316792259
H	0.000000000	-10.505113162	-1.909335146
H	0.000000000	-8.668643165	-0.138658680

$(CNC)_8[B_2(NHC)]_3$



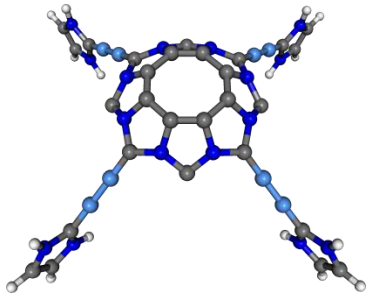
Total enthalpy, Htot (Utot + pV): -1874.786289 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1874.887395 hartrees

XYZ Coordinates

C	-0.181399018	-1.756721498	2.886647796
C	1.172692692	-1.322370311	2.822563073
C	1.803610622	-0.137118266	2.825636063
C	1.388591516	1.218575471	2.823078027
C	0.202320538	1.847437025	2.816531416
C	-1.163188588	1.450567126	2.881588366
C	-1.787184064	0.251277468	2.899591049
C	-1.369894830	-1.112324528	2.902037458
N	-0.323692419	-2.820074966	1.972178139
C	-1.577597078	-2.876054263	1.376297769
N	-2.207731794	-1.806933000	2.016451008
C	-3.273393017	-0.951513400	1.567628948
N	-2.869282535	0.355222482	2.012467330
C	-2.944876682	1.592032080	1.368645656
N	-1.875403497	2.249411372	1.964025355
C	-1.031299777	3.302332929	1.457589654
N	0.292777513	2.891423369	1.862287055
C	1.496341594	2.930485815	1.190633478
N	2.180261806	1.860751470	1.819992046
C	3.060482765	0.986064434	1.167072545
N	2.820146548	-0.229454964	1.823954725
C	2.852628587	-1.500747277	1.198777775

N	1.833011489	-2.140126832	1.871893086
C	0.965522698	-3.222185112	1.468585221
B	-4.441448904	-1.311838014	0.817821704
B	-5.675829197	-1.696236671	0.092267827
B	-1.398031851	4.465346529	0.706581560
B	-1.760372762	5.714229792	-0.003496925
B	1.314580733	-4.392000705	0.719605681
B	1.720129632	-5.627606933	0.009565581
C	-6.905753836	-2.083963023	-0.623889415
C	2.165942484	-6.851001313	-0.683797631
C	-2.090254648	6.974502268	-0.695624384
N	2.569270846	-8.046172207	-0.131986364
C	2.926347486	-8.959682850	-1.118105594
C	2.746376104	-8.347761004	-2.306843160
N	2.281075173	-7.065172597	-2.038682742
H	3.271411587	-9.951095656	-0.884757544
H	2.903971900	-8.703603419	-3.309299932
H	2.079717113	-6.358617503	-2.725513096
H	2.596167304	-8.213627142	0.859137200
N	-8.124084865	-2.446802864	-0.095731265
C	-9.038537859	-2.744094334	-1.100716006
C	-8.402282567	-2.570364336	-2.277433193
N	-7.104091029	-2.168299237	-1.983299818
H	-8.307600891	-2.482665654	0.892244131
H	-10.047416998	-3.048873170	-0.887180329
H	-8.750077582	-2.694293857	-3.287377023
H	-6.385984376	-1.964567720	-2.657270043
N	-2.406263671	8.194811626	-0.141855912
N	-2.151256766	7.208832455	-2.050651208
C	-2.487866345	8.531396142	-2.317172518
C	-2.646865919	9.146471778	-1.127133099
H	-1.950147662	6.504339410	-2.739618240
H	-2.582904501	8.908954029	-3.319536473
H	-2.907190659	10.163094018	-0.892314998
H	-2.444899832	8.355788463	0.849916518

$(CNC)_8[B_2(NHC)]_4$



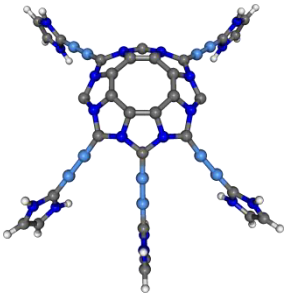
Total enthalpy, Htot (Utot + pV): -2150.682779 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2150.802353 hartrees

XYZ Coordinates

C	-0.191639089	-1.800756772	2.483981780
C	1.167806753	-1.384866169	2.484445930
C	1.800345052	-0.191889227	2.483162599
C	1.384181390	1.167426580	2.483845785
C	0.191639089	1.800756772	2.483981780
C	-1.167806753	1.384866169	2.484445930
C	-1.800345052	0.191889227	2.483162599
C	-1.384181390	-1.167426580	2.483845785
N	-0.307445079	-2.861232005	1.563540013
C	-1.547323451	-2.913969158	0.931254027
N	-2.197887622	-1.857314571	1.563448611
C	-3.252147812	-0.996467280	1.095462147
N	-2.860085631	0.307330981	1.562124735
C	-2.911736550	1.546402383	0.928752341
N	-1.857355827	2.198283409	1.563564021
C	-0.996457335	3.252911343	1.096454142
N	0.307445079	2.861232005	1.563540013
C	1.547323451	2.913969158	0.931254027
N	2.197887622	1.857314571	1.563448611
C	3.252147812	0.996467280	1.095462147
N	2.860085631	-0.307330981	1.562124735
C	2.911736550	-1.546402383	0.928752341
N	1.857355827	-2.198283409	1.563564021
C	0.996457335	-3.252911343	1.096454142
B	-4.402767430	-1.350235833	0.313494353
B	-5.614515787	-1.726305425	-0.450395097
B	-1.350457884	4.403513132	0.314962675
B	-1.727010049	5.615230159	-0.448581713
B	4.402767430	1.350235833	0.313494353
B	5.614515787	1.726305425	-0.450395097
B	1.350457884	-4.403513132	0.314962675
B	1.727010049	-5.615230159	-0.448581713
C	-6.816703206	-2.102523761	-1.214070592
C	2.104160900	-6.817157651	-1.211947007
C	6.816703206	2.102523761	-1.214070592
C	-2.104160900	6.817157651	-1.211947007
N	2.460726656	-8.061690526	-0.737164094
C	2.748798410	-8.935371937	-1.780421083
C	2.575329595	-8.250033698	-2.929269790
N	2.183943138	-6.961909445	-2.580891261
H	3.047653968	-9.954433094	-1.610766407
H	2.693317511	-8.557770601	-3.952988334
H	1.984805173	-6.214071843	-3.222640945
H	2.496609927	-8.285799372	0.242199643

N	8.055843525	2.477569996	-0.739154204
C	8.931928086	2.757081749	-1.782790171
C	8.253142681	2.561108330	-2.931922621
N	6.967183181	2.162706791	-2.583460726
H	6.224920089	1.944274760	-3.225499788
H	8.564429525	2.667246220	-3.955885589
H	9.947811677	3.066891352	-1.613252444
H	8.274171848	2.533187248	0.240705706
N	-8.055843525	-2.477569996	-0.739154204
C	-8.931928086	-2.757081749	-1.782790171
C	-8.253142681	-2.561108330	-2.931922621
N	-6.967183181	-2.162706791	-2.583460726
H	-8.274171848	-2.533187248	0.240705706
H	-9.947811677	-3.066891352	-1.613252444
H	-8.564429525	-2.667246220	-3.955885589
H	-6.224920089	-1.944274760	-3.225499788
N	-2.460726656	8.061690526	-0.737164094
N	-2.183943138	6.961909445	-2.580891261
C	-2.575329595	8.250033698	-2.929269790
C	-2.748798410	8.935371937	-1.780421083
H	-1.984805173	6.214071843	-3.222640945
H	-2.693317511	8.557770601	-3.952988334
H	-3.047653968	9.954433094	-1.610766407
H	-2.496609927	8.285799372	0.242199643

$(CNC)_8[B_2(NHC)]_5$



Total enthalpy, Htot (Utot + pV): -2426.558713 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2426.690538 hartrees

XYZ Coordinates

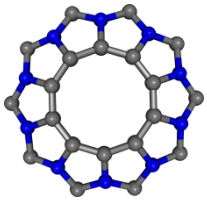
C	-0.201986023	-1.738545071	2.915085691
C	1.154087737	-1.327323940	2.869111747
C	1.806984515	-0.143907361	2.829065705
C	1.408598103	1.219218034	2.795756240
C	0.224694510	1.865976974	2.801029993
C	-1.137279935	1.465187724	2.844596539
C	-1.778286041	0.275329115	2.883890605

C	-1.391333591	-1.088403022	2.922872208
N	-0.323740616	-2.866446581	2.098992609
C	-1.653436664	-2.964130021	1.601769404
N	-2.282197114	-1.796176961	2.112981125
C	-3.284517489	-0.944212099	1.590049352
N	-2.860783848	0.376077633	1.990634379
C	-2.922357869	1.597042017	1.328883202
N	-1.840640832	2.255480439	1.917409029
C	-0.980998881	3.290030070	1.403578654
N	0.331058002	2.895749360	1.845517918
C	1.557468347	2.911973699	1.183511991
N	2.210723905	1.869356661	1.837356238
C	3.249329374	0.981045804	1.385719649
N	2.845183652	-0.304120817	1.893453083
C	2.871459986	-1.566665852	1.298427988
N	1.817260468	-2.179558320	1.967199237
C	0.931609171	-3.247148047	1.565113278
B	-2.218674285	-3.990142979	0.738002226
B	-2.777257513	-5.054792673	-0.110373683
B	-4.434208653	-1.323078840	0.804081160
B	-5.668616192	-1.712566324	0.089617448
B	-1.342752339	4.440611979	0.624347887
B	-1.721603033	5.685146490	-0.083534128
B	4.411240332	1.309747159	0.609035237
B	5.665805851	1.690918648	-0.079287971
B	1.253023335	-4.406828180	0.766898606
B	1.672493999	-5.620542155	0.032189379
C	-6.909668456	-2.102080998	-0.595340289
C	-3.317511732	-6.136809581	-0.946300036
C	2.139454866	-6.818229554	-0.680872188
C	6.925067225	2.101589842	-0.722523683
C	-2.098284846	6.939388830	-0.756876771
N	2.629816110	-7.997344179	-0.151160121
C	2.994301545	-8.888640149	-1.154202062
C	2.730691207	-8.288251843	-2.333475717
N	2.203251743	-7.034296798	-2.044792908
H	3.401699409	-9.860840563	-0.940228398
H	2.865598633	-8.638070217	-3.341573974
H	1.962848141	-6.327747900	-2.717857900
H	2.710302225	-8.159415813	0.837509865
N	8.112116939	2.461857752	-0.118221526
C	9.077496814	2.794588035	-1.062259977
C	8.510771634	2.645825608	-2.277284609
N	7.202336354	2.222875500	-2.068351141
H	6.522290417	2.040297512	-2.785792125
H	8.914903265	2.799710980	-3.261898907
H	10.069780143	3.103162410	-0.785284204
H	8.238048475	2.471609680	0.879030141

N	-8.167723707	-2.288503924	-0.053791744
C	-9.090108764	-2.645262085	-1.030975744
C	-8.425883946	-2.693045738	-2.204615469
N	-7.101183501	-2.366267426	-1.937757371
H	-8.366896210	-2.154665335	0.922271937
H	-10.125176886	-2.830805565	-0.805036623
H	-8.773115350	-2.927246595	-3.195182905
H	-6.358174336	-2.316573096	-2.612484133
N	-3.941394879	-7.306078650	-0.546122674
C	-4.301732783	-8.089267789	-1.634807399
C	-3.914920029	-7.426509407	-2.745983551
N	-3.322390177	-6.241102825	-2.327380245
H	-4.797517082	-9.037604013	-1.525054867
H	-4.010145380	-7.690466633	-3.784447515
H	-2.907561763	-5.543684434	-2.920039217
H	-4.095348982	-7.531391129	0.421135834
N	-2.433365213	8.149055934	-0.183780622
N	-2.199959643	7.188273192	-2.109820391
C	-2.583401397	8.502741787	-2.353268198
C	-2.728718415	9.101472509	-1.153301205
H	-2.014355113	6.491086415	-2.809843459
H	-2.716264055	8.887854748	-3.348524495
H	-3.012377219	10.108038905	-0.902473245
H	-2.455264784	8.297029142	0.810272905

4.4 $(CNC)_{10}[B_2(NHC)]_m$

$(CNC)_{10}$



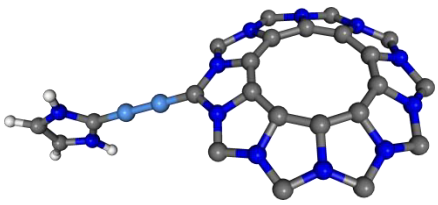
Total enthalpy, Htot (Utot + pV): -1308.981159 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1309.039495 hartrees

XYZ Coordinates

C	-2.207832011	-0.594286382	0.000000000
C	-1.785788307	-0.592843182	1.297701822
C	-0.682251140	-0.594913507	2.100266245
C	0.682462275	-0.596456443	2.100916468
C	1.785942125	-0.593551565	1.297985752
C	2.207297993	-0.592627417	0.000000000
C	0.682462275	-0.596456443	-2.100916468

C	-0.682251140	-0.594913507	-2.100266245
C	-1.785788307	-0.592843182	-1.297701822
N	-3.487261568	0.073852343	0.000000000
N	-2.820734639	0.074374018	-2.049938780
N	-1.077689646	0.071287088	-3.317648076
N	1.077935618	0.069835993	-3.318402251
N	3.486336617	0.076052276	0.000000000
N	2.820978367	0.073614806	2.050400209
N	1.077935618	0.069835993	3.318402251
N	-1.077689646	0.071287088	3.317648076
N	-2.820734639	0.074374018	2.049938780
N	2.820978367	0.073614806	-2.050400209
C	1.785942125	-0.593551565	-1.297985752
C	2.405843931	0.507726547	3.313070948
C	3.891766471	0.512036968	1.265317762
C	3.891766471	0.512036968	-1.265317762
C	2.405843931	0.507726547	-3.313070948
C	0.000154227	0.506512566	-4.094755530
C	-2.405672132	0.508969762	-3.312416571
C	-3.892222209	0.511140910	-1.264970972
C	-3.892222209	0.511140910	1.264970972
C	-2.405672132	0.508969762	3.312416571
C	0.000154227	0.506512566	4.094755530

$(CNC)_{10}[B_2(NHC)]$



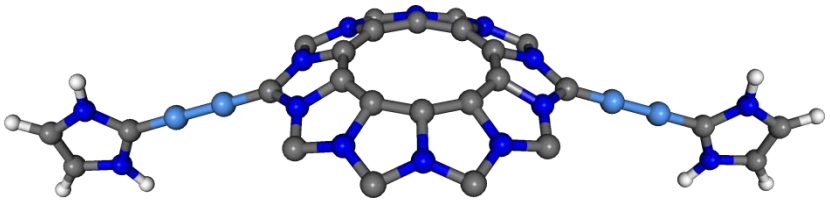
Total enthalpy, Htot (Utot + pV): -1584.895711 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1584.973637 hartrees

XYZ Coordinates

C	0.308451217	-3.883070498	0.679479616
C	0.440963839	-3.085114599	1.778687400
C	0.647686282	-1.805627793	2.192202817
C	0.852834156	-0.516036968	1.779577697
C	0.958432146	0.299657084	0.685999377
C	0.958432146	0.299657084	-0.685999377
C	0.647686282	-1.805627793	-2.192202817
C	0.440963839	-3.085114599	-1.778687400
C	0.308451217	-3.883070498	-0.679479616
N	-0.540019848	-4.977257997	1.078323397

N	-0.540019848	-4.977257997	-1.078323397
N	-0.318854574	-3.726302900	-2.822887087
N	0.032142645	-1.705808859	-3.488701996
N	0.575254271	1.600773127	-1.129765243
N	0.575254271	1.600773127	1.129765243
N	0.376190043	0.321121170	2.839901425
N	0.032142645	-1.705808859	3.488701996
N	-0.318854574	-3.726302900	2.822887087
N	0.376190043	0.321121170	-2.839901425
C	0.852834156	-0.516036968	-1.779577697
C	0.189659168	1.671434436	2.433632945
C	0.439574611	2.489322174	0.000000000
C	0.189659168	1.671434436	-2.433632945
C	-0.156176838	-0.374113652	-3.911596698
C	-0.594515020	-2.876966851	-3.905605708
C	-0.955924585	-4.898477047	-2.414668881
C	-1.095168750	-5.673946899	0.000000000
C	-0.955924585	-4.898477047	2.414668881
C	-0.594515020	-2.876966851	3.905605708
C	-0.156176838	-0.374113652	3.911596698
B	0.203258543	3.900172336	0.000000000
B	-0.048315027	5.361073814	0.000000000
C	-0.323436188	6.817501499	0.000000000
N	0.574137869	7.853182113	0.000000000
C	-0.078771587	9.080616100	0.000000000
C	-1.403101416	8.821123125	0.000000000
N	-1.545197953	7.438784909	0.000000000
H	0.454512543	10.014352861	0.000000000
H	-2.249223670	9.484782243	0.000000000
H	-2.420381242	6.941418139	0.000000000
H	1.572053397	7.723362511	0.000000000

