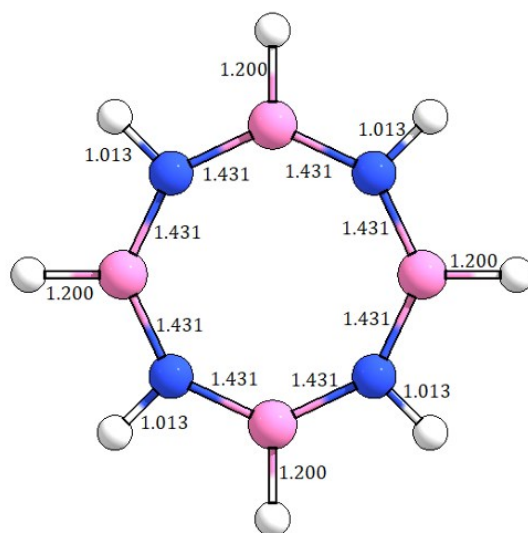


Electronic Supplementary Information

The planarised cyclooctatetraene neutral, the borazocine neutral and dianion monocycles were optimised with maximal symmetry (D_{4h} point group). The optimisation and frequency calculations were run on Gaussian 09 using B3LYP/6-31G**. The symmetry and charge of other azabore-annulenes are included, with imaginary frequencies. Finally, the $(B_4N_4H_8)_2Ti$ sandwich complex coordinates are given, alongside visual depiction of the six lowest energy active modes, calculated using MP2/6-31G** with QChem 5.2. Finally, the wB97X-2/6-31G** calculations were repeated for the $(B_4N_4H_8)_2Ti$ sandwich complex and the same structural information is given in full, these calculations were also carried out using QChem 5.2.

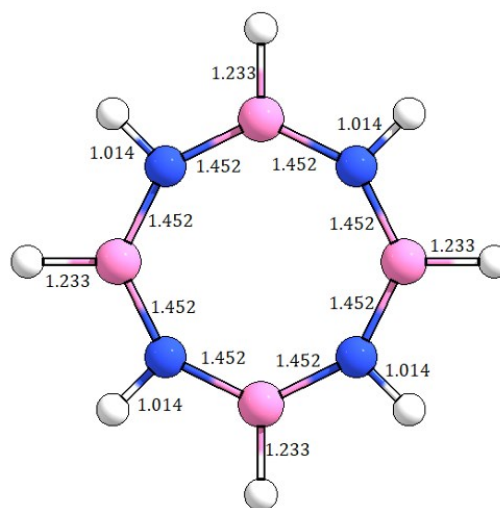
D_{4h} Borazocine Neutral Optimised

H	0.000000	3.106123	0.000000
H	-2.008126	2.008126	0.000000
H	-3.106123	0.000000	0.000000
H	2.008126	2.008126	0.000000
H	3.106123	0.000000	0.000000
H	0.000000	-3.106123	0.000000
H	2.008126	-2.008126	0.000000
H	-2.008126	-2.008126	0.000000
B	0.000000	1.906398	0.000000
B	-1.906398	0.000000	0.000000
B	0.000000	-1.906398	0.000000
B	1.906398	0.000000	0.000000
N	1.291967	1.291967	0.000000
N	-1.291967	1.291967	0.000000
N	-1.291967	-1.291967	0.000000
N	1.291967	-1.291967	0.000000



D_{4h} Borazocine Dianion Optimised

H	0.000000	3.179802	0.000000
H	-2.017268	2.017268	0.000000
H	-3.179802	0.000000	0.000000
H	2.017268	2.017268	0.000000
H	3.179802	0.000000	0.000000
H	0.000000	-3.179802	0.000000
H	2.017268	-2.017268	0.000000
H	-2.017268	-2.017268	0.000000
B	0.000000	1.946860	0.000000
B	-1.946860	0.000000	0.000000
B	0.000000	-1.946860	0.000000
B	1.946860	0.000000	0.000000
N	1.300130	1.300130	0.000000
N	-1.300130	1.300130	0.000000
N	-1.300130	-1.300130	0.000000
N	1.300130	-1.300130	0.000000



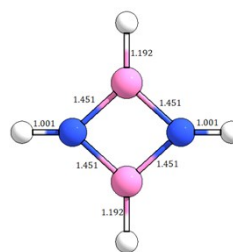
D_{4h} Cyclooctatetraene (COT) Neutral Optimised

C	0.672713	1.716417	0.000000
C	-0.672713	1.716417	0.000000

C	-1.716417	0.672713	0.000000
C	1.716417	0.672713	0.000000
C	-1.716417	-0.672713	0.000000
C	1.716417	-0.672713	0.000000
C	0.672713	-1.716417	0.000000
H	1.111484	2.712952	0.000000
H	-1.111484	2.712952	0.000000
H	-2.712952	1.111484	0.000000
H	2.712952	1.111484	0.000000
H	2.712952	-1.111484	0.000000
C	-0.672713	-1.716417	0.000000
H	-1.111484	-2.712952	0.000000
H	1.111484	-2.712952	0.000000
H	-2.712952	-1.111484	0.000000

D_{2h} $B_2N_2H_4$ Neutral Optimised

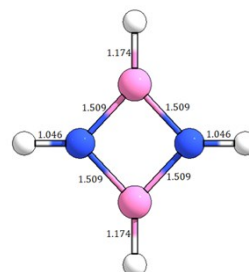
H	-0.000000	-2.170869	-0.000000
H	0.000000	2.170869	0.000000
B	0.000000	0.979129	-0.000000
B	-0.000000	-0.979129	-0.000000
N	-1.070374	0.000000	-0.000000
N	1.070374	-0.000000	-0.000000
H	2.071439	-0.000000	-0.000000
H	-2.071439	0.000000	0.000000



