Interplay of Donor-acceptor Interactions in
Stabilizing Boron Nitride Compounds: Insights
from Theory

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Isolated (BN)$_n$ ($n = 1–3$) Molecules

Isolated BN is a challenging system as the lowest singlet and triplet states both have multi-reference character and are nearly isoenergetic;\cite{1,2,3} the triplet state has been determined experimentally to be more stable by $0.71 \pm 0.09$ kcal/mol.\cite{4,5} The M05-2X/cc-pVTZ singlet-triplet gap is overestimated at 21.7 kcal/mol (with the triplet state as more stable) but this is in keeping with most DFT methods and also many ab initio approaches. However, the present work is focused on electronic and structural characterization of the singlet complexes rather than relative singlet-triplet energetics of the isolated species. For example, our computed M05-2X/cc-pVTZ bond lengths in the triplet and singlet states (1.315 Å and 1.261 Å, respectively) agree well with high-level CCSD(T)/aug-cc-pVQZ results of 1.329 Å and 1.270 Å.

Xu et al. have previously studied the singlet and triplet potential energy surfaces (PESs) of linear and cyclic B$_2$N$_2$ isomers by means of the coupled cluster CCSD method with the
Cui et al. have recently examined the B₂N₂ isomers with CCSD(T) single point computations based on DFT geometries. We will compare our results to the energies and geometries determined by Xu et al. as the relative stability of the linear isomers is strongly dependent on the electronic structure method used. For all the B₂N₂ isomers studied, the triplet states were found to be more stable than their corresponding singlet electronic arrangements; cyclic B₂N₂ and linear BNBN in their triplet states being the two lowest energy structures and nearly isoenergetic. Cyclic B₂N₂ and linear BNBN will be the two B₂N₂ isomers considered in our study, where upon complexation they undergo spin-forbidden process to form the singlet complex. On the triplet PES, the cyclic isomer is 1.0 kcal/mol (-0.3 kcal/mol) more stable than the linear form at the M05-2X/cc-pVTZ (CCSD/aug-cc-pVTZ) level of theory. On the singlet PES, the cyclic planar four-membered ring with D₂ℎ symmetry is most stable and the linear C∞v symmetric BNBN molecule is 25.1 kcal/mol higher in energy. The linear isomer with BNBN connectivity is 14.7, 20.9, and 46.6 kcal/mol more stable than the BNNB, NBBN, and BBNN isomers, respectively. They also concluded on the basis of short transannular B–B distances that a B–B bond exists within the singlet B₂N₂ heterocycle. Overall, our M05-2X/cc-pVTZ optimized geometries of linear BNBN and the D₂ℎ symmetric B₂N₂ rings are in reasonable agreement with the CCSD geometries determined by Xu et al. (Figure S1). However, singlet BNBN was found to adopt Cs symmetry as a global minimum instead of the reported C∞v symmetry, with the former geometry being 6.3 kcal/mol more stable than the latter at the M05-2X/cc-pVTZ level of theory. The calculated B-N bond lengths of the BNBN isomer at the M05-2X/cc-pVTZ level of theory (CCSD/aug-cc-pVTZ values in parentheses), with Cs (C∞v) symmetries, are 1.339 (1.397), 1.318 (1.289), and 1.332 (1.381) Å, respectively. The corresponding B-N bonds within the cyclic isomer B₂N₂ are each 1.392 (1.403) Å with a computed cross-ring B⋯B distance of 1.483 (1.491) Å. Additionally, the computed singlet-triplet gap (∆E S−T) value for the B₂N₂ molecule at the CCSD/aug-cc-pVTZ (20.0 kcal/mol) level of theory compares well with the ∆E S−T value of 13.2 kcal/mol obtained using M05-2X/cc-pVTZ; the corresponding
M05-2X (CCSD) $\Delta E_{S-T}$ values for the BNBN molecule are 40.1 (46.6) kcal/mol.

For B$_3$N$_3$, only the singlet isomer has been considered as all other isomers (regardless of spin-state) are significantly higher in energy; for example, linear BNBNBN in its triplet state is 75.2 kcal/mol higher in energy than the cyclic isomer in its singlet state at the CCSD(T)/cc-pVDZ level of theory. The B–N bond lengths in B$_3$N$_3$ are determined in the present M05-2X/cc-pVTZ study to be 1.354 Å; this is within 0.03 Å of the 1.3763 Å computed by Martin et al. at the CCSD(T)/cc-pVDZ level of theory. The M05-2X/cc-pVTZ computed B–N bond lengths in singlet cyclo-B$_3$N$_3$ decrease on average by 0.038 Å in relation to the intraring B–N distances in singlet cyclo-B$_2$N$_2$; this suggests a greater degree of B–N intraring resonance stabilization within B$_3$N$_3$ in relation to the B$_2$N$_2$, as later determined by NICS computations (see Table S1).