$(CNC)_{10}[B_2(NHC)]_2$



Total enthalpy, Htot (Utot + pV): -1860.802363 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -1860.895323 hartrees

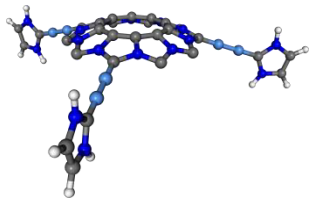
XYZ Coordinates

C	0.022269499	-3.919393044	0.741981241
C	0.201898147	-3.119602452	1.836147986

C	0.461192706	-1.844306272	2.251391981
C	0.715835999	-0.563353764	1.851138447
C	0.862072253	0.256125790	0.766639819
C	0.875223588	0.261651828	-0.599096336
C	0.502894500	-1.826849925	-2.107852740
C	0.236506738	-3.105581749	-1.707869410
C	0.036015206	-3.914203049	-0.623715041
N	-0.788615254	-5.009315714	1.177845187
N	-0.765218405	-5.001233709	-1.083937494
N	-0.472132599	-3.724609735	-2.786479613
N	-0.051273586	-1.707755423	-3.422861563
N	0.556854404	1.579072983	-1.044957126
N	0.535133452	1.569908743	1.217040404
N	0.284456125	0.284981329	2.920089416
N	-0.117221343	-1.735620623	3.556770925
N	-0.527829159	-3.746777195	2.895790192
N	0.337528081	0.307720843	-2.762485734
C	0.749603343	-0.549094293	-1.692696081
C	0.152870561	1.644333374	2.523802750
C	0.444054183	2.466133215	0.088685948
C	0.198218115	1.663817399	-2.357805979
C	-0.183795662	-0.376055978	-3.852214145
C	-0.686877861	-2.879827656	-3.866922441
C	-1.125735944	-4.925772531	-2.396853385
C	-1.215093438	-5.788660858	0.039628924
C	-1.175120116	-4.943949340	2.483858215
C	-0.761970389	-2.910809754	3.979071420
C	-0.256483849	-0.407433434	3.994730519
B	0.270586376	3.887512272	0.092692136
B	0.099848150	5.358725991	0.096811492
C	-0.081929808	6.827180890	0.100699458
N	0.881460684	7.804474069	0.140276949
C	0.310112552	9.072010401	0.129111403
C	-1.027459963	8.900335918	0.083724776
N	-1.260539818	7.530288010	0.065565589
H	0.902504332	9.969018541	0.154665679
H	-1.827147789	9.618895400	0.062490802
H	-2.165094625	7.090895334	0.030461931
H	1.867521264	7.608119828	0.173734554
B	-1.924116522	-7.032787401	0.028216837
B	-2.648143356	-8.324808696	0.017974775
C	-3.381293686	-9.610137348	0.008299307
N	-2.868099208	-10.883454236	0.024082234
C	-3.883545027	-11.833017335	0.007925278
C	-5.052201559	-11.159123388	-0.018150693
N	-4.740062851	-9.804826049	-0.018156287
H	-3.682099665	-12.889203216	0.016506941
H	-6.067004056	-11.514211402	-0.036547413

H	-5.405988322	-9.050747636	-0.037587246
H	-1.882287216	-11.082378542	0.047624906

$(CNC)_{10}[B_2(NHC)]_3$



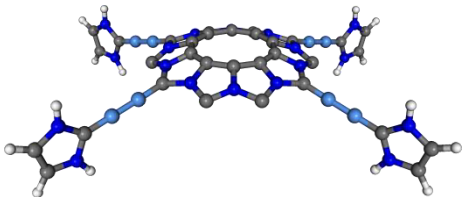
Total enthalpy, Htot (Utot + pV): -2136.703063 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2136.815335 hartrees

XYZ Coordinates

C	0.060759424	-3.916999209	0.849707130
C	0.131627583	-3.103542234	1.952718262
C	0.330916501	-1.817793713	2.362756413
C	0.583498845	-0.541609882	1.925755807
C	0.735637651	0.246902714	0.817908920
C	0.787697815	0.223373623	-0.548333687
C	0.515324844	-1.892681412	-2.043205127
C	0.262194976	-3.166816283	-1.629063076
C	0.086082109	-3.944089086	-0.518043066
N	-0.689236189	-5.054613292	1.248685450
N	-0.636230376	-5.106578498	-0.895354359
N	-0.360083503	-3.822251726	-2.734134527
N	0.017434469	-1.807872037	-3.376340564
N	0.470477688	1.529857750	-1.028240834
N	0.398136951	1.562882949	1.230482219
N	0.143894979	0.322761230	2.962805300
N	-0.228135904	-1.671919947	3.662455047
N	-0.557803031	-3.798925391	2.984141901
N	0.332474369	0.224885280	-2.728282133
C	0.715220911	-0.601586947	-1.631538811
C	0.001371566	1.659978776	2.541885203
C	0.316874014	2.432784754	0.085024187
C	0.159051645	1.584606446	-2.356876666
C	-0.127772676	-0.495948660	-3.831847479
C	-0.556000127	-3.026446491	-3.826681907
C	-0.855958554	-5.110365598	-2.319182571
C	-1.157000161	-5.815729695	0.159306032
C	-1.105308037	-4.994860417	2.594734025
C	-0.721600844	-2.941200617	4.128394085
C	-0.388215960	-0.371508747	4.068988327
B	0.121404521	3.852820713	0.051525276

B	-0.050496975	5.322269280	-0.000565519
C	-0.219988426	6.788080543	-0.067606268
N	0.753475791	7.759358154	-0.063641718
C	0.195107072	9.030170002	-0.144680108
C	-1.143457925	8.869893410	-0.199395392
N	-1.391640675	7.502868017	-0.151585671
H	0.796020507	9.921806849	-0.155904640
H	-1.934577178	9.595079840	-0.267337188
H	-2.299573331	7.070661795	-0.178481041
H	1.736618472	7.554013071	-0.012158945
B	-1.435876389	-6.141659549	-3.128981856
B	-2.017834449	-7.210116412	-3.971991325
C	-2.601339230	-8.272950514	-4.815425266
N	-1.957573551	-9.312833489	-5.444157838
C	-2.855773578	-10.106058543	-6.149471542
C	-4.080729515	-9.569553753	-5.970268909
N	-3.920987199	-8.453836669	-5.156736133
H	-2.543123041	-10.969892327	-6.708228490
H	-5.041890703	-9.875464040	-6.342978975
H	-4.658234826	-7.843522927	-4.847384255
H	-0.964278963	-9.459905433	-5.389382028
H	-0.668822277	-4.555257799	9.205829891
N	-1.664069281	-4.411975519	9.188892260
H	-2.189786895	-4.982273770	11.210193617
B	-1.257882279	-3.270613112	5.417282238
C	-2.531604979	-4.629329285	10.253691107
B	-1.797846688	-3.616384882	6.751281124
C	-2.341960729	-3.962947080	8.079660525
C	-3.771335478	-4.317631281	9.822116528
N	-3.651023831	-3.911967899	8.497960390
H	-4.718681841	-4.346422625	10.330063605
H	-4.407553866	-3.618665777	7.903577789

$(CNC)_{10}[B_2(NHC)]_4$



Total enthalpy, Htot (Utot + pV): -2412.594409 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2412.718547 hartrees

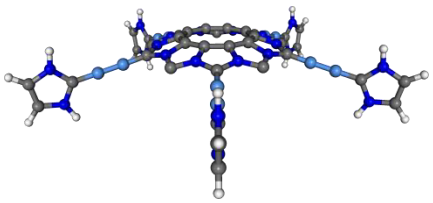
XYZ Coordinates

C	-0.686651967	-2.122546001	-1.211673611

C	0.686651967	-2.122546001	-1.211673611
C	1.781783055	-1.304873187	-1.212094823
C	2.193975732	0.000000000	-1.233143431
C	1.781783055	1.304873187	-1.212094823
C	0.686651967	2.122546001	-1.211673611
C	-1.781783055	1.304873187	-1.212094823
C	-2.193975732	0.000000000	-1.233143431
C	-1.781783055	-1.304873187	-1.212094823
N	-1.068442417	-3.388806441	-0.714755923
N	-2.882178030	-2.049283050	-0.709627092
N	-3.521852861	0.000000000	-0.721030019
N	-2.882178030	2.049283050	-0.709627092
N	1.068442417	3.388806441	-0.714755923
N	2.882178030	2.049283050	-0.709627092
N	3.521852861	0.000000000	-0.721030019
N	2.882178030	-2.049283050	-0.709627092
N	1.068442417	-3.388806441	-0.714755923
N	-1.068442417	3.388806441	-0.714755923
C	-0.686651967	2.122546001	-1.211673611
C	3.973539051	1.286197547	-0.366492939
C	2.478734591	3.409350906	-0.457781550
C	0.000000000	4.200003647	-0.364673049
C	-2.478734591	3.409350906	-0.457781550
C	-3.973539051	1.286197547	-0.366492939
C	-3.973539051	-1.286197547	-0.366492939
C	-2.478734591	-3.409350906	-0.457781550
C	0.000000000	-4.200003647	-0.364673049
C	2.478734591	-3.409350906	-0.457781550
C	3.973539051	-1.286197547	-0.366492939
B	3.301595769	4.515491763	-0.048680667
B	4.163574642	5.653557690	0.335944300
C	5.032635643	6.783074700	0.716520248
N	5.701157335	7.662315781	-0.106579525
C	6.423380461	8.593151368	0.631617060
C	6.216378565	8.310386165	1.934469499
N	5.369701579	7.208811473	1.982501531
H	7.012785637	9.363010092	0.166685013
H	6.590932213	8.786609471	2.822902785
H	5.036455966	6.760231572	2.818492391
H	5.660127017	7.613509553	-1.109899981
B	-3.301595769	-4.515491763	-0.048680667
B	-4.163574642	-5.653557690	0.335944300
C	-5.032635643	-6.783074700	0.716520248
N	-5.701157335	-7.662315781	-0.106579525
C	-6.423380461	-8.593151368	0.631617060
C	-6.216378565	-8.310386165	1.934469499
N	-5.369701579	-7.208811473	1.982501531
H	-7.012785637	-9.363010092	0.166685013

H	-6.590932213	-8.786609471	2.822902785
H	-5.036455966	-6.760231572	2.818492391
H	-5.660127017	-7.613509553	-1.109899981
H	5.660127017	-7.613509553	-1.109899981
N	5.701157335	-7.662315781	-0.106579525
H	7.012785637	-9.363010092	0.166685013
B	3.301595769	-4.515491763	-0.048680667
C	6.423380461	-8.593151368	0.631617060
B	4.163574642	-5.653557690	0.335944300
C	5.032635643	-6.783074700	0.716520248
C	6.216378565	-8.310386165	1.934469499
N	5.369701579	-7.208811473	1.982501531
H	6.590932213	-8.786609471	2.822902785
H	5.036455966	-6.760231572	2.818492391
B	-3.301595769	4.515491763	-0.048680667
B	-4.163574642	5.653557690	0.335944300
C	-5.032635643	6.783074700	0.716520248
N	-5.369701579	7.208811473	1.982501531
N	-5.701157335	7.662315781	-0.106579525
H	-5.660127017	7.613509553	-1.109899981
H	-5.036455966	6.760231572	2.818492391
C	-6.216378565	8.310386165	1.934469499
C	-6.423380461	8.593151368	0.631617060
H	-7.012785637	9.363010092	0.166685013
H	-6.590932213	8.786609471	2.822902785

$(CNC)_{10}[B_2(NHC)]_5$



Total enthalpy, Htot (Utot + pV): -2688.485591 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2688.629517 hartrees

XYZ Coordinates

C	1.311674040	-1.237093948	1.790582841
C	2.109215519	-1.235273978	0.692301388
C	2.109215519	-1.235273978	-0.692301388
C	1.311674040	-1.237093948	-1.790582841
C	-0.005102196	-1.238948495	-2.218942119
C	-1.296014553	-1.238163221	-1.799278645
C	-2.109497967	-1.235828734	0.678699073
C	-1.296014553	-1.238163221	1.799278645

C	-0.005102196	-1.238948495	2.218942119
N	2.113873490	-0.768065442	2.852633670
N	-0.029931063	-0.770588287	3.549863796
N	-2.057838994	-0.768654926	2.890612435
N	-3.381941774	-0.764237046	1.066035446
N	-2.057838994	-0.768654926	-2.890612435
N	-0.029931063	-0.770588287	-3.549863796
N	2.113873490	-0.768065442	-2.852633670
N	3.366738617	-0.765386334	-1.127229888
N	3.366738617	-0.765386334	1.127229888
N	-3.381941774	-0.764237046	-1.066035446
C	-2.109497967	-1.235828734	-0.678699073
C	1.305758321	-0.527555135	-4.013357830
C	-1.298447722	-0.439890002	-4.004516969
C	-3.410230660	-0.522388516	-2.479829289
C	-4.205902451	-0.432862895	0.000000000
C	-3.410230660	-0.522388516	2.479829289
C	-1.298447722	-0.439890002	4.004516969
C	1.305758321	-0.527555135	4.013357830
C	3.407355850	-0.437210509	2.474831542
C	4.220064773	-0.521297242	0.000000000
C	3.407355850	-0.437210509	-2.474831542
B	1.733646260	-0.137394532	-5.331693954
B	2.175473866	0.223244536	-6.695305203
C	2.618603590	0.575840434	-8.055420876
N	2.976643690	-0.268908711	-9.085524286
C	3.338652012	0.446168622	-10.221780338
C	3.213962073	1.755538286	-9.921316195
N	2.775265335	1.831582933	-8.604194827
H	3.648994947	-0.037272351	-11.130912698
H	3.395199481	2.631275551	-10.518609558
H	2.589213670	2.677841517	-8.094454486
H	2.968772427	-1.270429903	-8.999374578
B	1.733646260	-0.137394532	5.331693954
B	2.175473866	0.223244536	6.695305203
C	2.618603590	0.575840434	8.055420876
N	2.976643690	-0.268908711	9.085524286
C	3.338652012	0.446168622	10.221780338
C	3.213962073	1.755538286	9.921316195
N	2.775265335	1.831582933	8.604194827
H	3.648994947	-0.037272351	11.130912698
H	3.395199481	2.631275551	10.518609558
H	2.589213670	2.677841517	8.094454486
H	2.968772427	-1.270429903	8.999374578
H	9.493835069	-1.196429808	0.000000000
N	9.561261499	-0.193418452	0.000000000
H	11.710236077	0.074059319	0.000000000
B	5.604155642	-0.123932435	0.000000000

C	10.741703032	0.541551822	0.000000000
B	7.032331437	0.257240011	0.000000000
C	8.456865780	0.633230093	0.000000000
C	10.395441245	1.845536503	0.000000000
N	9.006148037	1.898490671	0.000000000
H	11.004774548	2.731669626	0.000000000
H	8.449733349	2.735746163	0.000000000
B	-4.530983917	-0.126206088	-3.292517877
B	-5.690664874	0.246400640	-4.129734758
C	-6.849536354	0.613447516	-4.961974462
N	-7.298693330	1.875212427	-5.291803518
H	-6.847331030	2.715895713	-4.975342764
H	-7.690254293	-1.222583358	-5.548795989
N	-7.746012593	-0.220080454	-5.597928676
C	-8.428754699	1.813550825	-6.099457181
H	-8.926128123	2.695849038	-6.461047527
C	-8.707684333	0.507391708	-6.290462845
H	-9.494476088	0.033854585	-6.850230084
B	-4.530983917	-0.126206088	3.292517877
B	-5.690664874	0.246400640	4.129734758
C	-6.849536354	0.613447516	4.961974462
N	-7.746012593	-0.220080454	5.597928676
H	-7.690254293	-1.222583358	5.548795989
H	-6.847331030	2.715895713	4.975342764
N	-7.298693330	1.875212427	5.291803518
C	-8.707684333	0.507391708	6.290462845
H	-9.494476088	0.033854585	6.850230084
C	-8.428754699	1.813550825	6.099457181
H	-8.926128123	2.695849038	6.461047527

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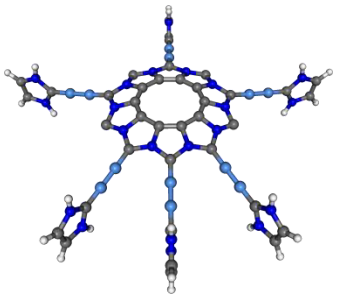


Total enthalpy, Htot (Utot + pV): -2964.362064 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -2964.518395 hartrees