Imaginary frequencies: 214.3i cm^{-1} (B_{3u}), 61.06i cm^{-1} (B_{2g})

D_{2h} $B_2N_2H_4$ Cation Optimised

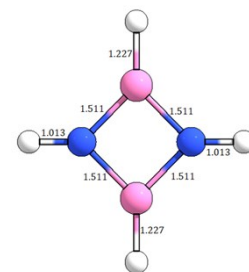
H	0.000000	-2.278754	-0.000000
H	-0.000000	2.278754	0.000000
B	-0.000000	1.104612	-0.000000
B	0.000000	-1.104612	-0.000000
N	-1.027525	-0.000000	-0.000000
N	1.027525	0.000000	-0.000000
H	2.073867	0.000000	-0.000000
H	-2.073867	-0.000000	0.000000



Imaginary frequencies: 377.2i cm^{-1} (B_{3u})

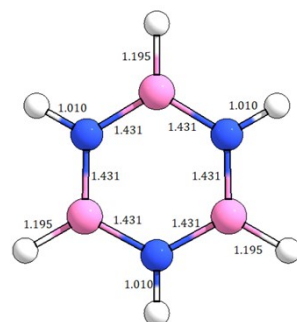
D_{2h} $B_2N_2H_4$ Anion Optimised

H	0.000000	-2.310983	-0.000000
H	-0.000000	2.310983	0.000000
B	-0.000000	1.084281	-0.000000
B	0.000000	-1.084281	-0.000000
N	-1.052779	-0.000000	-0.000000
N	1.052779	0.000000	-0.000000
H	2.066227	0.000000	-0.000000
H	-2.066227	-0.000000	0.000000



Imaginary frequencies: 1050i cm^{-1} (B_{1g}), 866.3 cm^{-1} (B_{3u}),
631.6 cm^{-1} (B_{2g})

D_{3h} $B_3N_3H_6$ Neutral Optimised

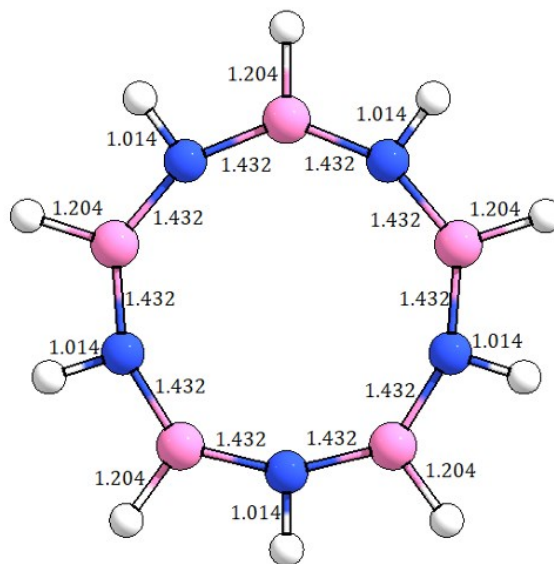


H	-2.64589324	0.00000000	0.00000000
H	1.32294662	-2.29141077	0.00000000
H	1.32294662	2.29141077	0.00000000
N	1.40941708	0.00000000	0.00000000
N	-0.70470854	1.22059099	0.00000000
N	-0.70470854	-1.22059099	0.00000000
B	0.72534573	1.25633566	0.00000000
B	-1.45069147	0.00000000	0.00000000
B	0.72534573	-1.25633566	0.00000000
H	2.41908988	0.00000000	0.00000000
H	-1.20954494	-2.09499329	0.00000000
H	-1.20954494	2.09499329	0.00000000

D_{5h} $B_5N_5H_{10}$ Neutral Optimised

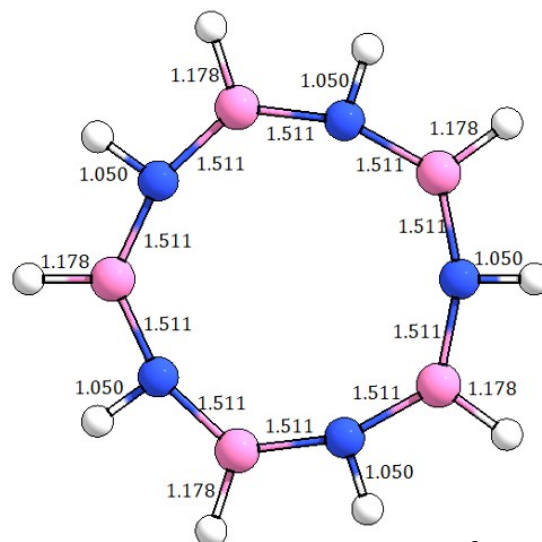
B	-1.390558	-1.913939	-0.000000
B	1.390558	-1.913939	-0.000000
B	2.249971	0.731060	0.000000
B	-0.000000	2.365759	0.000000
B	-2.249971	0.731060	0.000000
N	-2.145089	-0.696982	0.000000
N	0.000000	-2.255480	-0.000000
N	2.145089	-0.696982	-0.000000
N	1.325738	1.824722	0.000000
N	-1.325738	1.824722	0.000000
H	-0.000000	3.569521	0.000000
H	-3.394816	1.103043	0.000000
H	-3.109856	-1.010453	0.000000
H	-2.098112	-2.887803	-0.000000
H	0.000000	-3.269896	-0.000000
H	-1.921997	2.645401	0.000000
H	2.098112	-2.887803	-0.000000
H	1.921997	2.645401	0.000000
H	3.109856	-1.010453	-0.000000
H	3.394816	1.103043	0.000000

