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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;[1–3] the triplet state has been determined experimentally to be more stable by 0.71 ± 0.09 kcal/mol.[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_2N_2 isomers by means of the coupled cluster CCSD method with the

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aug-cc-pVTZ basis set.[6] Cui *et al.* have recently examined the B_2N_2 isomers with CCSD(T) single point computations based on DFT geometries.[7] 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.[7–10] For all the B_2N_2 isomers studied, the triplet states were found to be more stable than their corresponding singlet electronic arrangements; cyclic B_2N_2 and linear BNBN in their triplet states being the two lowest energy structures and nearly isoenergetic.[6,7] Cyclic B_2N_2 and linear BNBN will be the two B_2N_2 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 D_{2h} symmetry is most stable and the linear $C_{\infty v}$ 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 B_2N_2 heterocycle. Overall, our M05-2X/cc-pVTZ optimized geometries of linear BNBN and the D_{2h} symmetric B_2N_2 rings are in reasonable agreement with the CCSD geometries determined by Xu *et al.* (Figure S1). However, singlet BNBN was found to adopt C_s symmetry as a global minimum instead of the reported $C_{\infty v}$ 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 C_s ($C_{\infty v}$) 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 B_2N_2 are each 1.392 (1.403) Åwith a computed cross-ring B$\cdots$B distance of 1.483 (1.491) Å. Additionally, the computed singlet-triplet gap (ΔE_{S-T}) value for the B_2N_2 molecule at the CCSD/aug-cc-pVTZ (20.0 kcal/mol) level of theory compares well with the ΔE_{S-T} value of 13.2 kcal/mol obtained using M05-2X/cc-pVTZ; the corresponding

M05-2X (CCSD) ΔE_{S-T} values for the BNBN molecule are 40.1 (46.6) kcal/mol.

For B_3N_3, only the singlet isomer has been considered as all other isomers (regardless of spin-state) are significantly higher in energy;[8,11] 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.[11] The B–N bond lengths in B_3N_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.*[11] at the CCSD(T)/cc-pVDZ level of theory. The M05-2X/cc-pVTZ computed B–N bond lengths in singlet cyclo-B_3N_3 decrease on average by 0.038 Å in relation to the intraring B–N distances in singlet cyclo-B_2N_2; this suggests a greater degree of B–N intraring resonance stabilization within B_3N_3 in relation to the B_2N_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 $ImMe_2CH_2$ and Me_3PCH_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 $ImMe_2CH_2$·BNBN and $ImMe_2CH_2$·B_3N_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.

Species	NICS (0.0)	NICS $(0.0)_{zz}$	NICS (1.0)	NICS $(1.0)_{zz}$
B_2N_2	–44.50	–73.09	–6.28	–15.12
B_3N_3	–9.88	–7.04	–2.64	–6.51
C_2H_4	+33.58	+127.38	+20.85	+65.77
C_6H_6	–7.41	–16.09	–10.56	–31.06
$ImMe_2{\cdot}B_2N_2$	–11.03	–12.79	+1.29	+8.46
$(ImMe_2)_2{\cdot}B_2N_2$	+6.06	+36.05	+5.13	+13.74
$ImMe_2{\cdot}B_3N_3$	–6.24	+1.02	–3.52	–7.43
$(ImMe_2)_2{\cdot}B_3N_3$	–3.61	+2.42	–3.92	–8.55
$(ImMe_2)_3{\cdot}B_3N_3$	–1.02	–4.96	–3.97	–2.02
$ImMe_2CH_2{\cdot}B_2N_2$	–12.82	+25.83	+0.47	+8.60
$(ImMe_2CH_2)_2{\cdot}B_2N_2$	+4.42	+22.52	+3.06	+9.04
$ImMe_2CH_2{\cdot}B_3N_3$	–5.67	–11.08	–3.12	–0.20
$(ImMe_2CH_2)_2{\cdot}B_3N_3$	–3.56	+1.50	–3.87	–3.19
$(ImMe_2CH_2)_3{\cdot}B_3N_3$	–1.96	+2.45	–3.71	–2.37
$Me_3PCH_2{\cdot}B_2N_2$	-13.87	–19.71	–1.17	+2.55
$(Me_3PCH_2)_2{\cdot}B_2N_2$	+7.07	+36.58	+3.67	+12.62
$Me_3PCH_2{\cdot}B_3N_3$	–6.15	+1.42	–3.31	–6.95
$(Me_3PCH_2)_2{\cdot}B_3N_3$	–2.92	+5.36	–3.16	–6.39
$(Me_3PCH_2)_3{\cdot}B_3N_3$	–0.91	+4.71	–3.78	–3.37