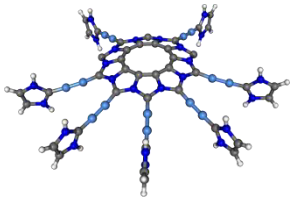
XYZ Coordinates

C	1.258990421	-1.228656149	-0.682945289
C	1.258990421	-1.228656149	0.682945289

C	1.242146234	-0.399636527	1.792278353
C	1.209631990	0.894645752	2.208567949
C	1.172649141	2.209815078	1.785168290
C	1.149657450	3.010398012	0.690342830
C	1.172649141	2.209815078	-1.785168290
C	1.209631990	0.894645752	-2.208567949
C	1.242146234	-0.399636527	-1.792278353
N	0.889851205	-2.506448059	-1.106358792
N	0.827741872	-1.172690679	-2.897182822
N	0.771559602	0.857147513	-3.547630831
N	0.700950614	3.001769715	-2.853261562
N	0.659603827	4.258485349	1.128414638
N	0.700950614	3.001769715	2.853261562
N	0.771559602	0.857147513	3.547630831
N	0.827741872	-1.172690679	2.897182822
N	0.889851205	-2.506448059	1.106358792
N	0.659603827	4.258485349	-1.128414638
C	1.149657450	3.010398012	-0.690342830
C	0.504067392	2.187348412	4.017099603
C	0.343564960	4.291050787	2.480234480
C	0.397948893	5.106924243	0.000000000
C	0.343564960	4.291050787	-2.480234480
C	0.504067392	2.187348412	-4.017099603
C	0.498865232	-0.422373333	-4.015351076
C	0.636478872	-2.539588172	-2.492908191
C	0.657175118	-3.356434969	0.000000000
C	0.636478872	-2.539588172	2.492908191
C	0.498865232	-0.422373333	4.015351076
B	0.137749388	2.608643689	5.344840314
B	-0.179742777	3.057807842	6.716882089
C	-0.477970009	3.515807745	8.084637295
N	0.407882813	3.915461751	9.064306623
C	-0.258332760	4.281375792	10.228549278
C	-1.577433774	4.117359989	9.997621082
N	-1.708315219	3.651375944	8.694156577
H	0.261874298	4.621894564	11.106057684
H	-2.426286345	4.287871589	10.635530744
H	-2.573614807	3.429292075	8.233217736
H	1.403127568	3.937709896	8.924942807
B	0.261556851	-3.688312012	-3.290760363
B	-0.071171459	-4.869188980	-4.108551846
C	-0.382910459	-6.046201628	-4.932235670
N	0.491959000	-6.876177572	-5.608937717
C	-0.186779536	-7.877667883	-6.292947050
C	-1.503007375	-7.699622869	-6.053204098
N	-1.620037454	-6.590971663	-5.222677481
H	0.322182928	-8.619651361	-6.882303500
H	-2.357036291	-8.256972331	-6.394998173

H	-2.479696175	-6.194267703	-4.885806653
H	1.487061319	-6.735783096	-5.604058477
H	1.487061319	-6.735783096	5.604058477
N	0.491959000	-6.876177572	5.608937717
H	0.322182928	-8.619651361	6.882303500
B	0.261556851	-3.688312012	3.290760363
C	-0.186779536	-7.877667883	6.292947050
B	-0.071171459	-4.869188980	4.108551846
C	-0.382910459	-6.046201628	4.932235670
C	-1.503007375	-7.699622869	6.053204098
N	-1.620037454	-6.590971663	5.222677481
H	-2.357036291	-8.256972331	6.394998173
H	-2.479696175	-6.194267703	4.885806653
B	-0.025826551	6.483887865	0.000000000
B	-0.426724243	7.906524161	0.000000000
C	-0.820702167	9.325873393	0.000000000
N	-2.092927328	9.860375311	0.000000000
H	-2.923272752	9.293698303	0.000000000
H	0.995803744	10.385602195	0.000000000
N	-0.007822549	10.441038117	0.000000000
C	-2.056846794	11.250288237	0.000000000
H	-2.950258324	11.848983669	0.000000000
C	-0.757153402	11.612308929	0.000000000
H	-0.301756023	12.586584229	0.000000000
B	0.137749388	2.608643689	-5.344840314
B	-0.179742777	3.057807842	-6.716882089
C	-0.477970009	3.515807745	-8.084637295
N	0.407882813	3.915461751	-9.064306623
H	1.403127568	3.937709896	-8.924942807
H	-2.573614807	3.429292075	-8.233217736
N	-1.708315219	3.651375944	-8.694156577
C	-0.258332760	4.281375792	-10.228549278
H	0.261874298	4.621894564	-11.106057684
C	-1.577433774	4.117359989	-9.997621082
H	-2.426286345	4.287871589	-10.635530744
H	-2.531330311	-7.696977168	0.000000000
B	0.255708292	-4.757461909	0.000000000
N	-1.675387053	-8.223067791	0.000000000
B	-0.101998043	-6.184984764	0.000000000
C	-0.429702588	-7.617098629	0.000000000
C	-1.566938600	-9.608764364	0.000000000
H	-2.426357279	-10.255671692	0.000000000
N	0.438673907	-8.696408687	0.000000000
C	-0.249278216	-9.903030540	0.000000000
H	1.437346398	-8.585060589	0.000000000
H	0.253389466	-10.854105211	0.000000000

$(CNC)_{10}[B_2(NHC)]_7$



Total enthalpy, Htot (Utot + pV): -3240.235926 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -3240.406644 hartrees

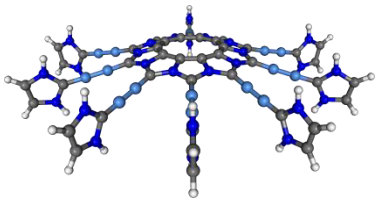
XYZ Coordinates

C	1.249280072	1.166576736	-0.810870262
C	1.268054896	1.181212215	0.558093478
C	0.464464231	1.180100150	1.681506817
C	-0.820814936	1.151388197	2.125230197
C	-2.138715011	1.116779708	1.728100982
C	-2.955237713	1.093709169	0.645667465
C	-2.197559582	1.105445127	-1.846284784
C	-0.897069946	1.122775047	-2.311880708
C	0.414157139	1.141023591	-1.916733599
N	2.528092183	0.826427735	-1.249388409
N	1.193742387	0.785096695	-3.016059476
N	-0.925860176	0.747744695	-3.656816853
N	-3.027577385	0.673554240	-2.901690530
N	-4.203406611	0.627760163	1.108223771
N	-2.916547067	0.663311069	2.813745816
N	-0.758304451	0.732902875	3.468542688
N	1.260186659	0.793720857	2.779863631
N	2.559310197	0.839170106	0.963553014
N	-4.241925512	0.634889864	-1.147682257
C	-2.975847379	1.090128479	-0.731040630
C	-2.080211970	0.466074101	3.962089182
C	-4.217345697	0.321463667	2.463563683
C	-5.074849591	0.385608446	-0.004848650
C	-4.314387234	0.342118631	-2.504296200
C	-2.242449264	0.484546865	-4.092233501
C	0.384714797	0.537389653	-4.150783057
C	2.543742511	0.583914724	-2.643943767
C	3.398560693	0.615549329	-0.154594425
C	2.623778923	0.621062861	2.355756945
C	0.532283208	0.477220029	3.916885115
B	-2.474331026	0.089313991	5.295651333
B	-2.888880057	-0.266852052	6.668404501
C	-3.309749686	-0.617979288	8.034956385
N	-3.656967650	0.227329847	9.069953528
C	-4.001175292	-0.486912770	10.212135247

C	-3.874433997	-1.796417096	9.913033414
N	-3.453488400	-1.873887183	8.590009854
H	-4.301816685	-0.003209114	11.124478212
H	-4.043335898	-2.671223846	10.515282316
H	-3.274621355	-2.720233081	8.077906022
H	-3.654500156	1.228409872	8.981008298
B	3.674727674	0.204044385	-3.475025559
B	4.846472787	-0.165950114	-4.283505238
C	6.034043630	-0.529186579	-5.068875305
N	6.903689280	0.302956684	-5.751671876
C	7.915930296	-0.417738831	-6.372333206
C	7.701724095	-1.721159369	-6.094276263
N	6.560013857	-1.787206188	-5.304589894
H	8.689750546	0.054501664	-6.951097748
H	8.254125607	-2.596823819	-6.386004704
H	6.149832814	-2.622646924	-4.925868927
H	6.791592622	1.300726118	-5.771572210
H	6.522776820	1.750879288	5.736888694
N	6.650516458	0.760688424	5.851422477
H	8.155293407	0.711555449	7.408566819
B	3.774069202	0.306849589	3.180220071
C	7.503879943	0.149434818	6.762914506
B	4.873258084	0.057476596	4.133826198
C	5.910711392	-0.174432391	5.147607599
C	7.331794365	-1.183084581	6.635660724
N	6.374836153	-1.379347768	5.646318227
H	7.804897139	-2.000655279	7.149844349
H	5.988606175	-2.264350339	5.368405853
B	-6.460549745	-0.007596543	0.023022740
B	-7.893655393	-0.364595768	0.068465209
C	-9.324117640	-0.706939658	0.132604183
N	-9.905426213	-1.958392893	0.173666937
H	-9.370041665	-2.809052035	0.166181255
H	-10.314453758	1.148368916	0.154348085
N	-10.407899886	0.147708487	0.169003819
C	-11.291523923	-1.869581951	0.235686686
H	-11.922479108	-2.739514174	0.275178212
C	-11.604707849	-0.557030094	0.232917364
H	-12.560456271	-0.065437365	0.269705798
B	-2.710754633	0.111814329	-5.413189025
B	-3.306332724	-0.213646086	-6.724598383
C	-3.980351473	-0.526454942	-7.993118142
N	-4.493333171	0.350108648	-8.933505259
H	-4.461466147	1.348192594	-8.819011152
H	-4.069632345	-2.626278627	-8.050919757
N	-4.273011998	-1.767468774	-8.530938410
C	-5.100580902	-0.330594104	-9.982627219
H	-5.564740191	0.179098287	-10.808395969

C	-4.964089431	-1.649337839	-9.731299092
H	-5.287300861	-2.505058524	-10.296812619
H	7.703156788	-2.508331955	0.437900597
B	4.806875242	0.241746825	-0.133777619
N	8.237292450	-1.657412089	0.414156675
B	6.231176238	-0.096848045	0.014302269
C	7.649412828	-0.417532536	0.227820914
C	9.609052367	-1.546256682	0.607516670
H	10.240945351	-2.401543845	0.770831206
N	8.726114749	0.449695377	0.306340626
C	9.913285193	-0.232230175	0.540136139
H	8.622989298	1.445583072	0.221381902
H	10.859517490	0.270821022	0.634241658
H	1.745381979	1.254131776	-9.241885890
B	0.779051595	0.149867767	-5.498166070
N	1.715919948	0.253994649	-9.334855450
B	1.120039914	-0.221088428	-6.879602727
C	1.423784758	-0.582179325	-8.270856948
C	1.930267024	-0.465022360	-10.504408246
H	2.168352798	0.010481598	-11.439791072
N	1.478794835	-1.841223209	-8.843811274
C	1.782502928	-1.772129542	-10.198456226
H	1.292404411	-2.679134107	-8.321106584
H	1.868499771	-2.648051311	-10.817519653

$(CNC)_{10}[B_2(NHC)]_8$



Total enthalpy, Htot (Utot + pV): -3516.111249 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -3516.298593 hartrees

XYZ Coordinates

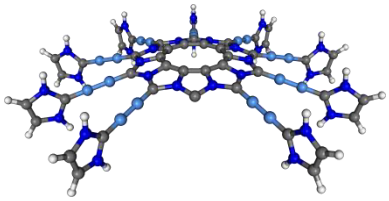
C	1.199895588	-1.032428509	-0.686588387
C	1.199895588	-1.032428509	0.686588387
C	1.190138544	-0.225759686	1.809206449
C	1.177875285	1.076469372	2.231522261
C	1.166136670	2.380217890	1.790443111
C	1.151420340	3.174132710	0.686712193
C	1.166136670	2.380217890	-1.790443111
C	1.177875285	1.076469372	-2.231522261
C	1.190138544	-0.225759686	-1.809206449

N	0.888283718	-2.324370057	-1.105247268
N	0.862309391	-1.028569436	-2.901158517
N	0.826597632	1.080762529	-3.581751211
N	0.762433131	3.198892888	-2.865001362
N	0.730120092	4.443279002	1.128576792
N	0.762433131	3.198892888	2.865001362
N	0.826597632	1.080762529	3.581751211
N	0.862309391	-1.028569436	2.901158517
N	0.888283718	-2.324370057	1.105247268
N	0.730120092	4.443279002	-1.128576792
C	1.151420340	3.174132710	-0.686712193
C	0.580830290	2.393101323	4.043977421
C	0.454355726	4.499661686	2.491295257
C	0.501873509	5.300436222	0.000000000
C	0.454355726	4.499661686	-2.491295257
C	0.580830290	2.393101323	-4.043977421
C	0.631397290	-0.239966983	-4.055189401
C	0.675446219	-2.373914071	-2.503736114
C	0.690546075	-3.184542368	0.000000000
C	0.675446219	-2.373914071	2.503736114
C	0.631397290	-0.239966983	4.055189401
B	0.229066266	2.835536152	5.379994215
B	-0.083763945	3.390268445	6.711785880
C	-0.388456891	4.003810503	8.011755885
N	0.492572583	4.465048006	8.975105714
C	-0.182574465	5.018204429	10.056999509
C	-1.502763835	4.901477594	9.802636850
N	-1.627169564	4.276062066	8.567221949
H	0.331224346	5.436376307	10.904484759
H	-2.355530029	5.199512122	10.386579518
H	-2.488377203	4.097026371	8.081495085
H	1.490008898	4.430774074	8.857878806
B	0.338364596	-3.530671038	-3.320928888
B	0.021894085	-4.703166727	-4.152398117
C	-0.283697153	-5.867782372	-4.993495872
N	0.596938839	-6.718265127	-5.641888589
C	-0.077413074	-7.704322917	-6.351084145
C	-1.397927410	-7.496616212	-6.161182171
N	-1.521933910	-6.385209530	-5.336471723
H	0.435512959	-8.458896047	-6.920973941
H	-2.249857759	-8.036432828	-6.535307885
H	-2.383160411	-5.972843133	-5.023912924
H	1.593837943	-6.603824234	-5.589903744
H	1.593837943	-6.603824234	5.589903744
N	0.596938839	-6.718265127	5.641888589
H	0.435512959	-8.458896047	6.920973941
B	0.338364596	-3.530671038	3.320928888
C	-0.077413074	-7.704322917	6.351084145

B	0.021894085	-4.703166727	4.152398117
C	-0.283697153	-5.867782372	4.993495872
C	-1.397927410	-7.496616212	6.161182171
N	-1.521933910	-6.385209530	5.336471723
H	-2.249857759	-8.036432828	6.535307885
H	-2.383160411	-5.972843133	5.023912924
B	0.133655033	6.694496520	0.000000000
B	-0.213858878	8.130969839	0.000000000
C	-0.554856924	9.562860897	0.000000000
N	-1.807008592	10.145544433	0.000000000
H	-2.657370512	9.609753780	0.000000000
H	1.299599648	10.555485929	0.000000000
N	0.298862595	10.648648206	0.000000000
C	-1.719052412	11.533005261	0.000000000
H	-2.589349995	12.164786032	0.000000000
C	-0.406826223	11.846632704	0.000000000
H	0.083919616	12.803588017	0.000000000
B	0.229066266	2.835536152	-5.379994215
B	-0.083763945	3.390268445	-6.711785880
C	-0.388456891	4.003810503	-8.011755885
N	0.492572583	4.465048006	-8.975105714
H	1.490008898	4.430774074	-8.857878806
H	-2.488377203	4.097026371	-8.081495085
N	-1.627169564	4.276062066	-8.567221949
C	-0.182574465	5.018204429	-10.056999509
H	0.331224346	5.436376307	-10.904484759
C	-1.502763835	4.901477594	-9.802636850
H	-2.355530029	5.199512122	-10.386579518
H	-2.344276789	-7.608987792	0.000000000
B	0.353925777	-4.603199537	0.000000000
N	-1.477263006	-8.116421600	0.000000000
B	0.046499130	-6.042243974	0.000000000
C	-0.245124727	-7.481446881	0.000000000
C	-1.337736704	-9.498975624	0.000000000
H	-2.182320145	-10.165237562	0.000000000
N	0.647347984	-8.542350519	0.000000000
C	-0.013817623	-9.764069921	0.000000000
H	1.643159990	-8.408414669	0.000000000
H	0.509433016	-10.704059413	0.000000000
H	1.473101761	-1.582423147	-9.127566666
B	0.271036366	-0.650928936	-5.405810649
N	0.475603841	-1.557597265	-9.246310398
B	-0.066146370	-0.984222570	-6.798731715
C	-0.389906069	-1.278134241	-8.201435886
C	-0.212420781	-1.770281672	-10.434214565
H	0.287978037	-1.999380558	-11.358567197
N	-1.634003846	-1.336246277	-8.807653669
C	-1.527633878	-1.633047036	-10.160879724

H	-2.486311395	-1.161458187	-8.305078756
H	-2.386484605	-1.720722668	-10.802708795
H	1.473101761	-1.582423147	9.127566666
B	0.271036366	-0.650928936	5.405810649
N	0.475603841	-1.557597265	9.246310398
B	-0.066146370	-0.984222570	6.798731715
C	-0.389906069	-1.278134241	8.201435886
C	-0.212420781	-1.770281672	10.434214565
H	0.287978037	-1.999380558	11.358567197
N	-1.634003846	-1.336246277	8.807653669
C	-1.527633878	-1.633047036	10.160879724
H	-2.486311395	-1.161458187	8.305078756
H	-2.386484605	-1.720722668	10.802708795

$(CNC)_{10}[B_2(NHC)]_9$



Total enthalpy, Htot (Utot + pV): -3791.987815 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -3792.186279 hartrees