Imaginary frequencies: $77.27i$ cm^{-1} , $77.27i$ cm^{-1}



D_{5h} $B_5N_5H_{10}$ Cation Optimised

B	2.04098143	1.48285981	0.00000000
B	-0.77958553	2.39931757	0.00000000
B	-2.52279179	0.00000000	0.00000000
B	-0.77958553	-2.39931757	0.00000000
B	2.04098143	-1.48285981	0.00000000
N	2.33223963	0.00000000	0.00000000
N	0.72070168	2.21809169	0.00000000
N	-1.88682149	1.37085606	0.00000000
N	-1.88682149	-1.37085606	0.00000000
N	0.72070168	-2.21809169	0.00000000
H	-1.14350639	-3.51935078	0.00000000
H	2.99373859	-2.17507840	0.00000000
H	3.38201797	0.00000000	0.00000000

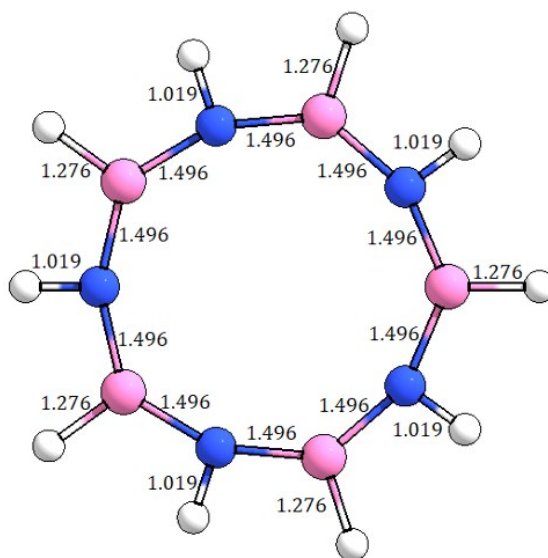


H	2.99373859	2.17507840	0.00000000
H	1.04510103	3.21649023	0.00000000
H	1.04510103	-3.21649023	0.00000000
H	-1.14350639	3.51935078	0.00000000
H	-2.73611002	-1.98790029	0.00000000
H	-2.73611002	1.98790029	0.00000000
H	-3.70046440	0.00000000	0.00000000

Imaginary frequencies: 8927i cm⁻¹, 8914i cm⁻¹, 1057i cm⁻¹, 1055i cm⁻¹, 992.6i cm⁻¹, 346.7i cm⁻¹, 345.6i cm⁻¹, 135.9i cm⁻¹, 134.6i cm⁻¹

D_{5h} B₅N₅H₁₀ Anion Optimised

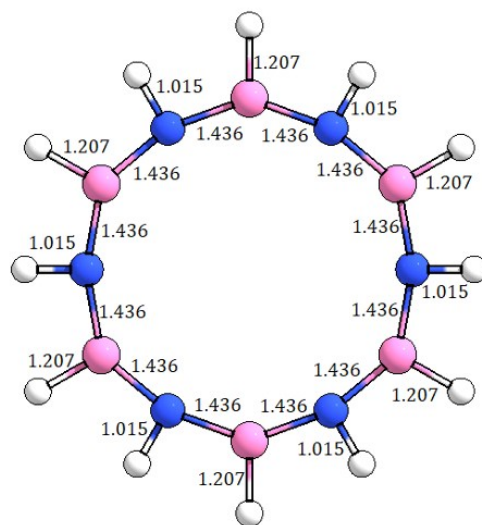
B	-1.457353	-2.005875	-0.000000
B	1.457353	-2.005875	-0.000000
B	2.358047	0.766176	0.000000
B	-0.000000	2.479397	0.000000
B	-2.358047	0.766176	0.000000
N	-2.228529	-0.724093	0.000000
N	0.000000	-2.343214	-0.000000
N	2.228529	-0.724093	-0.000000
N	1.377307	1.895700	0.000000
N	-1.377307	1.895700	0.000000
H	-0.000000	3.755105	0.000000
H	-3.571317	1.160391	0.000000
H	-3.197571	-1.038954	0.000000
H	-2.207195	-3.037944	-0.000000
H	0.000000	-3.362125	-0.000000
H	-1.976207	2.720016	0.000000
H	2.207195	-3.037944	-0.000000
H	1.976207	2.720016	0.000000
H	3.197571	-1.038954	-0.000000
H	3.571317	1.160391	0.000000



Imaginary frequencies: 575.6i cm⁻¹, 575.4i cm⁻¹, 480.0i cm⁻¹, 480.0i cm⁻¹, 399.1i cm⁻¹

D_{6h} B₆N₆H₁₂ Neutral Optimised

N	2.69643821	0.00000000	0.00000000
N	1.34821911	2.33518399	0.00000000
N	-1.34821911	2.33518399	0.00000000
N	-2.69643821	0.00000000	0.00000000
N	-1.34821911	-2.33518399	0.00000000
N	1.34821911	-2.33518399	0.00000000
B	2.44932263	-1.41411708	0.00000000
B	2.44932263	1.41411708	0.00000000
B	0.00000000	2.82823416	0.00000000
B	-2.44932263	1.41411708	0.00000000
B	-2.44932263	-1.41411708	0.00000000
B	0.00000000	-2.82823416	0.00000000
H	-3.49454397	-2.01757590	0.00000000
H	-1.85548598	-3.21379599	0.00000000
H	0.00000000	-4.03515180	0.00000000
H	1.85548598	-3.21379599	0.00000000