Overall, the optimized M05-2X/cc-pVTZ geometries and relative energies of the isolated (BN)$_n$ ($n = 1 - 3$) are in good agreement with available coupled cluster data, and hence we chose to conduct the remaining computations using the M05-2X/cc-pVTZ level of theory.

**Comparison of M05-2X/cc-pVTZ and BP86/TZ2P Geometries**

BP86/TZ2P optimized geometries show slightly (0.003-0.009 Å) shorter C–B and longer (0.001-0.029 Å) carbene attached B–N bonds compared to the geometries obtained by M05-2X. In the ImMe$_2$CH$_2$ and Me$_3$PCH$_2$ substituted adducts, the C–B and B–N bonds determined using BP86/TZ2P are 0.002-0.016 Å and 0.007-0.020 Å longer, respectively, than those determined using M05-2X/cc-pVTZ. Except in the case of the ImMe$_2$CH$_2$·BNBN and ImMe$_2$CH$_2$·B$_3$N$_3$ adducts, all the other BP86 optimized C-CH$_2$ and P-CH$_2$ ylidic bonds are 0.007-0.015 Å longer than the bond lengths obtained via M05-2X (coordinates of all optimized structures are presented in Tables S10 and S11).
Table S1: Calculated NICS Values of the $B_2N_2$ and $B_3N_3$ Rings of the Studied Complexes at the M05-2X/cc-pVTZ Level of Theory. The Corresponding Values Are Computed for Benzene ($C_6H_6$) and Cyclobutadiene ($C_2H_4$) as Aromatic and Anti-aromatic Molecules, Respectively.

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<th>Species</th>
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<th>NICS (1.0)</th>
<th>NICS (1.0)$_{zz}$</th>
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<td>-12.79</td>
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<td>+13.74</td>
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<td>+2.42</td>
<td>-3.92</td>
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</tr>
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<td>-4.96</td>
<td>-3.97</td>
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<td>ImMe$_2$CH$_2$·$B_3N_3$</td>
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Table S2: NBO Analysis for the Ligands at the M05-2X/cc-pVTZ Level of Theory

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<th>Bond A-B</th>
<th>Occ (A)</th>
<th>Hyb (A)</th>
<th>Hyb (B)</th>
<th>WBI</th>
</tr>
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<td>sp².70</td>
<td>66.4</td>
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<td>C-N₁ (π)</td>
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<td>C-N (σ)</td>
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<td>C-C(H₂) (σ)</td>
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<td>P-C(H₂) (σ)</td>
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<td>C(H₂) (LP)</td>
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S5
Table S3: NBO Analysis for the BN Systems at the M05-2X/cc-pVTZ Level of Theory. With the Exception of the Cyclic C=C Bond in the ImMe$_2$ and ImMe$_2$CH$_2$ Containing Complexes, All Other Double Bonds Have Been Omitted for Simplicity from the Above and Following Figures.

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<td>$C_{\infty}$</td>
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<td>B-N ($\pi_2$)</td>
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<td>71.2%</td>
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<td>⁶₅.₆</td>
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<td>P 1.₆₃₀</td>
<td>B-N (π₂)</td>
<td>1.₉₅₅</td>
<td>sp⁹⁹.⁹⁹</td>
<td>⁶₄.₇</td>
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<td>sp⁰.₈₈</td>
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<td>sp².₃⁶</td>
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<td>sp³.₃⁴</td>
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<td>1.₉₅₉</td>
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Table S4: NBO Analysis for the BNBN Systems at the M05-2X/cc-pVTZ Level of Theory