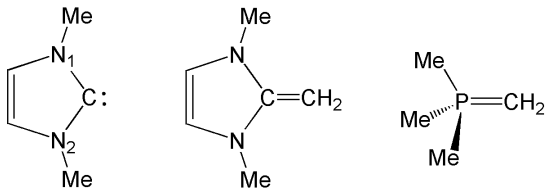


Table S2: NBO Analysis for the Ligands at the M05-2X/cc-pVTZ Level of Theory

Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
$ImMe_2$								
C_{2v}	C 0.070	C-N_1 (σ)	1.979	33.6	$sp^{2.70}$	66.4	$sp^{1.82}$	1.258
	N_1 -0.393	C-N_1 (π)	1.865	19.5	$p^{1.00}$	80.5	$p^{1.00}$	
	N_2 -0.393	C (LP)	1.921	-	$sp^{1.11}$	-	-	-
		N_2 (LP)	1.571	-	$p^{1.00}$	-	-	-
$ImMe_2CH_2$								
C_{2v}	C 0.366	C-N (σ)	1.979	38.6	$sp^{2.51}$	61.4	$sp^{2.00}$	1.091
	$C(H_2)$ -0.722	C-$C(H_2)$ (σ)	1.982	53.1	$sp^{1.32}$	46.9	$sp^{1.71}$	1.613
	N -0.384	C-$C(H_2)$ (π)	1.988	37.3	$p^{1.00}$	62.7	$p^{1.00}$	
		N (LP)	1.662	-	$p^{1.00}$	-	-	-
Me_3PCH_2								
C_s	P 1.567	P-$C(H_2)$ (σ)	1.987	43.7	$sp^{1.97}$	56.3	$sp^{2.02}$	1.328
	$C(H_2)$ -1.268	$C(H_2)$ (LP)	1.700	-	$sp^{19.69}$	-	-	-

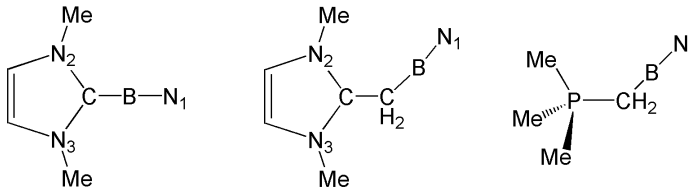
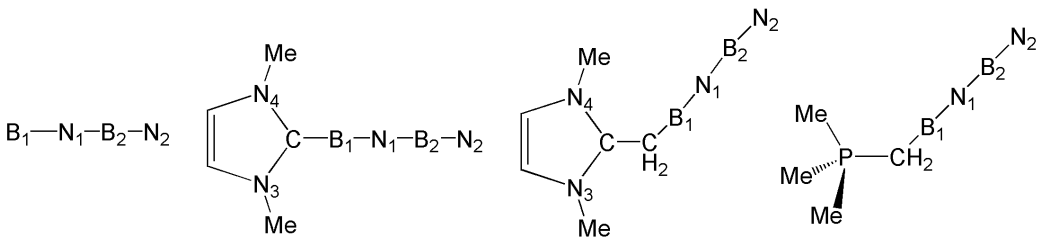


Table S3: NBO Analysis for the BN Systems at the M05-2X/cc-pVTZ Level of Theory. Wih the Exception of the Cyclic C=C Bond in the $ImMe_2$ and $ImMe_2CH_2$ Containing Complexes, All Other Double Bonds Have Been Omitted for Simplicity from the Above and Following Figures.

Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
BN (singlet)								
$C_{\infty v}$	B 0.861	B-N (σ)	1.985	15.2	$sp^{6.70}$	84.8	$sp^{0.01}$	3.012
	N -0.861	B-N (π_1)	2.000	28.8	$p^{1.00}$	71.2	$p^{1.00}$	
		B-N (π_2)	2.000	28.8	$p^{1.00}$	71.2	$p^{1.00}$	
		B-N(π_3)	1.975	33.0	$sp^{0.18}$	67.0	$sp^{99.99}$	
BN (triplet)								
$C_{\infty v}$	B 0.677	B-N(α)(σ)	1.000	23.9	$sp^{2.18}$	76.1	$sp^{1.34}$	0.546
	N -0.677	B-N(α) (π_1)	1.000	25.6	$p^{1.00}$	74.4	$p^{1.00}$	
		B-N (α) (π_2)	1.000	21.1	$p^{1.00}$	78.9	$p^{1.00}$	
		B (α) (LP)	0.997	-	$sp^{0.42}$	-	-	-
		N (α) (LP)	0.996	-	$sp^{0.73}$	-	-	-
		B-N (β)(σ)	1.000	23.6	$p^{1.00}$	76.4	$p^{1.00}$	0.449
		B-N (β)(π)	1.000	32.9	$sp^{0.17}$	67.1	$sp^{3.63}$	
		N (β) (LP)	0.950	-	$sp^{0.27}$	-		-
$ImMe_2$· BN								
C_{2v}	B 0.230	B-N_1 (σ)	1.994	30.0	$sp^{1.05}$	70.0	$sp^{0.69}$	2.622
	N_1 -0.753	B-N_1 (π_1)	1.963	37.6	$p^{1.00}$	62.4	$p^{1.00}$	
	C 0.203	B-N_1 (π_2)	1.892	39.1	$p^{1.00}$	60.9	$p^{1.00}$	
	N_2 -0.297	B-C (σ)	1.969	32.2	$sp^{0.95}$	67.8	$sp^{1.39}$	0.944
	N_3 -0.297	C-N_2 (σ)	1.981	38.2	$sp^{2.42}$	61.8	$sp^{1.90}$	1.266
		C-N_2 (π)	1.875	26.1	$p^{1.00}$	73.9	$p^{1.00}$	
		C-N_3 (σ)	1.981	38.2	$sp^{2.42}$	61.8	$sp^{1.90}$	1.266
		N_1 (LP)	1.966	-	$sp^{1.43}$	-	-	-
		N_3 (LP)	1.525	-	$p^{1.00}$	-	-	-

Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
$ImMe_2CH_2$· BN								
C_1	B 0.367	B-N_1 (σ)	1.988	34.1	$sp^{0.91}$	65.9	$sp^{2.84}$	2.656
	N_1 -0.887	B-N_1 (π_1)	1.974	33.6	$sp^{99.99}$	66.4	$sp^{99.99}$	
	N_2 -0.320	B-N_1 (π_2)	1.959	33.6	$sp^{99.99}$	66.4	$p^{1.00}$	
	N_3 -0.336	B-C(H_2)(σ)	1.914	29.0	$sp^{1.14}$	71.0	$sp^{3.06}$	0.772
	C(H_2) -0.821	C-N_2(σ)	1.982	39.4	$sp^{2.37}$	60.6	$sp^{1.76}$	1.288
	C 0.523	C-N_2 (π)	1.897	24.4	$p^{1.00}$	75.6	$p^{1.00}$	
		C-N_3 (σ)	1.982	39.1	$sp^{2.38}$	60.9	$sp^{1.74}$	1.271
		N_1 (LP)	1.951	-	$sp^{0.36}$	-	-	-
		N_3 (LP)	1.575	-	$p^{1.00}$	-	-	-
Me_3PCH_2 · BN								
C_s	B 0.382	B-N (σ)	1.995	29.2	$sp^{1.16}$	70.8	$sp^{0.65}$	2.604
	N -0.945	B-N (π_1)	1.973	34.4	$p^{1.00}$	65.6	$p^{1.00}$	
	P 1.630	B-N (π_2)	1.955	35.3	$sp^{99.99}$	64.7	$sp^{99.99}$	
	C(H_2) -1.046	B-C(H_2)(σ)	1.964	30.4	$sp^{0.88}$	69.6	$sp^{2.36}$	0.872
		P-C(H_2)(σ)	1.961	41.6	$sp^{2.66}$	58.4	$sp^{3.34}$	0.955
		N(LP)	1.959	-	$sp^{1.55}$	-	-	-