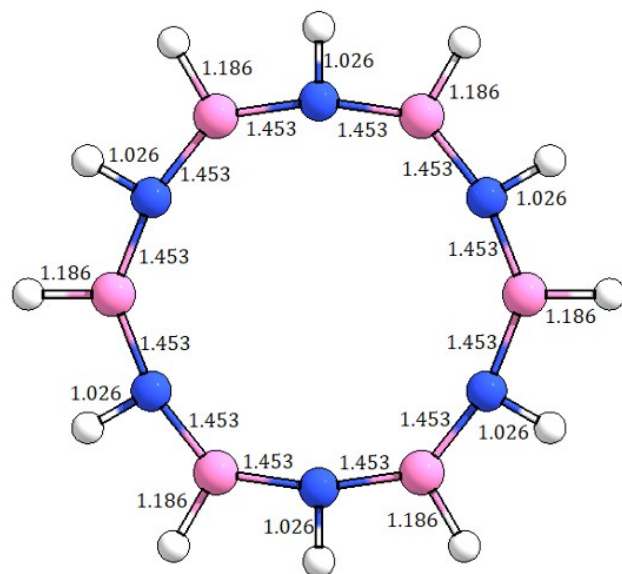
H	3.49454397	-2.01757590	0.00000000
H	3.71097197	0.00000000	0.00000000
H	3.49454397	2.01757590	0.00000000
H	1.85548598	3.21379599	0.00000000
H	0.00000000	4.03515180	0.00000000
H	-1.85548598	3.21379599	0.00000000
H	-3.49454397	2.01757590	0.00000000
H	-3.71097197	0.00000000	0.00000000

Imaginary frequencies: 113.6i cm⁻¹, 100.1i cm⁻¹

D_{6h} B₆N₆H₁₂ Cation Optimised

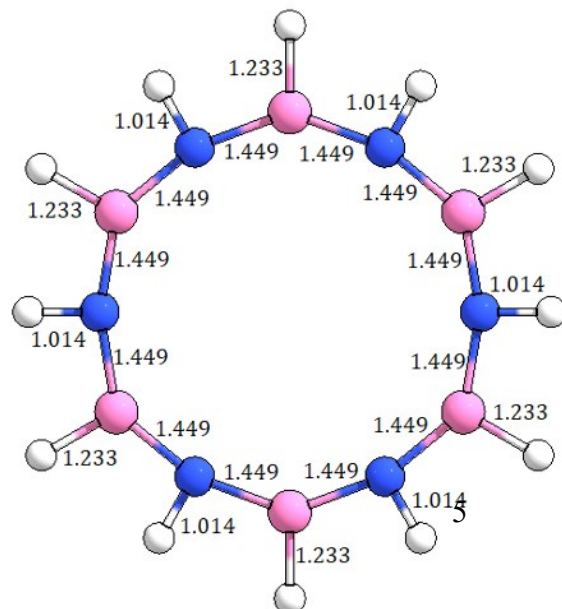
N	2.70272385	0.00000000	0.00000000
N	1.35136193	2.34062752	0.00000000
N	-1.35136193	2.34062752	0.00000000
N	-2.70272385	0.00000000	0.00000000
N	-1.35136193	-2.34062752	0.00000000
N	1.35136193	-2.34062752	0.00000000
B	2.48930154	-1.43719891	0.00000000
B	2.48930154	1.43719891	0.00000000
B	0.00000000	2.87439783	0.00000000
B	-2.48930154	1.43719891	0.00000000
B	-2.48930154	-1.43719891	0.00000000
B	0.00000000	-2.87439783	0.00000000
H	-3.51656154	-2.03028775	0.00000000
H	-1.86423368	-3.22894745	0.00000000
H	0.00000000	-4.06057551	0.00000000
H	1.86423368	-3.22894745	0.00000000
H	3.51656154	-2.03028775	0.00000000
H	3.72846736	0.00000000	0.00000000
H	3.51656154	2.03028775	0.00000000
H	1.86423368	3.22894745	0.00000000
H	0.00000000	4.06057551	0.00000000
H	-1.86423368	3.22894745	0.00000000
H	-3.51656154	2.03028775	0.00000000
H	-3.72846736	0.00000000	0.00000000

Imaginary frequencies: 392.5i cm⁻¹, 390.1i cm⁻¹, 348.4i cm⁻¹, 3.44.6i cm⁻¹, 272.2i cm⁻¹, 173.0i cm⁻¹, 111.6i cm⁻¹, 110.3i cm⁻¹



D_{6h} B₆N₆H₁₂ Anion Optimised

N	2.71434705	0.00000000	0.00000000
N	1.35717353	2.35069350	0.00000000
N	-1.35717353	2.35069350	0.00000000
N	-2.71434705	0.00000000	0.00000000
N	-1.35717353	-2.35069350	0.00000000
N	1.35717353	-2.35069350	0.00000000
B	2.47508520	-1.42899111	0.00000000
B	2.47508520	1.42899111	0.00000000
B	0.00000000	2.85798221	0.00000000
B	-2.47508520	1.42899111	0.00000000