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<th>Bond A-B</th>
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<th>Hyb (A)</th>
<th>Hyb (B)</th>
<th>WBI</th>
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<td>20.4</td>
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<td>(B) %</td>
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<td>80.7</td>
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<td>p(^{1.00})</td>
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<td>p(^{1.00})</td>
<td>78.5</td>
<td>p(^{1.00})</td>
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<tr>
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<td>sp(^{0.88})</td>
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<tr>
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<td>(B_1-N_1(π_1))</td>
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<td>26.9</td>
<td>p(^{1.00})</td>
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<td>sp(^{2.33})</td>
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<td>sp(^{1.93})</td>
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<td>Species</td>
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<td>Bond A-B</td>
<td>Occ (A)</td>
<td>Hyb (A)</td>
<td>Hyb (B)</td>
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<td>sp&lt;sup&gt;0.86&lt;/sup&gt;</td>
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<td>p&lt;sup&gt;1.00&lt;/sup&gt;</td>
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<td>sp&lt;sup&gt;99.99&lt;/sup&gt;</td>
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<td>sp&lt;sup&gt;1.16&lt;/sup&gt;</td>
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<td>sp&lt;sup&gt;0.90&lt;/sup&gt;</td>
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<td>sp&lt;sup&gt;65.94&lt;/sup&gt;</td>
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<td>1.952</td>
<td>39.1</td>
<td>sp&lt;sup&gt;3.15&lt;/sup&gt;</td>
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<td>sp&lt;sup&gt;1.31&lt;/sup&gt;</td>
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Table S5: NBO Analysis for $\text{B}_2\text{N}_2$ and Its Mono-substituted Complexes at the M05-2X/cc-pVTZ Level of Theory

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<th>Species</th>
<th>NBO Charge</th>
<th>Bond A-B</th>
<th>Occ (A)</th>
<th>Hyb (A)</th>
<th>Hyb (B)</th>
<th>WBI</th>
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<td>$\text{B}_2\text{N}<em>2$ (singlet) $D</em>{2h}$</td>
<td>B$_1$ 1.069</td>
<td>B$_1$-N$_1$ ($\sigma$)</td>
<td>1.853</td>
<td>29.3</td>
<td>sp$^{1.02}$</td>
<td>70.7</td>
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<td>B$_2$ 1.069</td>
<td>B$_1$-N$_2$ ($\sigma$)</td>
<td>1.853</td>
<td>29.3</td>
<td>sp$^{1.02}$</td>
<td>70.7</td>
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<td>B$_1$-N$_2$ ($\pi$)</td>
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<td>87.3</td>
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<td>B$_2$-N$_1$ ($\pi$)</td>
<td>1.853</td>
<td>29.3</td>
<td>sp$^{1.02}$</td>
<td>70.7</td>
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**B-N represents $B_1-N_1$, $B_1-N_2$, $B_2-N_1$, and $B_2-N_2$.**
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<th>Hyb (A)</th>
<th>Occ (B) %</th>
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Table S6: NBO Analysis for the Di-substituted B$_2$N$_2$ Complexes at the M05-2X/cc-pVTZ Level of Theory

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<th>Occ (A) %</th>
<th>Hyb (A)</th>
<th>(B) %</th>
<th>Hyb (B)</th>
<th>WBI</th>
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<td>(ImMe$_2$)$_2$ · B$_2$N$<em>2$ $C</em>{2v}$</td>
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<td>(B)</td>
<td>%</td>
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Table S7: NBO Analysis for B$_3$N$_3$ and Its Mono-substituted Complexes at the M05-2X/cc-pVTZ Level of Theory

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<th>Hyb (A)</th>
<th>Hyb (B)</th>
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![Diagrams of B$_3$N$_3$ and its mono-substituted complexes]
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Table S8: NBO Analysis for the Di-substituted $B_3N_3$ Complexes at the M05-2X/cc-pVTZ Level of Theory

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<th>Occ (A)</th>
<th>Hyb (A)</th>
<th>Hyb (B)</th>
<th>WBI</th>
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Table S9: NBO Analysis for the Tri-substituted B$_3$N$_3$ Complexes at the M05-2X/cc-pVTZ Level of Theory

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<th>Species</th>
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<th>Hyb (A)</th>
<th>B (%)</th>
<th>Hyb (B)</th>
<th>WBI</th>
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<td>B (%)</td>
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Table S10: Gas Phase Ground State M05-2X/cc-pVTZ Determined XYZ Coordinates (in Å) for All the Studied Species. Electronic Energies Are Also Given in Hartrees.

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Table S12: The M05-2X/cc-pVTZ Computed Complexation Energies\(^{(a)}\) (in kcal/mol) for the Attachment of Different ImMe\(_2\)·(BN)\(_x\) Donors to the BH\(_3\) and WCO\(_5\) Acceptor Groups\(^{(b)}\)

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\(^{(a)}\)See Table 2 for Definition of Each Term.