BNBN **ImMe$_2$.BNBN** **ImMe$_2$CH$_2$.BNBN** **Me$_3$PCH$_2$.BNBN**

Table S4: NBO Analysis for the BNBN Systems at the M05-2X/cc-pVTZ Level of Theory

Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
BNBN (singlet)								
C_s	B_1 0.703	B_1-N_1 (σ)	1.951	20.2	$sp^{1.19}$	79.8	$sp^{1.28}$	1.230
	B_2 0.879	B_1-N_1 (π)	1.873	11.3	$p^{1.00}$	88.7	$p^{1.00}$	
	N_1 -1.214	B_2-N_1 (σ)	1.986	25.4	$sp^{1.07}$	74.6	$sp^{1.06}$	1.340
	N_2 -0.368	B_2-N_1 (π)	1.774	17.6	$sp^{99.99}$	82.4	$sp^{12.42}$	
		B_2-N_2 (σ)	1.994	31.7	$sp^{0.95}$	68.3	$sp^{1.58}$	1.604
		B_2-N_2 (π)	1.992	20.4	$p^{1.00}$	79.6	$p^{1.00}$	
		N_2 (LP)	1.977	-	$sp^{0.63}$	-	-	-

Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
BNBN (triplet)								
C_s	B_1 0.945	B_1-N_1 (α) (σ)	0.994	19.3	$sp^{1.85}$	80.7	$sp^{0.87}$	0.443
	B_2 0.925	B_1-N_1 (α) (π_1)	0.967	19.5	$p^{1.00}$	80.5	$p^{1.00}$	
	N_1 -1.286	B_1-N_1 (α)(π_2)	0.962	18.7	$p^{1.00}$	81.3	$p^{1.00}$	
	N_2 -0.584	B_2-N_1 (α) (σ)	0.994	24.4	$sp^{1.11}$	75.6	$sp^{1.15}$	0.234
		B_2-N_2(α) (σ)	0.999	30.8	$sp^{0.90}$	69.2	$sp^{1.44}$	0.553
		B_2-N_2 (α)(π_1)	0.993	21.5	$p^{1.00}$	78.5	$p^{1.00}$	
		B_2-N_2 (α) (π_2)	0.989	25.8	$p^{1.00}$	74.2	$p^{1.00}$	
		B_1(α) (LP)	0.989	-	$sp^{0.53}$	-	-	-
		N_2(α) (LP)	0.987	-	$sp^{0.69}$	-	-	-
		B_1-N_1 (β) (σ)	0.994	20.3	$sp^{0.61}$	79.7	$sp^{0.95}$	0.370
		B_1-N_1 (β) (π_1)	0.964	15.4	$sp^{99.99}$	84.6	$sp^{99.99}$	
		B_1-N_1 (β)(π_2)	0.905	12.4	$p^{1.00}$	87.6	$p^{1.00}$	
		B_2-N_1 (β) (σ)	0.992	24.2	$sp^{1.14}$	75.8	$sp^{1.05}$	0.276
		B_2-N_2(β) (σ)	0.998	31.8	$sp^{0.91}$	68.2	$sp^{1.39}$	0.416
		B_2-N_2 (β)(π)	0.982	29.5	$sp^{99.99}$	70.5	$sp^{99.99}$	
		N_2(β) (LP)	0.985	-	$sp^{0.73}$	-	-	-