B	-2.47508520	-1.42899111	0.00000000
B	0.00000000	-2.85798221	0.00000000
H	-3.54276640	-2.04541713	0.00000000
H	-1.86402237	-3.22858145	0.00000000
H	0.00000000	-4.09083427	0.00000000
H	1.86402237	-3.22858145	0.00000000
H	3.54276640	-2.04541713	0.00000000
H	3.72804474	0.00000000	0.00000000
H	3.54276640	2.04541713	0.00000000
H	1.86402237	3.22858145	0.00000000
H	0.00000000	4.09083427	0.00000000
H	-1.86402237	3.22858145	0.00000000
H	-3.54276640	2.04541713	0.00000000
H	-3.72804474	0.00000000	0.00000000

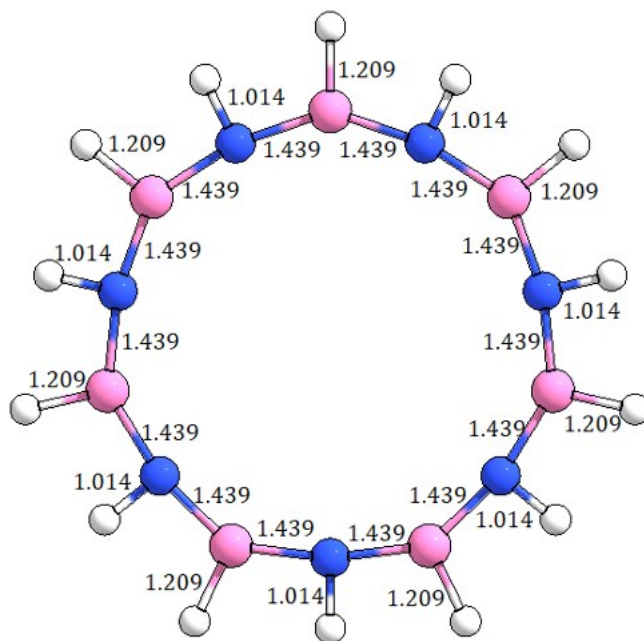
Imaginary frequencies: 48.8i cm⁻¹, 42.2i cm⁻¹

D_{7h} B₇N₇H₁₄ Neutral Optimised

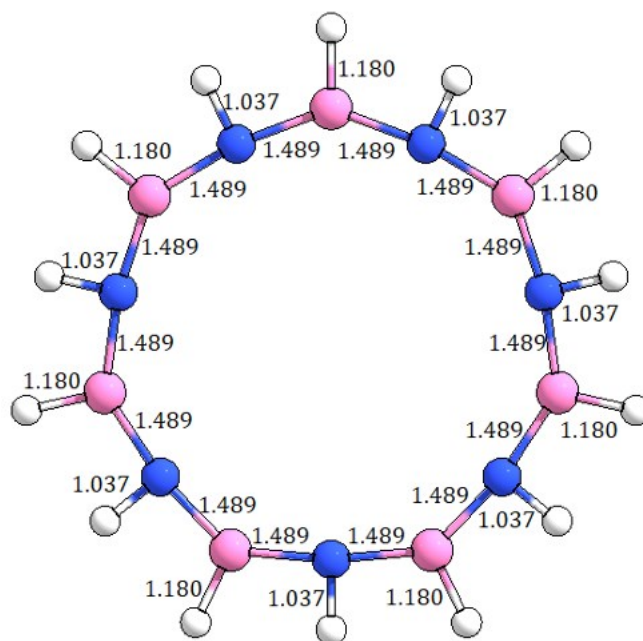
N	0.000000	3.140604	-0.000000
N	-2.455423	1.958134	-0.000000
N	-3.061862	-0.698850	-0.000000
N	-1.362657	-2.829586	-0.000000
N	1.362657	-2.829586	0.000000
N	3.061862	-0.698850	0.000000
N	2.455423	1.958134	0.000000
B	1.428198	2.965685	0.000000
B	-1.428198	2.965685	-0.000000
B	-3.209133	0.732464	-0.000000
B	-2.573525	-2.052317	-0.000000
B	-0.000000	-3.291662	-0.000000
B	2.573525	-2.052317	0.000000
B	3.209133	0.732464	0.000000
H	3.519071	-2.806366	0.000000
H	4.050685	-0.924542	0.000000
H	4.388210	1.001580	0.000000
H	3.248397	2.590510	0.000000
H	1.952937	4.055316	0.000000
H	0.000000	4.154856	-0.000000
H	-1.952937	4.055316	-0.000000
H	-3.248397	2.590510	-0.000000
H	-4.388210	1.001580	-0.000000
H	-4.050685	-0.924542	-0.000000
H	-3.519071	-2.806366	-0.000000
H	-1.802725	-3.743396	-0.000000
H	-0.000000	-4.501061	-0.000000
H	1.802725	-3.743396	0.000000

Imaginary frequencies: 159.7i cm⁻¹, 159.7i cm⁻¹, 99.15i cm⁻¹, 99.14i cm⁻¹, 98.82i cm⁻¹, 98.82i cm⁻¹,