\(^{(b)}\)For the Reaction: ImMe\(_2\)·(BN)\(_n\) + LA → ImMe\(_2\)·(BN)\(_n\)·LA \((n = 1–3)\)
Figure S1: M05-2X/cc-pVTZ Optimized Structures of the Isolated Species in the Gas Phase.
Figure S2: M05-2X/cc-pVTZ Calculated AIM Results, i.e., $\rho$ and H(r) (in Parenthesis), for All the Structures in This Study. Average Values of the $\rho$ and H(r) Are Provided for Some of the Two and Three-base Substituted Complexes.

BN (s)

BNBN (s)

B$_2$N$_2$ (s)

B$_2$N$_2$ (t)
B\textsubscript{3}N\textsubscript{3} (s)

************************************************************************

C\textsubscript{6}H\textsubscript{6}

************************************************************************

ImMe\textsubscript{2}

************************************************************************
ImMe₂CH₂

Me₃PCH₂

ImMe₂·BN
ImMe₂CH₂-BN

Me₃PCH₂-BN

ImMe₂BNBN
ImMe₂CH₂-BNBN

Me₃PCH₂-BNBN
ImMe$_2$·B$_2$N$_2$

ImMe$_2$CH$_2$·B$_2$N$_2$
Me₃PCH₂·B₂N₂

(ImMe₂)₂·B₂N₂
(ImMe₂CH₂)₂·B₂N₂

(Me₃PCH₂)₂·B₂N₂
\textbf{ImMe}_2\text{·B}_3\text{N}_3

\textbf{ImMe}_2\text{CH}_2\text{·B}_3\text{N}_3

\textbf{Me}_3\text{PCH}_2\text{·B}_3\text{N}_3
(ImMe$_2$)$_2$·B$_3$N$_3$

(ImMe$_2$CH$_2$)$_2$·B$_3$N$_3$

(Me$_3$PCH$_2$)$_2$·B$_3$N$_3$
(ImMe$_2$)$_3$·B$_3$N$_3$

(ImMe$_2$CH$_2$)$_3$·B$_3$N$_3$
\((\text{Me}_3\text{PCH}_2)_3\cdot\text{B}_3\text{N}_3\)
Figure S3: Highest Occupied (HOMO) and Lowest Unoccupied (LUMO) Molecular Orbitals of All the Studied Structures (Isovalue = 0.02) Computed at the M05-2X/cc-pVTZ Level of Theory. Energies (in eV) Are Also Given in Parentheses.
\[
\text{Me}_3\text{PCH}_2\cdot\text{B}_2\text{N}_2
\]

HOMO (-5.783)  LUMO (+0.711)

\[
\text{(ImMe)}_2\cdot\text{B}_2\text{N}_2
\]

HOMO (-4.320)  LUMO (+0.553)

\[
\text{(ImMeCH}_2\text{)}_2\cdot\text{B}_2\text{N}_2
\]

HOMO (-4.110)  LUMO (+1.137)

\[
\text{(Me}_3\text{PCH}_2\text{)}_2\cdot\text{B}_2\text{N}_2
\]

HOMO (-3.968)  LUMO (+1.586)

\[
\text{ImMe}_2\cdot\text{B}_3\text{N}_3
\]

HOMO (-8.073)  LUMO (-0.082)

\[
\text{ImMe}_2\text{CH}_2\cdot\text{B}_3\text{N}_3
\]

HOMO (-7.833)  LUMO (+0.406)

\[
\text{Me}_3\text{PCH}_2\cdot\text{B}_3\text{N}_3
\]

HOMO (-7.760)  LUMO (+0.800)

\[
\text{(ImMe)}_2\cdot\text{B}_3\text{N}_3
\]

HOMO (-6.392)  LUMO (+0.717)

\[
\text{(ImMeCH}_2\text{)}_2\cdot\text{B}_3\text{N}_3
\]

HOMO (-5.932)  LUMO (+1.262)

\[
\text{(Me}_3\text{PCH}_2\text{)}_2\cdot\text{B}_3\text{N}_3
\]

HOMO (-5.460)  LUMO (+1.509)

\[
\text{(ImMe)}_3\cdot\text{B}_3\text{N}_3
\]

HOMO (-5.340)  LUMO (+1.383)
References