XYZ Coordinates

C	1.188800547	-2.785223765	0.680634498
C	1.203030923	-1.991727602	1.799889531
C	1.222532320	-0.692815819	2.230515524
C	1.239418907	0.615059038	1.802308672
C	1.249457786	1.417809949	0.689057206
C	1.249457786	1.417809949	-0.689057206
C	1.222532320	-0.692815819	-2.230515524
C	1.203030923	-1.991727602	-1.799889531
C	1.188800547	-2.785223765	-0.680634498
N	0.837789914	-4.089813875	1.068360039
N	0.837789914	-4.089813875	-1.068360039
N	0.885282845	-2.794449434	-2.894794969
N	0.918022030	-0.689089971	-3.590356972
N	0.960509815	2.714925147	-1.106781374
N	0.960509815	2.714925147	1.106781374
N	0.945390039	1.418342096	2.901229984
N	0.918022030	-0.689089971	3.590356972
N	0.885282845	-2.794449434	2.894794969
N	0.945390039	1.418342096	-2.901229984
C	1.239418907	0.615059038	-1.802308672

C	0.764846619	2.766225161	2.506926747
C	0.771512321	3.575416069	0.000000000
C	0.764846619	2.766225161	-2.506926747
C	0.738247902	0.633683656	-4.063259322
C	0.704163304	-2.009184329	-4.059704548
C	0.664819956	-4.132789692	-2.495829303
C	0.579656677	-4.948743333	0.000000000
C	0.664819956	-4.132789692	2.495829303
C	0.704163304	-2.009184329	4.059704548
C	0.738247902	0.633683656	4.063259322
B	0.439725418	3.922767372	3.331736225
B	0.099156056	5.088179593	4.161376269
C	-0.247587176	6.249613493	4.989671183
N	0.599149932	7.138935309	5.632672583
C	-0.112890321	8.110538979	6.324723990
C	-1.424401837	7.854115601	6.131784341
N	-1.505502176	6.727147244	5.323346451
H	0.370225179	8.889964352	6.887159369
H	-2.296350206	8.368909241	6.494971419
H	-2.349643512	6.287199213	5.002253007
H	1.599646080	7.061373385	5.583614996
H	1.447588495	-3.720441220	9.085813949
N	0.445438243	-3.723882918	9.157353617
H	0.167846762	-4.401313699	11.196290944
B	0.359000077	-2.454922240	5.403778127
C	-0.293522280	-4.083782076	10.277852152
B	-0.003751776	-2.906533349	6.756588070
C	-0.376696201	-3.353947873	8.104527173
C	-1.597575312	-3.947651747	9.954582633
N	-1.646573058	-3.505611125	8.638502000
H	-2.483191564	-4.124796165	10.538955134
H	-2.478234698	-3.309690959	8.110109064
B	0.439725418	3.922767372	-3.331736225
B	0.099156056	5.088179593	-4.161376269
C	-0.247587176	6.249613493	-4.989671183
N	-1.505502176	6.727147244	-5.323346451
H	-2.349643512	6.287199213	-5.002253007
H	1.599646080	7.061373385	-5.583614996
N	0.599149932	7.138935309	-5.632672583
C	-1.424401837	7.854115601	-6.131784341
H	-2.296350206	8.368909241	-6.494971419
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H	0.370225179	8.889964352	-6.887159369
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C	-0.376696201	-3.353947873	-8.104527173
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H	1.447588495	-3.720441220	-9.085813949

H	-2.478234698	-3.309690959	-8.110109064
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H	0.167846762	-4.401313699	-11.196290944
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B	0.314427521	-5.257092746	3.343191279
N	-1.718098422	-7.950836186	5.396940929
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H	-2.571168376	-9.548555394	-6.585492693
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B	0.401020478	1.079494038	5.408411542
N	0.492499259	2.287319809	9.181708953
B	0.041218634	1.523490270	6.764228940
C	-0.330766673	1.962156359	8.115135285
C	-0.244909364	2.659401994	10.299061768
H	0.217751130	2.947003665	11.226649281
N	-1.600158330	2.154122919	8.637445830
C	-1.549204075	2.577196912	9.959642121
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H	-2.434215140	2.779707980	10.536634645
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N	-1.600158330	2.154122919	-8.637445830
B	0.041218634	1.523490270	-6.764228940
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H	-2.434215140	2.779707980	-10.536634645
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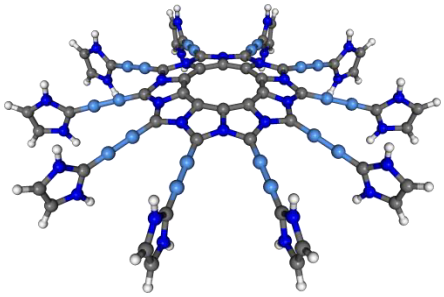
$(CNC)_{10}[B_2(NHC)]_{10}$



Total enthalpy, Htot (Utot + pV): -4067.869060 hartrees
Total Gibbs free energy, Gtot (Htot - T*S): -4068.072520 hartrees

XYZ Coordinates

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C	1.307451217	1.799555591	-1.329565576
C	0.000001983	2.224371599	-1.329565576
C	-1.307454426	1.799553259	-1.329565576
C	-2.115502491	0.687370512	-1.329565576
C	-2.115502491	-0.687370512	-1.329565576
C	0.000001983	-2.224371599	-1.329565576
C	1.307451217	-1.799555591	-1.329565576
C	2.115503716	-0.687366740	-1.329565576
N	3.407237816	1.107087402	-1.016126812
N	3.407237816	-1.107087402	-1.016126812
N	2.105797077	-2.898366906	-1.016126812
N	-0.000008299	-3.582584549	-1.016126812
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N	-2.105783649	-2.898376662	-1.016126812
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C	-4.265121053	0.000000000	-0.813106317
C	-3.450541545	-2.506965177	-0.813502381
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C	3.450555415	-2.506975254	-0.813106317
C	4.265103908	0.000000000	-0.813502381
C	3.450555415	2.506975254	-0.813106317
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N	-7.800569419	5.667445426	-0.479210117
C	-8.742461855	6.351770337	0.279092763
C	-8.441749788	6.133290232	1.577069887
N	-7.318055369	5.316878448	1.604056616
H	-9.534796277	6.927434991	-0.166053156
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H	-6.851181578	4.977674784	2.426358954
H	-7.758304236	5.636737973	-1.482435298
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C	8.434909311	-6.128320334	1.597149351
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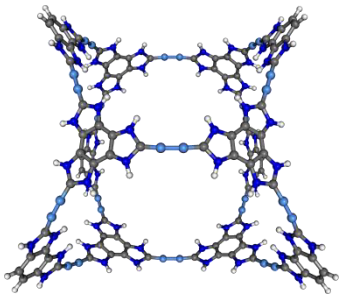
5 Other diboryne nanostructures

Compound 26



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N	33.862140000	41.017800000	45.747710000
N	30.973450000	39.583730000	46.551310000
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H	28.448340000	39.296420000	44.680040000
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H	26.147420000	36.549740000	49.989390000
H	24.233060000	35.014260000	51.786590000
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B	44.525580000	24.071100000	38.292000000
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C	46.069800000	23.424770000	34.951470000
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H	42.504310000	39.381140000	47.394660000
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H	45.199650000	40.560060000	41.994690000
H	39.872180000	40.614590000	46.639090000
H	39.426780000	42.403010000	43.014280000
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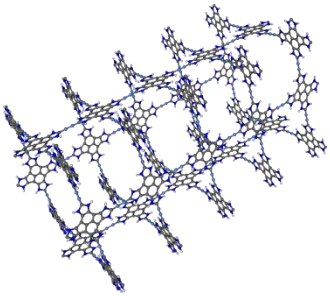
Compound 27 (5 rings)



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B	46.347480000	52.479660000	5.832220000
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B	59.999690000	45.916080000	13.848730000
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C	46.278720000	58.801380000	4.354230000
C	46.273920000	57.613620000	5.107390000
C	57.610320000	45.908580000	5.113400000
C	58.799580000	45.907980000	4.350930000
C	59.288460000	45.910140000	2.998740000
C	46.281420000	59.292660000	8.668330000
C	46.278540000	58.801440000	7.309580000
C	46.273680000	57.613680000	6.556610000
C	46.270440000	55.424460000	5.831940000
C	46.367400000	40.943820000	5.831930000
C	47.100420000	43.142760000	5.830740000
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C	58.799510000	45.907860000	7.312880000
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C	57.610080000	45.908640000	6.550650000
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C	48.801960000	46.711440000	5.831330000
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N	47.498820000	50.160660000	5.833310000
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H	48.391500000	41.426340000	5.831780000
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H	50.473010000	43.928400000	5.831520000
H	57.966590000	45.911520000	10.370160000
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B	46.286990000	53.952960000	20.373130000
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C	58.799580000	45.907980000	18.892930000
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B	59.999700000	74.084100000	55.981940000
B	46.288680000	60.000000000	55.984430000
B	46.288320000	60.000000000	57.473050000
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N	61.092720000	74.087460000	53.615660000
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N	63.722880000	74.088540000	50.544190000
N	74.692860000	69.872700000	49.458440000
N	69.878160000	75.121020000	49.458760000
N	69.861780000	72.941640000	49.458380000
N	77.308800000	72.940140000	49.458290000
N	72.500640000	69.839340000	49.459310000
N	77.312820000	75.066060000	49.458380000
N	72.549720000	78.200220000	49.457860000
N	74.685420000	78.166560000	49.457730000
H	64.072560000	74.090340000	47.420940000
H	73.737720000	64.075200000	47.423270000
H	62.032920000	74.088420000	44.919750000
H	73.715580000	62.034960000	44.923180000
H	73.715760000	62.034960000	53.992700000
H	62.032860000	74.088480000	53.996160000
H	73.737840000	64.075380000	51.492840000
H	64.073100000	74.090280000	51.494830000

H	75.642060000	78.501180000	49.457480000
H	69.526440000	76.071600000	49.457520000
H	69.489360000	71.999040000	49.457700000
H	71.562180000	69.458160000	49.457570000
H	71.607960000	78.573660000	49.457780000
H	77.660220000	76.017960000	49.457770000
H	75.645480000	69.527520000	49.457450000
H	77.657940000	71.989080000	49.457760000
B	73.712460000	66.047040000	63.999130000
B	66.060000000	74.073360000	63.998880000
B	67.540080000	74.051640000	64.000350000
B	73.651920000	67.520340000	64.000220000
C	73.721460000	60.000000000	63.310170000
C	62.389140000	74.091420000	63.281400000
C	73.725540000	62.386320000	63.275390000
C	61.199880000	74.092020000	62.518930000
C	73.720740000	61.198620000	62.522230000
C	60.710940000	74.089860000	61.166740000
C	73.717200000	60.707340000	61.163500000
C	73.710540000	60.000000000	58.973710000
C	73.711140000	60.000000000	69.026090000
C	73.718040000	60.707340000	66.836330000
C	60.711000000	74.090340000	66.832850000
C	73.720920000	61.198560000	65.477580000
C	61.199940000	74.092140000	65.480880000
C	73.725780000	62.386320000	64.724610000
C	62.389380000	74.091360000	64.718650000
C	73.721400000	60.000000000	64.689450000
C	74.778180000	75.469140000	63.998620000
C	73.580400000	74.696220000	63.998640000
C	74.291400000	76.839060000	63.998500000
C	73.729020000	64.575540000	63.999940000
C	69.015120000	74.039220000	64.000350000
C	71.197500000	73.288560000	63.999330000
C	73.575060000	73.320900000	63.999490000
C	71.208660000	74.751000000	63.999540000
C	75.959100000	73.285140000	63.999570000
C	75.960600000	74.723580000	63.999420000
C	78.177360000	74.003580000	64.000150000
C	73.632060000	79.056180000	63.999930000
C	72.387540000	75.491820000	63.999130000
C	72.899040000	76.857240000	63.998740000
C	72.372720000	72.533760000	63.999640000
C	74.770380000	72.545220000	63.999680000
C	73.610700000	69.006360000	64.000640000
C	72.878280000	71.172660000	63.999320000
C	74.274540000	71.186280000	63.998960000
C	64.576740000	74.085180000	63.999600000

N	63.722520000	74.088840000	62.913620000
N	73.729320000	63.713580000	62.912300000
N	61.092660000	74.086860000	59.841980000
N	73.711200000	61.092780000	59.840860000
N	73.711980000	61.092720000	68.159090000
N	61.092720000	74.087460000	68.157660000
N	73.729440000	63.713640000	65.087840000
N	63.722880000	74.088540000	65.086190000
N	74.692860000	69.872700000	64.000440000
N	69.878160000	75.121020000	64.000760000
N	69.861780000	72.941640000	64.000380000
N	77.308800000	72.940140000	64.000290000
N	72.500640000	69.839340000	64.001310000
N	77.312820000	75.066060000	64.000380000
N	72.549720000	78.200220000	63.999860000
N	74.685420000	78.166560000	63.999730000
H	64.072560000	74.090340000	61.962940000
H	73.737720000	64.075200000	61.965270000
H	62.032920000	74.088420000	59.461750000
H	73.715580000	62.034960000	59.465180000
H	73.715760000	62.034960000	68.534700000
H	62.032860000	74.088480000	68.538160000
H	73.737840000	64.075380000	66.034840000
H	64.073100000	74.090280000	66.036830000
H	75.642060000	78.501180000	63.999480000
H	69.526440000	76.071600000	63.999520000
H	69.489360000	71.999040000	63.999700000
H	71.562180000	69.458160000	63.999570000
H	71.607960000	78.573660000	63.999780000
H	77.660220000	76.017960000	63.999770000
H	75.645480000	69.527520000	63.999450000
H	77.657940000	71.989080000	63.999760000

6 CIF Files

Compound $(3BB)_n$

```
#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_chemical_name_common                  'XCrySDen XSF file'
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_cell_length_a                    22.23043
_cell_length_b                    26.07444
_cell_length_c                    26.04923
_cell_angle_alpha                  88.19770
_cell_angle_beta                  90.01337
_cell_angle_gamma                   90.00793
_space_group_name_H-M_alt           'P 1'
_space_group_IT_number              1

loop_
_space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
  B1       1.0    0.868102     0.999839    -0.000063    Biso  1.000000 B
  B2       1.0    0.934168     0.999891     0.000020    Biso  1.000000 B
  B3       1.0    0.434144     0.999979     0.999299    Biso  1.000000 B
  B4       1.0    0.368109     0.000099     0.999336    Biso  1.000000 B
  C1       1.0    0.500634     0.999920     0.999353    Biso  1.000000 C
  C2       1.0    0.598081     0.972670     0.999508    Biso  1.000000 C
  C3       1.0    0.598111     0.027119     0.999361    Biso  1.000000 C
  C4       1.0    0.651152     0.056027     0.999225    Biso  1.000000 C
  C5       1.0    0.704144     0.027087     0.999458    Biso  1.000000 C
  C6       1.0    0.704121     0.972632     0.999760    Biso  1.000000 C
  C7       1.0    0.651088     0.943727     0.999792    Biso  1.000000 C
  C8       1.0    0.801607     0.999840     0.999807    Biso  1.000000 C
  C9       1.0    0.516689     0.094351     0.999391    Biso  1.000000 C
  C10      1.0    0.785573     0.094295     0.999359    Biso  1.000000 C
  C11      1.0    0.785501     0.905397     0.000111    Biso  1.000000 C
  C12      1.0    0.516603     0.905476     0.999185    Biso  1.000000 C
  C13      1.0    0.301596     0.000134     0.999451    Biso  1.000000 C
  C14      1.0    0.204214     0.002154     0.026715    Biso  1.000000 C
  C15      1.0    0.204074     0.998073     0.972513    Biso  1.000000 C
  C16      1.0    0.285708     0.007484     0.093511    Biso  1.000000 C
  C17      1.0    0.285226     0.992701     0.905453    Biso  1.000000 C
  C18      1.0    0.150989     0.995937     0.943816    Biso  1.000000 C
  C19      1.0    0.098047     0.998034     0.972694    Biso  1.000000 C
  C20      1.0    0.098180     0.002058     0.026897    Biso  1.000000 C
  C21      1.0    0.151282     0.004229     0.055594    Biso  1.000000 C
  C22      1.0    0.000648     0.999962     0.999945    Biso  1.000000 C
```