D_{7h} B₇N₇H₁₄ Cation Optimised



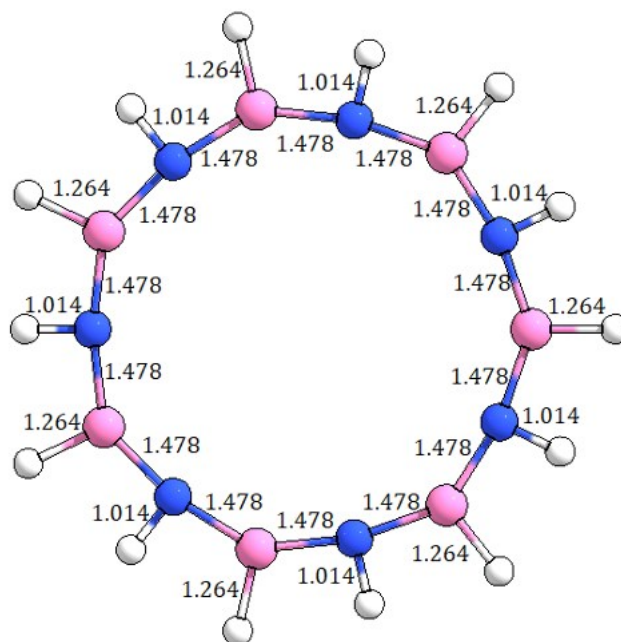
N	0.000000	3.213482	-0.000000
N	-2.512402	2.003573	-0.000000
N	-3.132914	-0.715067	-0.000000
N	-1.394278	-2.895248	-0.000000
N	1.394278	-2.895248	0.000000
N	3.132914	-0.715067	0.000000
N	2.512402	2.003573	0.000000
B	1.482514	3.078472	0.000000
B	-1.482514	3.078472	-0.000000
B	-3.331179	0.760320	-0.000000
B	-2.671398	-2.130369	-0.000000
B	-0.000000	-3.416846	-0.000000
B	2.671398	-2.130369	0.000000
B	3.331179	0.760320	0.000000
H	3.594223	-2.866297	0.000000
H	4.144193	-0.945885	0.000000
H	4.481922	1.022970	0.000000
H	3.323385	2.650311	0.000000
H	1.994643	4.141919	0.000000
H	0.000000	4.250768	-0.000000
H	-1.994643	4.141919	-0.000000
H	-3.323385	2.650311	-0.000000
H	-4.481922	1.022970	-0.000000
H	-4.144193	-0.945885	-0.000000
H	-3.594223	-2.866297	-0.000000
H	-1.844339	-3.829810	-0.000000
H	-0.000000	-4.597183	-0.000000
H	1.844339	-3.829810	0.000000



Imaginary frequencies: 1472i cm⁻¹, 1472i cm⁻¹, 1216 i cm⁻¹, 1216i cm⁻¹, 754.4i cm⁻¹, 754.4i cm⁻¹, 200.4i cm⁻¹, 200.4i cm⁻¹, 163.2i cm⁻¹, 129.0i cm⁻¹, 129.0i cm⁻¹,

D_{7h} B₇N₇H₁₄ Anion Optimised

N	0.000000	3.220409	-0.000000
N	-2.517817	2.007892	-0.000000
N	-3.139666	-0.716608	-0.000000
N	-1.397283	-2.901488	-0.000000
N	1.397283	-2.901488	0.000000
N	3.139666	-0.716608	0.000000
N	2.517817	2.007892	0.000000
B	1.467432	3.047154	0.000000
B	-1.467432	3.047154	-0.000000
B	-3.297290	0.752585	-0.000000
B	-2.644221	-2.108696	-0.000000
B	-0.000000	-3.382085	-0.000000
B	2.644221	-2.108696	0.000000
B	3.297290	0.752585	0.000000
H	3.632318	-2.896677	0.000000
H	4.128235	-0.942243	0.000000
H	4.529427	1.033812	0.000000
H	3.310587	2.640105	0.000000

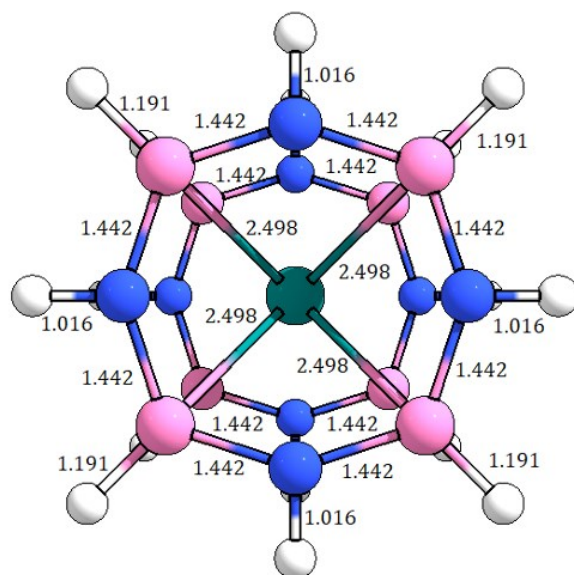


H	2.015784	4.185820	0.000000
H	0.000000	4.234400	-0.000000
H	-2.015784	4.185820	-0.000000
H	-3.310587	2.640105	-0.000000
H	-4.529427	1.033812	-0.000000
H	-4.128235	-0.942243	-0.000000
H	-3.632318	-2.896677	-0.000000
H	-1.837237	-3.815063	-0.000000
H	-0.000000	-4.645909	-0.000000
H	1.837237	-3.815063	0.000000

Imaginary frequencies: 20.84i cm⁻¹, 20.84 i cm⁻¹

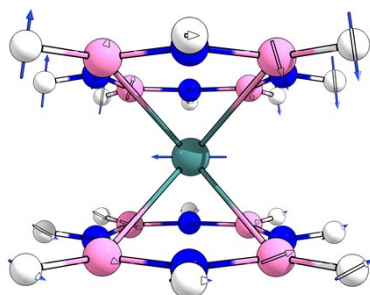
D_{4h} (B₄N₄H₈)₂Ti Neutral Optimised

1	2.214075890	2.214075890	1.519332700
1	0.000000000	2.817793100	1.459995830
1	-2.214075890	2.214075890	1.519332700
1	2.817793100	0.000000000	1.459995830
1	2.214075890	-2.214075890	1.519332700
1	-2.214075890	-2.214075890	1.519332700
1	0.000000000	-2.817793100	1.459995830
1	-2.817793100	0.000000000	1.459995830
5	1.372658650	1.372658650	1.572875590
5	-1.372658650	1.372658650	1.572875590
5	-1.372658650	-1.372658650	1.572875590
5	1.372658650	-1.372658650	1.572875590
7	1.812573570	0.000000000	1.610736080
7	0.000000000	1.812573570	1.610736080
7	-1.812573570	0.000000000	1.610736080
7	0.000000000	-1.812573570	1.610736080
22	0.000000000	0.000000000	0.000000000
1	2.214075890	2.214075890	-1.519332700
1	0.000000000	2.817793100	-1.459995830
1	-2.214075890	2.214075890	-1.519332700
1	2.817793100	0.000000000	-1.459995830
1	2.214075890	-2.214075890	-1.519332700
1	-2.214075890	-2.214075890	-1.519332700
1	0.000000000	-2.817793100	-1.459995830
1	-2.817793100	0.000000000	-1.459995830
5	1.372658650	1.372658650	-1.572875590
5	-1.372658650	1.372658650	-1.572875590
5	-1.372658650	-1.372658650	-1.572875590
5	1.372658650	-1.372658650	-1.572875590
7	1.812573570	0.000000000	-1.610736080
7	0.000000000	1.812573570	-1.610736080
7	-1.812573570	0.000000000	-1.610736080
7	0.000000000	-1.812573570	-1.610736080
1	3.910257785	9.142071234	1.571545277
1	1.698292820	9.747968506	1.528447259
1	-0.513667621	9.142065153	1.571428563
1	4.516104842	6.930945702	1.460133516

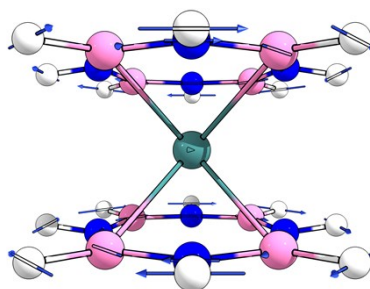


1	3.914479211	4.713912006	1.467535251
1	-0.517881160	4.713905651	1.467334541
1	1.698302275	4.112388305	1.391924167
1	-1.119497375	6.930942363	1.459958146
5	3.069115729	8.299010931	1.600888252
5	0.327473659	8.299007761	1.600830566
5	0.323797959	5.553696221	1.545048717
5	3.072794031	5.553703148	1.545146517
7	3.510878604	6.925798753	1.610821616
7	1.698292382	8.738858694	1.651900175
7	-0.114286435	6.925792931	1.610748803
7	1.698295164	5.113735347	1.569824077
22	1.698298065	6.952344818	-0.000000217
1	3.917792138	9.048015215	-1.402501000
1	1.698268516	9.644330459	-1.308445796
1	-0.521260381	9.048027566	-1.402487962
1	4.516057557	6.822956556	-1.460111313
1	3.906891075	4.619862664	-1.636374610
1	-0.510356531	4.619875374	-1.636482676
1	1.698255687	4.008743579	-1.611796197
1	-1.119538151	6.822957775	-1.460108307
5	3.075593194	8.210434607	-1.496808647
5	0.320934542	8.210443032	-1.496797599
5	0.330282177	5.465133075	-1.649178619
5	3.066255030	5.465118325	-1.649130010
7	3.510836619	6.835302301	-1.610835436
7	1.698262490	8.647617419	-1.524126770
7	-0.114312257	6.835313537	-1.610800851
7	1.698266028	5.022477838	-1.697529447