C23	1.0	0.016540	0.992749	0.905889	Biso	1.000000 C
C24	1.0	0.016978	0.007217	0.093952	Biso	1.000000 C
N1	1.0	0.538544	0.042186	0.999471	Biso	1.000000 N
N2	1.0	0.538497	0.957631	0.999316	Biso	1.000000 N
N3	1.0	0.763719	0.042129	0.999514	Biso	1.000000 N
N4	1.0	0.763683	0.957567	-0.000050	Biso	1.000000 N
N5	1.0	0.263809	0.003398	0.041600	Biso	1.000000 N
N6	1.0	0.263590	0.996869	0.957427	Biso	1.000000 N
N7	1.0	0.038461	0.996827	0.957798	Biso	1.000000 N
N8	1.0	0.038661	0.003169	0.041977	Biso	1.000000 N
H1	1.0	0.651148	0.097764	0.998983	Biso	1.000000 H
H2	1.0	0.651043	0.901992	0.000047	Biso	1.000000 H
H3	1.0	0.467406	0.092543	0.002518	Biso	1.000000 H
H4	1.0	0.528887	0.115212	0.963498	Biso	1.000000 H
H5	1.0	0.535108	0.114770	0.032214	Biso	1.000000 H
H6	1.0	0.467291	0.907297	0.996453	Biso	1.000000 H
H7	1.0	0.529221	0.884369	0.034829	Biso	1.000000 H
H8	1.0	0.534621	0.885301	0.966057	Biso	1.000000 H
H9	1.0	0.834916	0.907123	0.000025	Biso	1.000000 H
H10	1.0	0.769999	0.885755	0.965744	Biso	1.000000 H
H11	1.0	0.770206	0.883823	0.034675	Biso	1.000000 H
H12	1.0	0.769949	0.113987	0.033643	Biso	1.000000 H
H13	1.0	0.770425	0.115828	0.964720	Biso	1.000000 H
H14	1.0	0.834983	0.092551	0.999612	Biso	1.000000 H
H15	1.0	0.335106	0.008341	0.091677	Biso	1.000000 H
H16	1.0	0.271306	0.974278	0.117566	Biso	1.000000 H
H17	1.0	0.269328	0.042964	0.110516	Biso	1.000000 H
H18	1.0	0.270632	0.025827	0.881365	Biso	1.000000 H
H19	1.0	0.268815	0.957151	0.888585	Biso	1.000000 H
H20	1.0	0.334637	0.991926	0.907111	Biso	1.000000 H
H21	1.0	0.031333	0.025761	0.881750	Biso	1.000000 H
H22	1.0	0.967143	0.992298	0.907722	Biso	1.000000 H
H23	1.0	0.032489	0.957075	0.888990	Biso	1.000000 H
H24	1.0	0.967569	0.007562	0.092278	Biso	1.000000 H
H25	1.0	0.032916	0.042934	0.110793	Biso	1.000000 H
H26	1.0	0.031957	0.974243	0.118068	Biso	1.000000 H
H27	1.0	0.151391	0.007301	0.097134	Biso	1.000000 H
H28	1.0	0.150897	0.992869	0.902274	Biso	1.000000 H

Compound $(5BB)_n$

#==

CRYSTAL DATA

#--

```
data_VESTA_phase_1


_chemical_name_common                  'XCrySDen XSF file'
_cell_length_a                         27.13193
_cell_length_b                         26.59245
_cell_length_c                         26.15771
_cell_angle_alpha                      91.01731
_cell_angle_beta                       90.01233
_cell_angle_gamma                      90.00921
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
  B1      1.0   0.391896   0.000454   0.997720   Biso  1.000000 B
  B2      1.0   0.446045   0.000300   0.997861   Biso  1.000000 B
  B3      1.0   0.891894   0.999845   0.999752   Biso  1.000000 B
  B4      1.0   0.946069   0.999944   -0.000096  Biso  1.000000 B
  C1      1.0   0.214464   0.948740   0.981429   Biso  1.000000 C
  C2      1.0   0.257805   0.974736   0.989765   Biso  1.000000 C
  C3      1.0   0.169012   0.974133   0.990119   Biso  1.000000 C
  C4      1.0   0.169048   0.026336   0.007412   Biso  1.000000 C
  C5      1.0   0.214527   0.051870   0.015537   Biso  1.000000 C
  C6      1.0   0.257840   0.025993   0.006669   Biso  1.000000 C
  C7      1.0   0.123519   0.948671   0.981951   Biso  1.000000 C
  C8      1.0   0.080204   0.974492   0.990829   Biso  1.000000 C
  C9      1.0   0.080238   0.025714   0.007908   Biso  1.000000 C
  C10     1.0   0.123590   0.051663   0.016188   Biso  1.000000 C
  C11     1.0   0.000488   0.000011   0.999798   Biso  1.000000 C
  C12     1.0   0.337503   0.000442   0.997849   Biso  1.000000 C
  C13     1.0   0.013468   0.911353   0.970511   Biso  1.000000 C
  C14     1.0   0.013589   0.088677   0.029058   Biso  1.000000 C
  C15     1.0   0.324557   0.089163   0.026966   Biso  1.000000 C
  C16     1.0   0.324449   0.911628   0.969051   Biso  1.000000 C
  C17     1.0   0.824876   0.035824   0.913260   Biso  1.000000 C
  C18     1.0   0.837469   0.999744   0.999497   Biso  1.000000 C
```

C19	1.0	0.757862	0.010020	0.974153	Biso	1.000000	C
C20	1.0	0.714613	0.020543	0.948750	Biso	1.000000	C
C21	1.0	0.757651	0.989369	0.024077	Biso	1.000000	C
C22	1.0	0.824150	0.963698	0.085632	Biso	1.000000	C
C23	1.0	0.669044	0.010328	0.973341	Biso	1.000000	C
C24	1.0	0.623685	0.020694	0.948382	Biso	1.000000	C
C25	1.0	0.714199	0.978888	0.049119	Biso	1.000000	C
C26	1.0	0.668824	0.989215	0.024159	Biso	1.000000	C
C27	1.0	0.513843	0.036265	0.911953	Biso	1.000000	C
C28	1.0	0.580238	0.010333	0.973458	Biso	1.000000	C
C29	1.0	0.623240	0.979017	0.048744	Biso	1.000000	C
C30	1.0	0.580017	0.989591	0.023334	Biso	1.000000	C
C31	1.0	0.500440	0.000176	0.998083	Biso	1.000000	C
C32	1.0	0.513056	0.964124	0.084372	Biso	1.000000	C
N1	1.0	0.031316	0.960354	0.986446	Biso	1.000000	N
N2	1.0	0.031365	0.039716	0.012906	Biso	1.000000	N
N3	1.0	0.306647	0.960659	0.984942	Biso	1.000000	N
N4	1.0	0.306695	0.040178	0.010993	Biso	1.000000	N
N5	1.0	0.806781	0.015656	0.960618	Biso	1.000000	N
N6	1.0	0.806462	0.983776	0.038068	Biso	1.000000	N
N7	1.0	0.531449	0.016250	0.959577	Biso	1.000000	N
N8	1.0	0.531097	0.983944	0.036838	Biso	1.000000	N
H1	1.0	0.310526	0.882535	0.994725	Biso	1.000000	H
H2	1.0	0.364938	0.912578	0.970716	Biso	1.000000	H
H3	1.0	0.312589	0.902507	0.929729	Biso	1.000000	H
H4	1.0	0.027066	0.882258	0.996370	Biso	1.000000	H
H5	1.0	0.025629	0.902113	0.931329	Biso	1.000000	H
H6	1.0	0.972969	0.912474	0.971811	Biso	1.000000	H
H7	1.0	0.973078	0.087369	0.028539	Biso	1.000000	H
H8	1.0	0.026553	0.117788	0.002877	Biso	1.000000	H
H9	1.0	0.026438	0.098047	0.067979	Biso	1.000000	H
H10	1.0	0.365023	0.088369	0.024751	Biso	1.000000	H
H11	1.0	0.313206	0.098003	0.066506	Biso	1.000000	H
H12	1.0	0.310198	0.118370	0.001684	Biso	1.000000	H
H13	1.0	0.813093	0.075145	0.909128	Biso	1.000000	H
H14	1.0	0.810038	0.985967	0.118314	Biso	1.000000	H
H15	1.0	0.473374	0.037592	0.913854	Biso	1.000000	H
H16	1.0	0.811164	0.013517	0.880406	Biso	1.000000	H
H17	1.0	0.524188	0.988381	0.116893	Biso	1.000000	H
H18	1.0	0.864636	0.965569	0.085036	Biso	1.000000	H
H19	1.0	0.528378	0.074410	0.906419	Biso	1.000000	H
H20	1.0	0.865358	0.034108	0.914312	Biso	1.000000	H
H21	1.0	0.472601	0.962844	0.082099	Biso	1.000000	H
H22	1.0	0.812447	0.924340	0.089648	Biso	1.000000	H
H23	1.0	0.525220	0.012101	0.879466	Biso	1.000000	H
H24	1.0	0.527486	0.925986	0.090174	Biso	1.000000	H
H25	1.0	0.123769	0.090855	0.029188	Biso	1.000000	H
H26	1.0	0.214432	0.091035	0.028536	Biso	1.000000	H

```
  H27      1.0   0.214328    0.909570    0.968452    Biso  1.000000 H
  H28      1.0   0.123632    0.909493    0.968914    Biso  1.000000 H
  H29      1.0   0.623187    0.963213    0.086905    Biso  1.000000 H
  H30      1.0   0.713907    0.963049    0.087263    Biso  1.000000 H
  H31      1.0   0.714609    0.036381    0.910607    Biso  1.000000 H
  H32      1.0   0.623974    0.036504    0.910224    Biso  1.000000 H
```

Compound $(12BB)_n$

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#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_chemical_name_common                  'XCrySDen XSF file'
_cell_length_a                         20.11168
_cell_length_b                         18.39321
_cell_length_c                         18.35849
_cell_angle_alpha                      89.84661
_cell_angle_beta                       90.16254
_cell_angle_gamma                      89.52755
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
  B1       1.0   0.354872    0.997230    -0.001611    Biso  1.000000 B
  B2       1.0   0.427953    0.000166    -0.000910    Biso  1.000000 B
  B3       1.0   0.854872   -0.001421    -0.000524    Biso  1.000000 B
  B4       1.0   0.927864    0.001877     0.001138    Biso  1.000000 B
  C1       1.0   0.175769    0.957837     0.008780    Biso  1.000000 C
  C2       1.0   0.107413    0.982801     0.037687    Biso  1.000000 C
```

C3	1.0	0.107242	0.040369	0.989700	Biso	1.000000	C
C4	1.0	0.175608	0.015456	0.960666	Biso	1.000000	C
C5	1.0	0.001199	0.002747	0.002125	Biso	1.000000	C
C6	1.0	0.281646	0.996283	0.997370	Biso	1.000000	C
C7	1.0	0.018439	0.901606	0.091232	Biso	1.000000	C
C8	1.0	0.017496	0.108293	0.918712	Biso	1.000000	C
C9	1.0	0.265620	0.891346	0.081457	Biso	1.000000	C
C10	1.0	0.264941	0.097720	0.908632	Biso	1.000000	C
C11	1.0	0.517604	0.915379	0.894960	Biso	1.000000	C
C12	1.0	0.765436	0.907888	0.899713	Biso	1.000000	C
C13	1.0	0.501201	0.001266	-0.001540	Biso	1.000000	C
C14	1.0	0.606941	0.988901	0.958766	Biso	1.000000	C
C15	1.0	0.675907	0.960266	0.982708	Biso	1.000000	C
C16	1.0	0.607049	0.037751	0.015469	Biso	1.000000	C
C17	1.0	0.675943	0.009079	0.039472	Biso	1.000000	C
C18	1.0	0.781638	0.997186	-0.000291	Biso	1.000000	C
C19	1.0	0.518067	0.090357	0.098842	Biso	1.000000	C
C20	1.0	0.765408	0.082096	0.103757	Biso	1.000000	C
N1	1.0	0.043704	0.956870	0.042738	Biso	1.000000	N
N2	1.0	0.043323	0.050405	0.964417	Biso	1.000000	N
N3	1.0	0.239589	0.948312	0.034637	Biso	1.000000	N
N4	1.0	0.239289	0.041724	0.956161	Biso	1.000000	N
N5	1.0	0.543328	0.963315	0.950529	Biso	1.000000	N
N6	1.0	0.739452	0.955819	0.955266	Biso	1.000000	N
N7	1.0	0.543501	0.042497	0.042837	Biso	1.000000	N
N8	1.0	0.739412	0.034907	0.047797	Biso	1.000000	N
H1	1.0	0.223958	0.862646	0.106435	Biso	1.000000	H
H2	1.0	0.297274	0.915261	0.123703	Biso	1.000000	H
H3	1.0	0.296400	0.853057	0.049920	Biso	1.000000	H
H4	1.0	0.057317	0.860579	0.100947	Biso	1.000000	H
H5	1.0	0.974753	0.876710	0.065799	Biso	1.000000	H
H6	1.0	0.002810	0.925599	0.143364	Biso	1.000000	H
H7	1.0	0.972858	0.088675	0.890704	Biso	1.000000	H
H8	1.0	0.055414	0.123903	0.879017	Biso	1.000000	H
H9	1.0	0.003284	0.155864	0.951611	Biso	1.000000	H
H10	1.0	0.295439	0.135452	0.940341	Biso	1.000000	H
H11	1.0	0.223036	0.126635	0.883333	Biso	1.000000	H
H12	1.0	0.296899	0.073433	0.866508	Biso	1.000000	H
H13	1.0	0.486687	0.946085	0.855765	Biso	1.000000	H
H14	1.0	0.795950	0.939077	0.861456	Biso	1.000000	H
H15	1.0	0.488863	0.135204	0.074602	Biso	1.000000	H
H16	1.0	0.559590	0.889667	0.866802	Biso	1.000000	H
H17	1.0	0.723761	0.882761	0.870931	Biso	1.000000	H
H18	1.0	0.723737	0.105086	0.134621	Biso	1.000000	H
H19	1.0	0.485164	0.059763	0.135095	Biso	1.000000	H
H20	1.0	0.486160	0.873921	0.920276	Biso	1.000000	H
H21	1.0	0.794578	0.125708	0.078677	Biso	1.000000	H
H22	1.0	0.797409	0.865496	0.924303	Biso	1.000000	H

```
  H23      1.0    0.560068     0.112259     0.129699    Biso  1.000000 H
  H24      1.0    0.798845     0.051292     0.140365    Biso  1.000000 H
```

Compound $(14BB)_n$