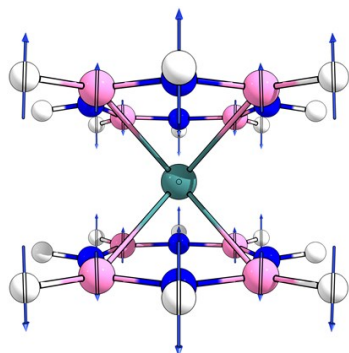
Mode 1: 54.69 cm^{-1}



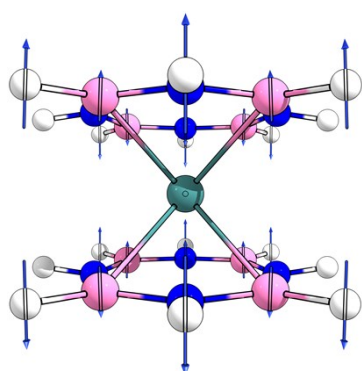
Mode 2: 86.87 cm^{-1}



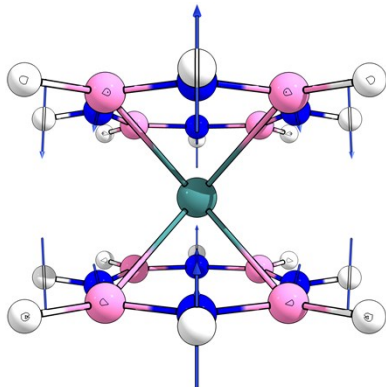
Mode 3: 127.6 cm^{-1}



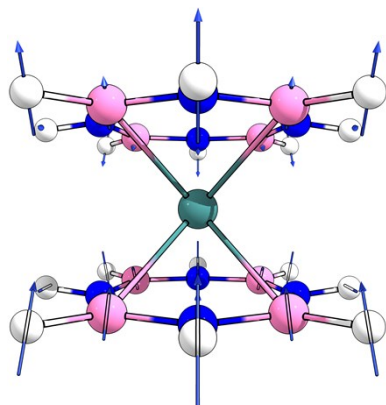
Mode 4: 159.1 cm^{-1}



Mode 5: 176.1 cm^{-1}

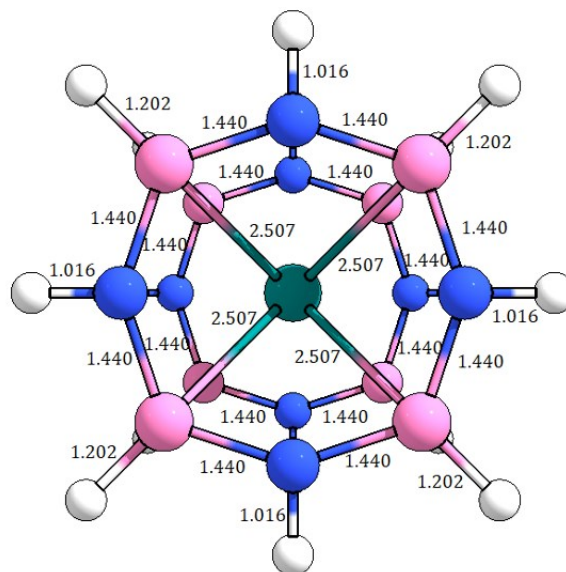


Mode 6: 176.5 cm^{-1}

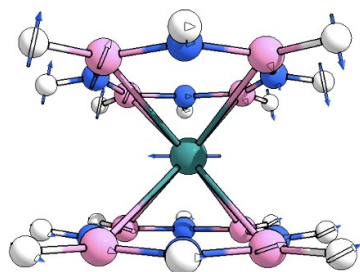


D_{4h} (B₄N₄H₈)₂Ti Neutral Optimised at wb97X-2/6-31G level of theory**

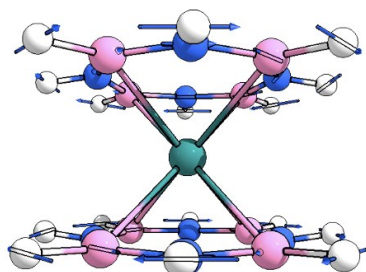
H	2.21754768	2.21754768	1.53106902
H	0.00000000	2.81865901	1.48466093
H	-2.21754768	2.21754768	1.53106902
H	2.81865901	0.00000000	1.48466093
H	2.21754768	-2.21754768	1.53106902
H	-2.21754768	-2.21754768	1.53106902
H	0.00000000	-2.81865901	1.48466093
H	-2.81865901	0.00000000	1.48466093
B	1.36904752	1.36904752	1.59239279
B	-1.36904752	1.36904752	1.59239279
B	-1.36904752	-1.36904752	1.59239279
B	1.36904752	-1.36904752	1.59239279
N	1.81456970	0.00000000	1.63924512
N	0.00000000	1.81456970	1.63924512
N	-1.81456970	0.00000000	1.63924512
N	0.00000000	-1.81456970	1.63924512
Ti	0.00000000	0.00000000	0.00000000
H	2.21754768	2.21754768	-1.53106902
H	0.00000000	2.81865901	-1.48466093
H	-2.21754768	2.21754768	-1.53106902
H	2.81865901	0.00000000	-1.48466093
H	2.21754768	-2.21754768	-1.53106902
H	-2.21754768	-2.21754768	-1.53106902
H	0.00000000	-2.81865901	-1.48466093
H	-2.81865901	0.00000000	-1.48466093
B	1.36904752	1.36904752	-1.59239279
B	-1.36904752	1.36904752	-1.59239279
B	-1.36904752	-1.36904752	-1.59239279
B	1.36904752	-1.36904752	-1.59239279
N	1.81456970	0.00000000	-1.63924512
N	0.00000000	1.81456970	-1.63924512
N	-1.81456970	0.00000000	-1.63924512
N	0.00000000	-1.81456970	-1.63924512



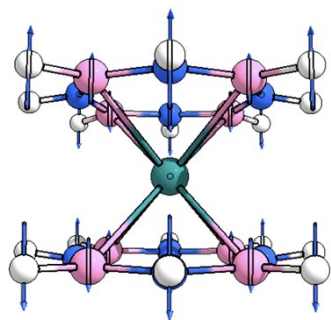
Mode 1: 59.35 cm⁻¹



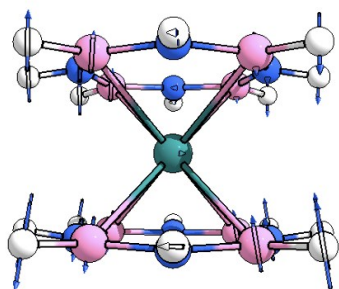
Mode 2: 109.03 cm⁻¹



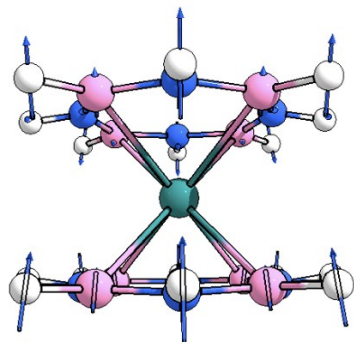
Mode 3: 121.53 cm^{-1}



Mode 4: 140.02 cm^{-1}



Mode 5: 175.52 cm^{-1}



Mode 6: 180.6 cm^{-1}