```
#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_chemical_name_common                  'XCrySDen XSF file'
_cell_length_a                         31.70100
_cell_length_b                         30.00000
_cell_length_c                         30.00000
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
  B1       1.0    0.407611     0.003818     0.014210    Biso  1.000000 B
  B2       1.0    0.453883     0.002723     0.014479    Biso  1.000000 B
  B3       1.0    0.907692     0.997912     0.004508    Biso  1.000000 B
  B4       1.0    0.953870     0.999615     0.000689    Biso  1.000000 B
  C1       1.0    0.218218     0.021612     0.993439    Biso  1.000000 C
  C2       1.0    0.217404     0.991357     0.029081    Biso  1.000000 C
  C3       1.0    0.143202     0.990280     0.026221    Biso  1.000000 C
  C4       1.0    0.143984     0.020555     0.990577    Biso  1.000000 C
  C5       1.0    0.106888     0.034817     0.969784    Biso  1.000000 C
  C6       1.0    0.069069     0.017671     0.986034    Biso  1.000000 C
```

C7	1.0	0.068351	0.987125	0.021919	Biso	1.000000	C
C8	1.0	0.105312	0.972965	0.042543	Biso	1.000000	C
C9	1.0	0.256257	0.036908	0.975504	Biso	1.000000	C
C10	1.0	0.293234	0.020846	0.994632	Biso	1.000000	C
C11	1.0	0.292384	0.990377	0.030543	Biso	1.000000	C
C12	1.0	0.254521	0.975117	0.048306	Biso	1.000000	C
C13	1.0	0.000509	0.000503	0.000930	Biso	1.000000	C
C14	1.0	0.361067	0.004635	0.013606	Biso	1.000000	C
C15	1.0	0.013384	0.053655	0.938264	Biso	1.000000	C
C16	1.0	0.010765	0.947047	0.063603	Biso	1.000000	C
C17	1.0	0.350665	0.058053	0.950468	Biso	1.000000	C
C18	1.0	0.347650	0.951550	0.076364	Biso	1.000000	C
C19	1.0	0.510687	0.938453	0.960874	Biso	1.000000	C
C20	1.0	0.500399	0.001430	0.014498	Biso	1.000000	C
C21	1.0	0.513929	0.063721	0.068099	Biso	1.000000	C
C22	1.0	0.568158	0.981685	0.999050	Biso	1.000000	C
C23	1.0	0.569082	0.017474	0.029650	Biso	1.000000	C
C24	1.0	0.605087	0.962290	0.983194	Biso	1.000000	C
C25	1.0	0.606964	0.034929	0.045237	Biso	1.000000	C
C26	1.0	0.643119	0.979818	0.998971	Biso	1.000000	C
C27	1.0	0.644041	0.015365	0.029315	Biso	1.000000	C
C28	1.0	0.717356	0.978955	0.997470	Biso	1.000000	C
C29	1.0	0.718287	0.014531	0.027795	Biso	1.000000	C
C30	1.0	0.754446	0.960562	0.980205	Biso	1.000000	C
C31	1.0	0.756349	0.033235	0.042116	Biso	1.000000	C
C32	1.0	0.792358	0.979050	0.994528	Biso	1.000000	C
C33	1.0	0.793301	0.014959	0.024982	Biso	1.000000	C
C34	1.0	0.847409	0.934308	0.954282	Biso	1.000000	C
C35	1.0	0.850649	0.060371	0.060608	Biso	1.000000	C
C36	1.0	0.861106	0.997394	0.006931	Biso	1.000000	C
N1	1.0	0.027586	0.024869	0.973840	Biso	1.000000	N
N2	1.0	0.026595	0.977093	0.029906	Biso	1.000000	N
N3	1.0	0.335154	0.028876	0.985127	Biso	1.000000	N
N4	1.0	0.333810	0.981206	0.041335	Biso	1.000000	N
N5	1.0	0.526248	0.972692	0.990504	Biso	1.000000	N
N6	1.0	0.527694	0.028676	0.038430	Biso	1.000000	N
N7	1.0	0.833745	0.968980	0.984408	Biso	1.000000	N
N8	1.0	0.835211	0.025352	0.031863	Biso	1.000000	N
H1	1.0	0.339832	0.092497	0.956025	Biso	1.000000	H
H2	1.0	0.339662	0.046812	0.917498	Biso	1.000000	H
H3	1.0	0.385334	0.057128	0.951384	Biso	1.000000	H
H4	1.0	0.382342	0.951337	0.076328	Biso	1.000000	H
H5	1.0	0.335938	0.917483	0.070503	Biso	1.000000	H
H6	1.0	0.336236	0.963151	0.109050	Biso	1.000000	H
H7	1.0	0.022897	0.088353	0.944575	Biso	1.000000	H
H8	1.0	0.978795	0.051729	0.936881	Biso	1.000000	H
H9	1.0	0.026578	0.042876	0.906082	Biso	1.000000	H
H10	1.0	0.976206	0.946712	0.060482	Biso	1.000000	H

H11	1.0	0.019478	0.958689	0.097154	Biso	1.000000 H
H12	1.0	0.023099	0.913115	0.058477	Biso	1.000000 H
H13	1.0	0.520952	0.905238	0.972168	Biso	1.000000 H
H14	1.0	0.525209	0.057514	0.102269	Biso	1.000000 H
H15	1.0	0.834883	0.901753	0.964901	Biso	1.000000 H
H16	1.0	0.842345	0.053660	0.095637	Biso	1.000000 H
H17	1.0	0.476032	0.940021	0.961133	Biso	1.000000 H
H18	1.0	0.525846	0.096324	0.056832	Biso	1.000000 H
H19	1.0	0.837193	0.092767	0.050786	Biso	1.000000 H
H20	1.0	0.882070	0.933447	0.954945	Biso	1.000000 H
H21	1.0	0.522222	0.943961	0.926678	Biso	1.000000 H
H22	1.0	0.479245	0.064128	0.067883	Biso	1.000000 H
H23	1.0	0.836709	0.941163	0.920016	Biso	1.000000 H
H24	1.0	0.885154	0.061534	0.057233	Biso	1.000000 H
H25	1.0	0.755925	0.060839	0.065739	Biso	1.000000 H
H26	1.0	0.752591	0.932985	0.956622	Biso	1.000000 H
H27	1.0	0.608768	0.062508	0.068793	Biso	1.000000 H
H28	1.0	0.605459	0.934681	0.959595	Biso	1.000000 H
H29	1.0	0.255889	0.060359	0.947772	Biso	1.000000 H
H30	1.0	0.252795	0.951588	0.075927	Biso	1.000000 H
H31	1.0	0.108676	0.058432	0.942242	Biso	1.000000 H
H32	1.0	0.105753	0.949571	0.070314	Biso	1.000000 H
O1	1.0	0.181500	0.037901	0.974367	Biso	1.000000 O
O2	1.0	0.179822	0.976166	0.047074	Biso	1.000000 O
O3	1.0	0.679762	0.960182	0.983270	Biso	1.000000 O
O4	1.0	0.681647	0.032783	0.045142	Biso	1.000000 O

Compound $(16BB)_n$

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#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_VESTA_phase_1


_chemical_name_common                  'XCrySDen XSF file'
_cell_length_a                         27.18266
_cell_length_b                         27.01391
_cell_length_c                         27.13095
_cell_angle_alpha                      90.07735
_cell_angle_beta                       89.05315
_cell_angle_gamma                      89.97718
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1
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loop_
_space_group_symop_operation_xyz
  'x, y, z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
  B1      1.0   0.611660    0.218583    0.989414    Biso  1.000000 B
  B2      1.0   0.610618    0.273045    0.986798    Biso  1.000000 B
  B3      1.0   0.619125    0.718654    0.998463    Biso  1.000000 B
  B4      1.0   0.620151    0.773143    0.000358    Biso  1.000000 B
  C1      1.0   0.604937    0.524703    0.888787    Biso  1.000000 C
  C2      1.0   0.609599    0.541655    0.939389    Biso  1.000000 C
  C3      1.0   0.613037    0.584395    0.967880    Biso  1.000000 C
  C4      1.0   0.617396    0.582815    0.021256    Biso  1.000000 C
  C5      1.0   0.618528    0.538461    0.047299    Biso  1.000000 C
  C6      1.0   0.617571    0.664248    0.996795    Biso  1.000000 C
  C7      1.0   0.622227    0.518531    0.096871    Biso  1.000000 C
  C8      1.0   0.596810    0.501410    0.807270    Biso  1.000000 C
  C9      1.0   0.603839    0.473237    0.887304    Biso  1.000000 C
  C10     1.0   0.607712    0.453283    0.936863    Biso  1.000000 C
  C11     1.0   0.610989    0.496625    0.966902    Biso  1.000000 C
  C12     1.0   0.609278    0.408904    0.962843    Biso  1.000000 C
  C13     1.0   0.612818    0.164248    0.992605    Biso  1.000000 C
  C14     1.0   0.511444    0.019707    0.003610    Biso  1.000000 C
  C15     1.0   0.610613    0.327509    0.987289    Biso  1.000000 C
  C16     1.0   0.671354    0.952888    0.999031    Biso  1.000000 C
  C17     1.0   0.641599    0.996485    0.998804    Biso  1.000000 C
  C18     1.0   0.591065    0.995501    0.000688    Biso  1.000000 C
  C19     1.0   0.619636    0.827575    0.001372    Biso  1.000000 C
  C20     1.0   0.563112    0.950784    0.003037    Biso  1.000000 C
  C21     1.0   0.591340    0.907767    0.002495    Biso  1.000000 C
  C22     1.0   0.587745    0.083186    0.997815    Biso  1.000000 C
  C23     1.0   0.644871    0.908781    0.000466    Biso  1.000000 C
  C24     1.0   0.561321    0.039120    0.000698    Biso  1.000000 C
  C25     1.0   0.641302    0.084237    0.995779    Biso  1.000000 C
  C26     1.0   0.669543    0.041244    0.996670    Biso  1.000000 C
  C27     1.0   0.801822   -0.000196    0.996721    Biso  1.000000 C
  C28     1.0   0.721252    0.972355    0.997382    Biso  1.000000 C
  C29     1.0   0.720187    0.023818    0.995994    Biso  1.000000 C
  C30     1.0   0.512505    0.968238    0.004952    Biso  1.000000 C
```

C31	1.0	0.430940	0.992431	0.009661	Biso	1.000000	C
C32	1.0	0.613574	0.407389	0.016262	Biso	1.000000	C
C33	1.0	0.615155	0.495167	0.017264	Biso	1.000000	C
C34	1.0	0.616561	0.450133	0.044785	Biso	1.000000	C
C35	1.0	0.621077	0.467070	0.095406	Biso	1.000000	C
C36	1.0	0.628162	0.490397	0.177026	Biso	1.000000	C
N1	1.0	0.600655	0.539973	0.840304	Biso	1.000000	N
N2	1.0	0.613396	0.634106	0.955937	Biso	1.000000	N
N3	1.0	0.619859	0.631729	0.035911	Biso	1.000000	N
N4	1.0	0.626484	0.530873	0.146202	Biso	1.000000	N
N5	1.0	0.598944	0.460921	0.838026	Biso	1.000000	N
N6	1.0	0.607649	0.359933	0.948162	Biso	1.000000	N
N7	1.0	0.462121	0.032565	0.006508	Biso	1.000000	N
N8	1.0	0.578951	0.858185	0.003212	Biso	1.000000	N
N9	1.0	0.463761	0.953509	0.008571	Biso	1.000000	N
N10	1.0	0.659157	0.859674	0.000108	Biso	1.000000	N
N11	1.0	0.653594	0.133775	0.992854	Biso	1.000000	N
N12	1.0	0.768974	0.038659	0.995633	Biso	1.000000	N
N13	1.0	0.770625	0.959611	0.997792	Biso	1.000000	N
N14	1.0	0.573377	0.132186	0.995952	Biso	1.000000	N
N15	1.0	0.613982	0.357734	0.028169	Biso	1.000000	N
N16	1.0	0.624699	0.451827	0.143952	Biso	1.000000	N
H1	1.0	0.600128	0.575407	0.828424	Biso	1.000000	H
H2	1.0	0.610845	0.648531	0.921686	Biso	1.000000	H
H3	1.0	0.623276	0.644120	0.070886	Biso	1.000000	H
H4	1.0	0.628296	0.565538	0.160110	Biso	1.000000	H
H5	1.0	0.596961	0.426273	0.824130	Biso	1.000000	H
H6	1.0	0.604780	0.347547	0.913147	Biso	1.000000	H
H7	1.0	0.688024	0.147846	0.990715	Biso	1.000000	H
H8	1.0	0.544477	0.844089	0.003945	Biso	1.000000	H
H9	1.0	0.784291	0.924839	0.998898	Biso	1.000000	H
H10	1.0	0.451562	0.918215	0.010476	Biso	1.000000	H
H11	1.0	0.781207	0.073985	0.994878	Biso	1.000000	H
H12	1.0	0.448466	0.067365	0.006643	Biso	1.000000	H
H13	1.0	0.694144	0.846947	0.998433	Biso	1.000000	H
H14	1.0	0.538376	0.144862	0.996117	Biso	1.000000	H
H15	1.0	0.616933	0.343271	0.062352	Biso	1.000000	H
H16	1.0	0.624892	0.416395	0.155883	Biso	1.000000	H

Compound 27

#==========

CRYSTAL DATA

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data_VESTA_phase_1


_chemical_name_common                  'XCrySDen XSF file'
_cell_length_a                         60.00000
_cell_length_b                         60.00000
_cell_length_c                         14.54169
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                      90
_space_group_name_H-M_alt              'P 1'
_space_group_IT_number                 1

loop_
_space_group_symop_operation_xyz
   'x, y, z'

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   B1       1.0     0.898991     0.765444     0.400977     Biso  1.000000 B
   B2       1.0     0.874323     0.765806     0.401078     Biso  1.000000 B
   B3       1.0     0.771450     0.899216     0.400994     Biso  1.000000 B
   B4       1.0     0.772458     0.874661     0.401069     Biso  1.000000 B
   B5       1.0     0.771450     0.100784     0.400994     Biso  1.000000 B
   B6       1.0     0.772458     0.125339     0.401069     Biso  1.000000 B
   B7       1.0     0.874323     0.234194     0.401078     Biso  1.000000 B
   B8       1.0     0.898991     0.234556     0.400977     Biso  1.000000 B
   B9       1.0     0.125668     0.765806     0.401078     Biso  1.000000 B
   B10      1.0     0.101000     0.765444     0.400977     Biso  1.000000 B
   B11      1.0     0.228541     0.899216     0.400994     Biso  1.000000 B
   B12      1.0     0.227532     0.874661     0.401069     Biso  1.000000 B
   B13      1.0     0.228541     0.100784     0.400994     Biso  1.000000 B
   B14      1.0     0.101000     0.234556     0.400977     Biso  1.000000 B
   B15      1.0     0.125668     0.234194     0.401078     Biso  1.000000 B
   B16      1.0     0.227532     0.125339     0.401069     Biso  1.000000 B
   B17      1.0     0.999995     0.765265     0.849691     Biso  1.000000 B
   B18      1.0     0.999995     0.234735     0.849691     Biso  1.000000 B
   B19      1.0     0.771478     0.000000     0.849862     Biso  1.000000 B
   B20      1.0     0.228513     0.000000     0.849862     Biso  1.000000 B
   B21      1.0     0.771472     0.000000     0.952231     Biso  1.000000 B
   B22      1.0     0.999995     0.234732     0.952347     Biso  1.000000 B
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B23	1.0	0.999995	0.765268	0.952347	Biso	1.000000	B
B24	1.0	0.228519	0.000000	0.952231	Biso	1.000000	B
C1	1.0	0.771370	0.988211	0.205994	Biso	1.000000	C
C2	1.0	0.771312	0.980023	0.299431	Biso	1.000000	C
C3	1.0	0.771232	0.960227	0.351224	Biso	1.000000	C
C4	1.0	0.960172	0.765143	0.351637	Biso	1.000000	C
C5	1.0	0.979993	0.765133	0.299204	Biso	1.000000	C
C6	1.0	0.988141	0.765169	0.206217	Biso	1.000000	C
C7	1.0	0.771357	0.988211	0.596102	Biso	1.000000	C
C8	1.0	0.771309	0.980024	0.502664	Biso	1.000000	C
C9	1.0	0.771228	0.960228	0.450884	Biso	1.000000	C
C10	1.0	0.771174	0.923741	0.401050	Biso	1.000000	C
C11	1.0	0.772790	0.682397	0.401049	Biso	1.000000	C
C12	1.0	0.785007	0.719046	0.400967	Biso	1.000000	C
C13	1.0	0.761801	0.719349	0.400951	Biso	1.000000	C
C14	1.0	0.988141	0.765161	0.595863	Biso	1.000000	C
C15	1.0	0.979992	0.765131	0.502891	Biso	1.000000	C
C16	1.0	0.793532	0.741803	0.400994	Biso	1.000000	C
C17	1.0	0.960168	0.765144	0.450474	Biso	1.000000	C
C18	1.0	0.753687	0.742181	0.400959	Biso	1.000000	C
C19	1.0	0.813180	0.754150	0.401022	Biso	1.000000	C
C20	1.0	0.923712	0.765247	0.401026	Biso	1.000000	C
C21	1.0	0.849739	0.766013	0.401078	Biso	1.000000	C
C22	1.0	0.773651	0.755063	0.400960	Biso	1.000000	C
C23	1.0	0.733981	0.754606	0.401014	Biso	1.000000	C
C24	1.0	0.813366	0.778524	0.401008	Biso	1.000000	C
C25	1.0	0.773740	0.777985	0.401019	Biso	1.000000	C
C26	1.0	0.697035	0.766607	0.401064	Biso	1.000000	C
C27	1.0	0.734006	0.778581	0.401024	Biso	1.000000	C
C28	1.0	0.793779	0.791104	0.401029	Biso	1.000000	C
C29	1.0	0.753817	0.790913	0.401032	Biso	1.000000	C
C30	1.0	0.785352	0.813789	0.401007	Biso	1.000000	C
C31	1.0	0.762082	0.813562	0.400982	Biso	1.000000	C
C32	1.0	0.773146	0.849894	0.401098	Biso	1.000000	C
C33	1.0	0.771232	0.039772	0.351224	Biso	1.000000	C
C34	1.0	0.771312	0.019977	0.299431	Biso	1.000000	C
C35	1.0	0.771370	0.011789	0.205994	Biso	1.000000	C
C36	1.0	0.771482	0.000000	0.055407	Biso	1.000000	C
C37	1.0	0.771300	0.000000	0.353616	Biso	1.000000	C
C38	1.0	0.960172	0.234857	0.351637	Biso	1.000000	C
C39	1.0	0.979993	0.234867	0.299204	Biso	1.000000	C
C40	1.0	0.988141	0.234831	0.206217	Biso	1.000000	C
C41	1.0	0.761801	0.280651	0.400951	Biso	1.000000	C
C42	1.0	0.753687	0.257819	0.400959	Biso	1.000000	C
C43	1.0	0.773651	0.244937	0.400960	Biso	1.000000	C
C44	1.0	0.773740	0.222015	0.401019	Biso	1.000000	C
C45	1.0	0.793532	0.258197	0.400994	Biso	1.000000	C
C46	1.0	0.785007	0.280954	0.400967	Biso	1.000000	C

C47	1.0	0.753817	0.209087	0.401032	Biso	1.000000	C
C48	1.0	0.762082	0.186438	0.400982	Biso	1.000000	C
C49	1.0	0.785352	0.186211	0.401007	Biso	1.000000	C
C50	1.0	0.793779	0.208896	0.401029	Biso	1.000000	C
C51	1.0	0.773146	0.150106	0.401098	Biso	1.000000	C
C52	1.0	0.733981	0.245393	0.401014	Biso	1.000000	C
C53	1.0	0.734006	0.221419	0.401024	Biso	1.000000	C
C54	1.0	0.697035	0.233393	0.401064	Biso	1.000000	C
C55	1.0	0.813180	0.245850	0.401022	Biso	1.000000	C
C56	1.0	0.813366	0.221476	0.401008	Biso	1.000000	C
C57	1.0	0.849739	0.233987	0.401078	Biso	1.000000	C
C58	1.0	0.772790	0.317603	0.401049	Biso	1.000000	C
C59	1.0	0.771174	0.076259	0.401050	Biso	1.000000	C
C60	1.0	0.771228	0.039772	0.450884	Biso	1.000000	C
C61	1.0	0.771309	0.019976	0.502664	Biso	1.000000	C
C62	1.0	0.771357	0.011789	0.596102	Biso	1.000000	C
C63	1.0	0.771301	0.000000	0.448466	Biso	1.000000	C
C64	1.0	0.771472	0.000000	0.746687	Biso	1.000000	C
C65	1.0	0.923712	0.234753	0.401026	Biso	1.000000	C
C66	1.0	0.960168	0.234856	0.450474	Biso	1.000000	C
C67	1.0	0.979992	0.234869	0.502891	Biso	1.000000	C
C68	1.0	0.988141	0.234839	0.595863	Biso	1.000000	C
C69	1.0	0.039819	0.765143	0.351637	Biso	1.000000	C
C70	1.0	0.228759	0.960227	0.351224	Biso	1.000000	C
C71	1.0	0.999995	0.765110	0.353549	Biso	1.000000	C
C72	1.0	0.019998	0.765133	0.299204	Biso	1.000000	C
C73	1.0	0.228679	0.980023	0.299431	Biso	1.000000	C
C74	1.0	0.011849	0.765169	0.206217	Biso	1.000000	C
C75	1.0	0.228620	0.988211	0.205994	Biso	1.000000	C
C76	1.0	0.999995	0.765240	0.055533	Biso	1.000000	C
C77	1.0	0.999995	0.765230	0.746518	Biso	1.000000	C
C78	1.0	0.228634	0.988211	0.596102	Biso	1.000000	C
C79	1.0	0.011850	0.765161	0.595863	Biso	1.000000	C
C80	1.0	0.228682	0.980024	0.502664	Biso	1.000000	C
C81	1.0	0.019999	0.765131	0.502891	Biso	1.000000	C
C82	1.0	0.999995	0.765113	0.448544	Biso	1.000000	C
C83	1.0	0.228763	0.960228	0.450884	Biso	1.000000	C
C84	1.0	0.039823	0.765144	0.450474	Biso	1.000000	C
C85	1.0	0.150252	0.766013	0.401078	Biso	1.000000	C
C86	1.0	0.214638	0.813789	0.401007	Biso	1.000000	C
C87	1.0	0.076279	0.765247	0.401026	Biso	1.000000	C
C88	1.0	0.246303	0.742181	0.400959	Biso	1.000000	C
C89	1.0	0.226340	0.755063	0.400960	Biso	1.000000	C
C90	1.0	0.226251	0.777985	0.401019	Biso	1.000000	C
C91	1.0	0.302956	0.766607	0.401064	Biso	1.000000	C
C92	1.0	0.246173	0.790913	0.401032	Biso	1.000000	C
C93	1.0	0.265985	0.778581	0.401024	Biso	1.000000	C
C94	1.0	0.186625	0.778524	0.401008	Biso	1.000000	C

C95	1.0	0.266010	0.754606	0.401014	Biso	1.000000 C
C96	1.0	0.206212	0.791104	0.401029	Biso	1.000000 C
C97	1.0	0.186811	0.754150	0.401022	Biso	1.000000 C
C98	1.0	0.206459	0.741803	0.400994	Biso	1.000000 C
C99	1.0	0.227201	0.682397	0.401049	Biso	1.000000 C
C100	1.0	0.228817	0.923741	0.401050	Biso	1.000000 C
C101	1.0	0.238190	0.719349	0.400951	Biso	1.000000 C
C102	1.0	0.214984	0.719046	0.400967	Biso	1.000000 C
C103	1.0	0.237909	0.813562	0.400982	Biso	1.000000 C
C104	1.0	0.226845	0.849894	0.401098	Biso	1.000000 C
C105	1.0	0.999995	0.234760	0.055533	Biso	1.000000 C
C106	1.0	0.228691	0.000000	0.353616	Biso	1.000000 C
C107	1.0	0.039819	0.234857	0.351637	Biso	1.000000 C
C108	1.0	0.228759	0.039772	0.351224	Biso	1.000000 C
C109	1.0	0.999995	0.234889	0.353549	Biso	1.000000 C
C110	1.0	0.019998	0.234867	0.299204	Biso	1.000000 C
C111	1.0	0.228679	0.019977	0.299431	Biso	1.000000 C
C112	1.0	0.011849	0.234831	0.206217	Biso	1.000000 C
C113	1.0	0.228620	0.011789	0.205994	Biso	1.000000 C
C114	1.0	0.228509	0.000000	0.055407	Biso	1.000000 C
C115	1.0	0.228519	0.000000	0.746687	Biso	1.000000 C
C116	1.0	0.999995	0.234770	0.746518	Biso	1.000000 C
C117	1.0	0.228634	0.011789	0.596102	Biso	1.000000 C
C118	1.0	0.011850	0.234839	0.595863	Biso	1.000000 C
C119	1.0	0.228682	0.019976	0.502664	Biso	1.000000 C
C120	1.0	0.019999	0.234869	0.502891	Biso	1.000000 C
C121	1.0	0.999995	0.234887	0.448544	Biso	1.000000 C
C122	1.0	0.228763	0.039772	0.450884	Biso	1.000000 C
C123	1.0	0.039823	0.234856	0.450474	Biso	1.000000 C
C124	1.0	0.228690	0.000000	0.448466	Biso	1.000000 C
C125	1.0	0.246303	0.257819	0.400959	Biso	1.000000 C
C126	1.0	0.226340	0.244937	0.400960	Biso	1.000000 C
C127	1.0	0.238190	0.280651	0.400951	Biso	1.000000 C
C128	1.0	0.228817	0.076259	0.401050	Biso	1.000000 C
C129	1.0	0.150252	0.233987	0.401078	Biso	1.000000 C
C130	1.0	0.186625	0.221476	0.401008	Biso	1.000000 C
C131	1.0	0.226251	0.222015	0.401019	Biso	1.000000 C
C132	1.0	0.186811	0.245850	0.401022	Biso	1.000000 C
C133	1.0	0.265985	0.221419	0.401024	Biso	1.000000 C
C134	1.0	0.266010	0.245393	0.401014	Biso	1.000000 C
C135	1.0	0.302956	0.233393	0.401064	Biso	1.000000 C
C136	1.0	0.227201	0.317603	0.401049	Biso	1.000000 C
C137	1.0	0.206459	0.258197	0.400994	Biso	1.000000 C
C138	1.0	0.214984	0.280954	0.400967	Biso	1.000000 C
C139	1.0	0.206212	0.208896	0.401029	Biso	1.000000 C
C140	1.0	0.246173	0.209087	0.401032	Biso	1.000000 C
C141	1.0	0.226845	0.150106	0.401098	Biso	1.000000 C
C142	1.0	0.214638	0.186211	0.401007	Biso	1.000000 C

C143	1.0	0.237909	0.186438	0.400982	Biso	1.000000	C
C144	1.0	0.076279	0.234753	0.401026	Biso	1.000000	C
N1	1.0	0.771471	0.981787	0.115039	Biso	1.000000	N
N2	1.0	0.771169	0.938107	0.326255	Biso	1.000000	N
N3	1.0	0.937949	0.765186	0.326346	Biso	1.000000	N
N4	1.0	0.981780	0.765219	0.115116	Biso	1.000000	N
N5	1.0	0.771458	0.981788	0.687065	Biso	1.000000	N
N6	1.0	0.771166	0.938106	0.475862	Biso	1.000000	N
N7	1.0	0.790829	0.696663	0.401044	Biso	1.000000	N
N8	1.0	0.755234	0.697224	0.401035	Biso	1.000000	N
N9	1.0	0.981779	0.765209	0.686967	Biso	1.000000	N
N10	1.0	0.835355	0.747983	0.401106	Biso	1.000000	N
N11	1.0	0.937942	0.765191	0.475749	Biso	1.000000	N
N12	1.0	0.711444	0.748899	0.401080	Biso	1.000000	N
N13	1.0	0.835628	0.784306	0.401080	Biso	1.000000	N
N14	1.0	0.711510	0.784331	0.401074	Biso	1.000000	N
N15	1.0	0.791647	0.836011	0.401144	Biso	1.000000	N
N16	1.0	0.755110	0.835455	0.401084	Biso	1.000000	N
N17	1.0	0.771169	0.061893	0.326255	Biso	1.000000	N
N18	1.0	0.771471	0.018213	0.115039	Biso	1.000000	N
N19	1.0	0.937949	0.234814	0.326346	Biso	1.000000	N
N20	1.0	0.981780	0.234781	0.115116	Biso	1.000000	N
N21	1.0	0.755110	0.164545	0.401084	Biso	1.000000	N
N22	1.0	0.791647	0.163989	0.401144	Biso	1.000000	N
N23	1.0	0.711444	0.251101	0.401080	Biso	1.000000	N
N24	1.0	0.711510	0.215669	0.401074	Biso	1.000000	N
N25	1.0	0.835355	0.252017	0.401106	Biso	1.000000	N
N26	1.0	0.835628	0.215694	0.401080	Biso	1.000000	N
N27	1.0	0.755234	0.302776	0.401035	Biso	1.000000	N
N28	1.0	0.790829	0.303337	0.401044	Biso	1.000000	N
N29	1.0	0.771166	0.061894	0.475862	Biso	1.000000	N
N30	1.0	0.771458	0.018212	0.687065	Biso	1.000000	N
N31	1.0	0.937942	0.234809	0.475749	Biso	1.000000	N
N32	1.0	0.981779	0.234791	0.686967	Biso	1.000000	N
N33	1.0	0.062042	0.765186	0.326346	Biso	1.000000	N
N34	1.0	0.228822	0.938107	0.326255	Biso	1.000000	N
N35	1.0	0.018211	0.765219	0.115116	Biso	1.000000	N
N36	1.0	0.228520	0.981787	0.115039	Biso	1.000000	N
N37	1.0	0.228533	0.981788	0.687065	Biso	1.000000	N
N38	1.0	0.018212	0.765209	0.686967	Biso	1.000000	N
N39	1.0	0.228824	0.938106	0.475862	Biso	1.000000	N
N40	1.0	0.062048	0.765191	0.475749	Biso	1.000000	N
N41	1.0	0.208344	0.836011	0.401144	Biso	1.000000	N
N42	1.0	0.288480	0.784331	0.401074	Biso	1.000000	N
N43	1.0	0.244881	0.835455	0.401084	Biso	1.000000	N
N44	1.0	0.288547	0.748899	0.401080	Biso	1.000000	N
N45	1.0	0.164636	0.747983	0.401106	Biso	1.000000	N
N46	1.0	0.209162	0.696663	0.401044	Biso	1.000000	N

N47	1.0	0.244757	0.697224	0.401035	Biso	1.000000	N
N48	1.0	0.164363	0.784306	0.401080	Biso	1.000000	N
N49	1.0	0.062042	0.234814	0.326346	Biso	1.000000	N
N50	1.0	0.228822	0.061893	0.326255	Biso	1.000000	N
N51	1.0	0.018211	0.234781	0.115116	Biso	1.000000	N
N52	1.0	0.228520	0.018213	0.115039	Biso	1.000000	N
N53	1.0	0.228533	0.018212	0.687065	Biso	1.000000	N
N54	1.0	0.018212	0.234791	0.686967	Biso	1.000000	N
N55	1.0	0.228824	0.061894	0.475862	Biso	1.000000	N
N56	1.0	0.062048	0.234809	0.475749	Biso	1.000000	N
N57	1.0	0.244881	0.164545	0.401084	Biso	1.000000	N
N58	1.0	0.164636	0.252017	0.401106	Biso	1.000000	N
N59	1.0	0.164363	0.215694	0.401080	Biso	1.000000	N
N60	1.0	0.288480	0.215669	0.401074	Biso	1.000000	N
N61	1.0	0.208344	0.163989	0.401144	Biso	1.000000	N
N62	1.0	0.288547	0.251101	0.401080	Biso	1.000000	N
N63	1.0	0.209162	0.303337	0.401044	Biso	1.000000	N
N64	1.0	0.244757	0.302776	0.401035	Biso	1.000000	N
H1	1.0	0.771397	0.966084	0.089204	Biso	1.000000	H
H2	1.0	0.771029	0.932080	0.261130	Biso	1.000000	H
H3	1.0	0.932115	0.765161	0.260970	Biso	1.000000	H
H4	1.0	0.966109	0.765193	0.088968	Biso	1.000000	H
H5	1.0	0.771395	0.966084	0.712895	Biso	1.000000	H
H6	1.0	0.771027	0.932077	0.540985	Biso	1.000000	H
H7	1.0	0.806525	0.690439	0.401039	Biso	1.000000	H
H8	1.0	0.739290	0.691647	0.401018	Biso	1.000000	H
H9	1.0	0.841217	0.732140	0.401021	Biso	1.000000	H
H10	1.0	0.966110	0.765192	0.713133	Biso	1.000000	H
H11	1.0	0.932106	0.765162	0.541122	Biso	1.000000	H
H12	1.0	0.705654	0.733034	0.401038	Biso	1.000000	H
H13	1.0	0.841835	0.800016	0.401033	Biso	1.000000	H
H14	1.0	0.705692	0.800182	0.401037	Biso	1.000000	H
H15	1.0	0.807288	0.842364	0.401024	Biso	1.000000	H
H16	1.0	0.739233	0.841208	0.401016	Biso	1.000000	H
H17	1.0	0.771029	0.067920	0.261130	Biso	1.000000	H
H18	1.0	0.771397	0.033916	0.089204	Biso	1.000000	H
H19	1.0	0.932115	0.234839	0.260970	Biso	1.000000	H
H20	1.0	0.966109	0.234807	0.088968	Biso	1.000000	H
H21	1.0	0.739290	0.308353	0.401018	Biso	1.000000	H
H22	1.0	0.806525	0.309561	0.401039	Biso	1.000000	H
H23	1.0	0.841217	0.267860	0.401021	Biso	1.000000	H
H24	1.0	0.841835	0.199984	0.401033	Biso	1.000000	H
H25	1.0	0.807288	0.157636	0.401024	Biso	1.000000	H
H26	1.0	0.739233	0.158792	0.401016	Biso	1.000000	H
H27	1.0	0.705692	0.199818	0.401037	Biso	1.000000	H
H28	1.0	0.705654	0.266966	0.401038	Biso	1.000000	H
H29	1.0	0.771027	0.067923	0.540985	Biso	1.000000	H
H30	1.0	0.771395	0.033916	0.712895	Biso	1.000000	H

H31	1.0	0.932106	0.234838	0.541122	Biso	1.000000 H
H32	1.0	0.966110	0.234808	0.713133	Biso	1.000000 H
H33	1.0	0.067876	0.765161	0.260970	Biso	1.000000 H
H34	1.0	0.228962	0.932080	0.261130	Biso	1.000000 H
H35	1.0	0.033882	0.765193	0.088968	Biso	1.000000 H
H36	1.0	0.228593	0.966084	0.089204	Biso	1.000000 H
H37	1.0	0.228596	0.966084	0.712895	Biso	1.000000 H
H38	1.0	0.033881	0.765192	0.713133	Biso	1.000000 H
H39	1.0	0.228964	0.932077	0.540985	Biso	1.000000 H
H40	1.0	0.067885	0.765162	0.541122	Biso	1.000000 H
H41	1.0	0.158774	0.732140	0.401021	Biso	1.000000 H
H42	1.0	0.294299	0.800182	0.401037	Biso	1.000000 H
H43	1.0	0.260701	0.691647	0.401018	Biso	1.000000 H
H44	1.0	0.260758	0.841208	0.401016	Biso	1.000000 H
H45	1.0	0.193466	0.690439	0.401039	Biso	1.000000 H
H46	1.0	0.192703	0.842364	0.401024	Biso	1.000000 H
H47	1.0	0.294337	0.733034	0.401038	Biso	1.000000 H
H48	1.0	0.158156	0.800016	0.401033	Biso	1.000000 H
H49	1.0	0.067876	0.234839	0.260970	Biso	1.000000 H
H50	1.0	0.228962	0.067920	0.261130	Biso	1.000000 H
H51	1.0	0.033882	0.234807	0.088968	Biso	1.000000 H
H52	1.0	0.228593	0.033916	0.089204	Biso	1.000000 H
H53	1.0	0.228596	0.033916	0.712895	Biso	1.000000 H
H54	1.0	0.033881	0.234808	0.713133	Biso	1.000000 H
H55	1.0	0.228964	0.067923	0.540985	Biso	1.000000 H
H56	1.0	0.067885	0.234838	0.541122	Biso	1.000000 H
H57	1.0	0.260701	0.308353	0.401018	Biso	1.000000 H
H58	1.0	0.158774	0.267860	0.401021	Biso	1.000000 H
H59	1.0	0.158156	0.199984	0.401033	Biso	1.000000 H
H60	1.0	0.192703	0.157636	0.401024	Biso	1.000000 H
H61	1.0	0.193466	0.309561	0.401039	Biso	1.000000 H
H62	1.0	0.294337	0.266966	0.401038	Biso	1.000000 H
H63	1.0	0.260758	0.158792	0.401016	Biso	1.000000 H
H64	1.0	0.294299	0.199818	0.401037	Biso	1.000000 H

Compound 28

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CRYSTAL DATA

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data_VESTA_phase_1

_chemical_name_common 'XCrySDen XSF file'

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_cell_length_c                    28.72471
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_cell_angle_beta                   90.04631
_cell_angle_gamma                     89.94547
_space_group_name_H-M_alt           'P 1'
_space_group_IT_number              1

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  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_B_iso_or_equiv
  _atom_site_type_symbol
  B1       1.0    0.651228     0.223791     0.001279    Biso  1.000000 B
  B2       1.0    0.649453     0.278136     0.000992    Biso  1.000000 B
  B3       1.0    0.370429     0.000368     0.012720    Biso  1.000000 B
  B4       1.0    0.422943     0.998899     0.010154    Biso  1.000000 B
  B5       1.0    0.427759     0.525501     0.501279    Biso  1.000000 B
  B6       1.0    0.375249     0.526794     0.504150    Biso  1.000000 B
  B7       1.0    0.146404     0.302629     0.512317    Biso  1.000000 B
  B8       1.0    0.148432     0.248293     0.512561    Biso  1.000000 B
  B9       1.0    0.154874     0.017067     0.788123    Biso  1.000000 B
  B10      1.0    0.153460     0.022378     0.737380    Biso  1.000000 B
  B11      1.0    0.644939     0.504134     0.776533    Biso  1.000000 B
  B12      1.0    0.643638     0.509042     0.725755    Biso  1.000000 B
  B13      1.0    0.143216     0.748376     0.513116    Biso  1.000000 B
  B14      1.0    0.145854     0.802586     0.513242    Biso  1.000000 B
  B15      1.0    0.652719     0.723884     0.000996    Biso  1.000000 B
  B16      1.0    0.655536     0.778063     0.001232    Biso  1.000000 B
  B17      1.0    0.859787     0.522596     0.503868    Biso  1.000000 B
  B18      1.0    0.912263     0.523600     0.507444    Biso  1.000000 B
  B19      1.0    0.885934     0.002715     0.006731    Biso  1.000000 B
  B20      1.0    0.938422     0.003565     0.010002    Biso  1.000000 B
  B21      1.0    0.646624     0.504369     0.225962    Biso  1.000000 B
  B22      1.0    0.645380     0.509020     0.276825    Biso  1.000000 B
  B23      1.0    0.152922     0.017285     0.237072    Biso  1.000000 B
  B24      1.0    0.152157     0.021698     0.287960    Biso  1.000000 B
  C1       1.0    0.647905     0.527491     0.903361    Biso  1.000000 C
  C2       1.0    0.648327     0.545392     0.950154    Biso  1.000000 C
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C3	1.0	0.648988	0.589234	0.976100	Biso	1.000000	C
C4	1.0	0.648854	0.589290	0.026156	Biso	1.000000	C
C5	1.0	0.648344	0.545462	0.052149	Biso	1.000000	C
C6	1.0	0.650726	0.669677	0.001022	Biso	1.000000	C
C7	1.0	0.648217	0.527574	0.098953	Biso	1.000000	C
C8	1.0	0.155148	0.012279	0.839222	Biso	1.000000	C
C9	1.0	0.646153	0.502390	0.827776	Biso	1.000000	C
C10	1.0	0.129738	0.006449	0.914320	Biso	1.000000	C
C11	1.0	0.180195	0.006399	0.914524	Biso	1.000000	C
C12	1.0	0.647388	0.475298	0.902952	Biso	1.000000	C
C13	1.0	0.111859	0.005394	0.961128	Biso	1.000000	C
C14	1.0	0.197635	0.005201	0.961553	Biso	1.000000	C
C15	1.0	0.647593	0.456860	0.949766	Biso	1.000000	C
C16	1.0	0.648003	0.501035	0.977304	Biso	1.000000	C
C17	1.0	0.239933	0.004503	0.987729	Biso	1.000000	C
C18	1.0	0.069257	0.005204	0.986747	Biso	1.000000	C
C19	1.0	0.647785	0.413088	0.976000	Biso	1.000000	C
C20	1.0	0.154610	0.005022	0.988644	Biso	1.000000	C
C21	1.0	0.990900	0.004639	0.011149	Biso	1.000000	C
C22	1.0	0.652297	0.169445	0.001499	Biso	1.000000	C
C23	1.0	0.553098	0.025704	0.003420	Biso	1.000000	C
C24	1.0	0.648550	0.332498	0.000962	Biso	1.000000	C
C25	1.0	0.707520	0.957042	0.000532	Biso	1.000000	C
C26	1.0	0.678988	0.001081	0.000272	Biso	1.000000	C
C27	1.0	0.629784	0.000563	0.000756	Biso	1.000000	C
C28	1.0	0.655941	0.832304	0.001275	Biso	1.000000	C
C29	1.0	0.602127	0.956026	0.001564	Biso	1.000000	C
C30	1.0	0.629396	0.912559	0.001289	Biso	1.000000	C
C31	1.0	0.627554	0.088541	0.001644	Biso	1.000000	C
C32	1.0	0.681141	0.913008	0.000780	Biso	1.000000	C
C33	1.0	0.601197	0.044500	0.001807	Biso	1.000000	C
C34	1.0	0.679317	0.089175	0.001077	Biso	1.000000	C
C35	1.0	0.706680	0.045653	0.000730	Biso	1.000000	C
C36	1.0	0.833016	0.002262	0.004220	Biso	1.000000	C
C37	1.0	0.317974	0.002505	0.013139	Biso	1.000000	C
C38	1.0	0.755652	0.975755	0.001186	Biso	1.000000	C
C39	1.0	0.755201	0.027716	0.001361	Biso	1.000000	C
C40	1.0	0.553634	0.973758	0.003210	Biso	1.000000	C
C41	1.0	0.475847	0.998945	0.007462	Biso	1.000000	C
C42	1.0	0.154335	0.005658	0.036329	Biso	1.000000	C
C43	1.0	0.647899	0.413059	0.026215	Biso	1.000000	C
C44	1.0	0.239760	0.005469	0.038124	Biso	1.000000	C
C45	1.0	0.068852	0.006235	0.037110	Biso	1.000000	C
C46	1.0	0.648090	0.501043	0.025017	Biso	1.000000	C
C47	1.0	0.647904	0.456850	0.052532	Biso	1.000000	C
C48	1.0	0.197146	0.006570	0.063861	Biso	1.000000	C
C49	1.0	0.111199	0.006841	0.063314	Biso	1.000000	C
C50	1.0	0.647962	0.475367	0.099376	Biso	1.000000	C

C51	1.0	0.128661	0.008729	0.110335	Biso	1.000000	C
C52	1.0	0.179128	0.008618	0.110673	Biso	1.000000	C
C53	1.0	0.647498	0.502593	0.174627	Biso	1.000000	C
C54	1.0	0.153392	0.013528	0.185838	Biso	1.000000	C
C55	1.0	0.042549	0.550802	0.512830	Biso	1.000000	C
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C57	1.0	0.119207	0.525421	0.513506	Biso	1.000000	C
C58	1.0	0.168409	0.525789	0.513052	Biso	1.000000	C
C59	1.0	0.091469	0.480894	0.513064	Biso	1.000000	C
C60	1.0	0.042998	0.498844	0.512626	Biso	1.000000	C
C61	1.0	0.196192	0.570239	0.512361	Biso	1.000000	C
C62	1.0	0.244643	0.552336	0.510840	Biso	1.000000	C
C63	1.0	0.245011	0.500388	0.510644	Biso	1.000000	C
C64	1.0	0.196859	0.481747	0.512055	Biso	1.000000	C
C65	1.0	0.322353	0.526859	0.506828	Biso	1.000000	C
C66	1.0	0.117259	0.613483	0.513202	Biso	1.000000	C
C67	1.0	0.169020	0.613776	0.512705	Biso	1.000000	C
C68	1.0	0.142730	0.694131	0.512958	Biso	1.000000	C
C69	1.0	0.118662	0.437294	0.512646	Biso	1.000000	C
C70	1.0	0.170413	0.437770	0.512109	Biso	1.000000	C
C71	1.0	0.145397	0.356957	0.512112	Biso	1.000000	C
C72	1.0	0.965175	0.524165	0.510003	Biso	1.000000	C
C73	1.0	0.480218	0.523543	0.500812	Biso	1.000000	C
C74	1.0	0.558288	0.521565	0.526189	Biso	1.000000	C
C75	1.0	0.558437	0.521138	0.475789	Biso	1.000000	C
C76	1.0	0.600610	0.520805	0.552338	Biso	1.000000	C
C77	1.0	0.618119	0.519254	0.599357	Biso	1.000000	C
C78	1.0	0.643316	0.513453	0.674633	Biso	1.000000	C
C79	1.0	0.601032	0.520222	0.450014	Biso	1.000000	C
C80	1.0	0.643610	0.521206	0.525211	Biso	1.000000	C
C81	1.0	0.619038	0.518352	0.403180	Biso	1.000000	C
C82	1.0	0.668577	0.519098	0.599492	Biso	1.000000	C
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C84	1.0	0.686384	0.520471	0.552680	Biso	1.000000	C
C85	1.0	0.644792	0.513095	0.328036	Biso	1.000000	C
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C87	1.0	0.686994	0.519942	0.450536	Biso	1.000000	C
C88	1.0	0.728973	0.520757	0.527076	Biso	1.000000	C
C89	1.0	0.729362	0.520388	0.476712	Biso	1.000000	C
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C91	1.0	0.149681	0.193950	0.512644	Biso	1.000000	C
C92	1.0	0.150727	0.113342	0.487547	Biso	1.000000	C
C93	1.0	0.150583	0.113420	0.537772	Biso	1.000000	C
C94	1.0	0.150865	0.069504	0.461293	Biso	1.000000	C
C95	1.0	0.150921	0.050883	0.414483	Biso	1.000000	C
C96	1.0	0.150798	0.069698	0.564091	Biso	1.000000	C
C97	1.0	0.150987	0.051315	0.610936	Biso	1.000000	C
C98	1.0	0.152199	0.024254	0.686138	Biso	1.000000	C

C99	1.0	0.151441	0.023503	0.339287	Biso	1.000000 C
C100	1.0	0.150613	0.998682	0.414992	Biso	1.000000 C
C101	1.0	0.150379	0.980898	0.461826	Biso	1.000000 C
C102	1.0	0.150626	0.025370	0.488889	Biso	1.000000 C
C103	1.0	0.149848	0.937122	0.487886	Biso	1.000000 C
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C105	1.0	0.149952	0.937270	0.537938	Biso	1.000000 C
C106	1.0	0.150659	0.025474	0.536605	Biso	1.000000 C
C107	1.0	0.150559	0.981158	0.563803	Biso	1.000000 C
C108	1.0	0.150870	0.999122	0.610567	Biso	1.000000 C
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N2	1.0	0.650014	0.638320	0.963138	Biso	1.000000 N
N3	1.0	0.649640	0.638450	0.038979	Biso	1.000000 N
N4	1.0	0.648083	0.542772	0.144615	Biso	1.000000 N
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N6	1.0	0.194493	0.009749	0.868763	Biso	1.000000 N
N7	1.0	0.646311	0.461361	0.856774	Biso	1.000000 N
N8	1.0	0.021881	0.004193	0.973545	Biso	1.000000 N
N9	1.0	0.287461	0.002711	0.975137	Biso	1.000000 N
N10	1.0	0.648164	0.363917	0.963115	Biso	1.000000 N
N11	1.0	0.505609	0.039883	0.006077	Biso	1.000000 N
N12	1.0	0.616609	0.863325	0.001633	Biso	1.000000 N
N13	1.0	0.506407	0.958606	0.005633	Biso	1.000000 N
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N16	1.0	0.802514	0.042687	0.003148	Biso	1.000000 N
N17	1.0	0.803166	0.961413	0.002731	Biso	1.000000 N
N18	1.0	0.613675	0.137519	0.001990	Biso	1.000000 N
N19	1.0	0.648240	0.363835	0.038908	Biso	1.000000 N
N20	1.0	0.287338	0.004607	0.050973	Biso	1.000000 N
N21	1.0	0.021125	0.006186	0.049377	Biso	1.000000 N
N22	1.0	0.647654	0.461524	0.145595	Biso	1.000000 N
N23	1.0	0.114195	0.011573	0.156062	Biso	1.000000 N
N24	1.0	0.192986	0.011453	0.156617	Biso	1.000000 N
N25	1.0	0.291924	0.567307	0.508547	Biso	1.000000 N
N26	1.0	0.292448	0.486037	0.508188	Biso	1.000000 N
N27	1.0	0.103798	0.662634	0.513293	Biso	1.000000 N
N28	1.0	0.181961	0.662971	0.512525	Biso	1.000000 N
N29	1.0	0.105978	0.387942	0.512565	Biso	1.000000 N
N30	1.0	0.184120	0.388748	0.511672	Biso	1.000000 N
N31	1.0	0.994996	0.565048	0.511430	Biso	1.000000 N
N32	1.0	0.995731	0.483788	0.511047	Biso	1.000000 N
N33	1.0	0.510750	0.522910	0.538805	Biso	1.000000 N
N34	1.0	0.510859	0.522086	0.462958	Biso	1.000000 N
N35	1.0	0.603919	0.515917	0.645150	Biso	1.000000 N
N36	1.0	0.605190	0.515300	0.357239	Biso	1.000000 N
N37	1.0	0.682729	0.515740	0.645254	Biso	1.000000 N
N38	1.0	0.683978	0.515221	0.357810	Biso	1.000000 N

N39	1.0	0.776346	0.521418	0.540295	Biso	1.000000	N
N40	1.0	0.777085	0.520698	0.464444	Biso	1.000000	N
N41	1.0	0.150383	0.162535	0.474761	Biso	1.000000	N
N42	1.0	0.150012	0.162618	0.550551	Biso	1.000000	N
N43	1.0	0.151339	0.064626	0.368246	Biso	1.000000	N
N44	1.0	0.151666	0.065272	0.657124	Biso	1.000000	N
N45	1.0	0.150848	0.983378	0.369358	Biso	1.000000	N
N46	1.0	0.148882	0.887950	0.475140	Biso	1.000000	N
N47	1.0	0.148994	0.888211	0.550980	Biso	1.000000	N
N48	1.0	0.151489	0.983997	0.656214	Biso	1.000000	N
H1	1.0	0.647176	0.577608	0.845046	Biso	1.000000	H
H2	1.0	0.650894	0.651545	0.930189	Biso	1.000000	H
H3	1.0	0.649908	0.651858	0.071885	Biso	1.000000	H
H4	1.0	0.647834	0.577784	0.157213	Biso	1.000000	H
H5	1.0	0.228292	0.011714	0.855982	Biso	1.000000	H
H6	1.0	0.081938	0.011479	0.855512	Biso	1.000000	H
H7	1.0	0.645483	0.426768	0.843246	Biso	1.000000	H
H8	1.0	0.009137	0.002219	0.940575	Biso	1.000000	H
H9	1.0	0.300585	0.000574	0.942334	Biso	1.000000	H
H10	1.0	0.648417	0.350711	0.930132	Biso	1.000000	H
H11	1.0	0.725569	0.152386	0.000563	Biso	1.000000	H
H12	1.0	0.582797	0.849646	0.001732	Biso	1.000000	H
H13	1.0	0.816659	0.926633	0.003398	Biso	1.000000	H
H14	1.0	0.493557	0.923595	0.006240	Biso	1.000000	H
H15	1.0	0.815480	0.077639	0.004229	Biso	1.000000	H
H16	1.0	0.492026	0.074609	0.007137	Biso	1.000000	H
H17	1.0	0.728835	0.850832	0.000483	Biso	1.000000	H
H18	1.0	0.579524	0.150325	0.002107	Biso	1.000000	H
H19	1.0	0.648529	0.350462	0.071816	Biso	1.000000	H
H20	1.0	0.300382	0.004635	0.083878	Biso	1.000000	H
H21	1.0	0.007705	0.006717	0.082114	Biso	1.000000	H
H22	1.0	0.647042	0.426939	0.159124	Biso	1.000000	H
H23	1.0	0.226681	0.012630	0.169787	Biso	1.000000	H
H24	1.0	0.080323	0.012571	0.168762	Biso	1.000000	H
H25	1.0	0.981443	0.599807	0.510803	Biso	1.000000	H
H26	1.0	0.982830	0.448803	0.509977	Biso	1.000000	H
H27	1.0	0.072168	0.374276	0.513027	Biso	1.000000	H
H28	1.0	0.218217	0.375781	0.511476	Biso	1.000000	H
H29	1.0	0.305909	0.451246	0.507280	Biso	1.000000	H
H30	1.0	0.304925	0.602265	0.507920	Biso	1.000000	H
H31	1.0	0.215822	0.676518	0.512439	Biso	1.000000	H
H32	1.0	0.069785	0.675817	0.513683	Biso	1.000000	H
H33	1.0	0.497618	0.524487	0.571633	Biso	1.000000	H
H34	1.0	0.497828	0.522577	0.430051	Biso	1.000000	H
H35	1.0	0.570144	0.514416	0.658044	Biso	1.000000	H
H36	1.0	0.571494	0.513995	0.344077	Biso	1.000000	H
H37	1.0	0.716500	0.514201	0.658223	Biso	1.000000	H
H38	1.0	0.717856	0.514005	0.345129	Biso	1.000000	H

H39	1.0	0.789108	0.522598	0.573292	Biso	1.000000 H
H40	1.0	0.790499	0.520941	0.431702	Biso	1.000000 H
H41	1.0	0.150192	0.175823	0.441821	Biso	1.000000 H
H42	1.0	0.151942	0.099187	0.354665	Biso	1.000000 H
H43	1.0	0.149314	0.175915	0.583497	Biso	1.000000 H
H44	1.0	0.152292	0.099887	0.670614	Biso	1.000000 H
H45	1.0	0.150991	0.948347	0.356817	Biso	1.000000 H
H46	1.0	0.148037	0.874497	0.442262	Biso	1.000000 H
H47	1.0	0.148355	0.875050	0.583959	Biso	1.000000 H
H48	1.0	0.152082	0.949040	0.668903	Biso	1.000000 H

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