$ImMe_2$· BNBN								
C_{2v}	B_1 0.608	B_1-N_1 (σ)	1.982	25.7	$sp^{1.12}$	74.3	$sp^{0.88}$	2.062
	B_2 0.519	B_1-N_1 (π_1)	1.941	26.9	$p^{1.00}$	73.1	$p^{1.00}$	
	N_1 -0.851	B_1-N_1 (π_2)	1.903	27.5	$p^{1.00}$	72.5	$p^{1.00}$	
	N_2 -0.829	B_2-N_1 (σ)	1.980	23.8	$sp^{1.17}$	76.2	$sp^{1.14}$	0.915
	N_3 -0.281	B_2-N_2 (σ)	1.990	30.3	$sp^{0.86}$	69.7	$sp^{0.84}$	2.431
	N_4 -0.281	B_2-N_2 (π_1)	1.926	33.7	$p^{1.00}$	66.3	$p^{1.00}$	
	C 0.140	B_2-N_2 (π_2)	1.827	35.8	$p^{1.00}$	64.2	$p^{1.00}$	
		B_1-C (σ)	1.969	33.3	$sp^{0.90}$	66.7	$sp^{1.48}$	0.966
		C-N_3 (σ)	1.982	38.7	$sp^{2.33}$	61.3	$sp^{1.93}$	1.262
		C-N_4 (σ)	1.982	38.7	$sp^{2.33}$	61.3	$sp^{1.93}$	1.262
		C-N_4(π)	1.875	28.1	$p^{1.00}$	71.9	$p^{1.00}$	
		N_2 (LP)	1.965	-	$sp^{1.17}$	-	-	-
		N_3 (LP)	1.513	-	$p^{1.00}$	-	-	-
$ImMe_2CH_2$· BNBN								
C_1	B_1 0.838	B_1-N_1 (σ)	1.986	25.1	$sp^{1.20}$	74.9	$sp^{0.86}$	2.018
	B_2 0.602	B_1-N_1 (π_1)	1.935	21.7	$sp^{99.99}$	78.3	$sp^{1.00}$	
	N_1 -1.006	B_1-N_1 (π_2)	1.936	24.9	$sp^{99.99}$	75.1	$p^{1.00}$	
	N_2 -1.062	B_2-N_1 (σ)	1.977	23.6	$sp^{1.13}$	76.4	$sp^{1.16}$	0.866
	N_3 -0.275	B_2-N_2 (σ)	1.992	29.4	$sp^{0.90}$	70.6	$sp^{0.78}$	2.449
	N_4 -0.311	B_2-N_2 (π_1)	1.957	31.1	$sp^{99.99}$	68.9	$sp^{99.99}$	
	$C(H_2)$ -0.794	B_2-N_2 (π_2)	1.941	31.7	$sp^{99.99}$	68.3	$sp^{99.99}$	
	C 0.479	B_1-$C(H_2)$ (σ)	1.954	33.1	$sp^{0.85}$	66.9	$sp^{2.83}$	0.898
		C-$C(H_2)$ (σ)	1.965	50.7	$sp^{1.65}$	49.3	$sp^{2.86}$	1.026
		C-N_3 (σ)	1.982	38.8	$sp^{2.17}$	61.2	$sp^{1.88}$	1.315
		C-N_3 (π)	1.886	29.7	$sp^{99.99}$	70.3	$p^{1.00}$	
		C-N_4 (σ)	1.981	38.3	$sp^{2.26}$	61.7	$sp^{1.88}$	1.269
		N_2 (LP)	1.951	-	$sp^{1.32}$	-	-	-
		N_4 (LP)	1.536	-	$p^{1.00}$	-	-	-

Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
$Me_3PCH_2 \cdot BNBN$								
C_s	B_1 0.858	B_1-N_1 (σ)	1.986	25.2	$sp^{1.23}$	74.8	$sp^{0.86}$	1.997
	B_2 0.625	B_1-N_1 (π_1)	1.936	25.1	$p^{1.00}$	74.9	$p^{1.00}$	
	N_1 -1.013	B_1-N_1 (π_2)	1.930	20.7	$sp^{99.99}$	79.3	$sp^{99.99}$	
	N_2 -1.072	B_2-N_1 (σ)	1.976	23.7	$sp^{1.12}$	76.3	$sp^{1.16}$	0.875
	$C(H_2)$ -1.075	B_2-N_2 (σ)	1.992	29.5	$sp^{0.90}$	70.5	$sp^{0.80}$	2.406
	P 1.617	B_2-N_2 (π_1)	1.943	29.9	$sp^{99.99}$	70.1	$sp^{65.94}$	
		B_2-N_2 (π_2)	1.932	31.6	$p^{1.00}$	68.4	$p^{1.00}$	
		B_1-$C(H_2)$ (σ)	1.975	32.5	$sp^{0.83}$	67.5	$sp^{2.54}$	0.931
		P-$C(H_2)$ (σ)	1.952	39.1	$sp^{3.15}$	60.9	$sp^{3.21}$	0.906
		N_2 (LP)	1.952	-	$sp^{1.31}$	-	-	-

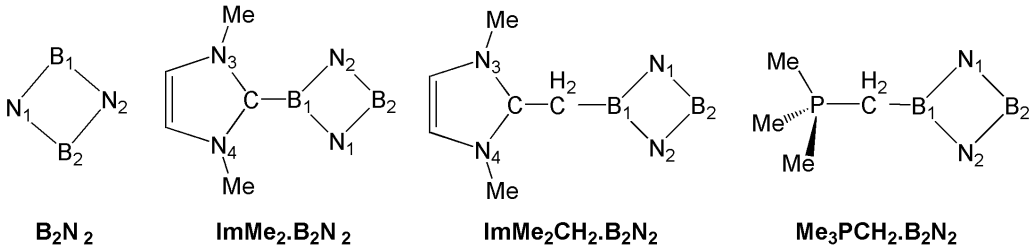


Table S5: NBO Analysis for B_2N_2 and Its Mono-substituted Complexes at the M05-2X/cc-pVTZ Level of Theory

Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
B_2N_2 (singlet)								
D_{2h}	B_1 1.069	B_1-N_1 (σ)	1.853	29.3	$sp^{1.02}$	70.7	$sp^{2.81}$	1.221
	B_2 1.069	B_1-N_2 (σ)	1.853	29.3	$sp^{1.02}$	70.7	$sp^{2.81}$	1.221
	N_1 -1.069	B_1-N_2 (π)	1.745	12.7	$p^{1.00}$	87.3	$p^{1.00}$	
	N_2 -1.069	B_2-N_1 (σ)	1.853	29.3	$sp^{1.02}$	70.7	$sp^{2.81}$	1.221
		B_2-N_1 (π)	1.745	12.7	$p^{1.00}$	87.3	$p^{1.00}$	
		B_2-N_2 (σ)	1.853	29.3	$sp^{1.02}$	70.7	$sp^{2.81}$	1.221
		N_1 (LP)	1.884	-	$sp^{1.08}$	-	-	-
		N_2 (LP)	1.884	-	$sp^{1.08}$	-	-	-

Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
B_2N_2 (triplet)								
D_{2h}	B_1 0.737	B_1-N_1(α) (σ)	0.961	33.0	$sp^{1.03}$	67.0	$sp^{2.96}$	0.281
	B_2 0.737	B_1-N_1 (α) (π)	0.907	9.2	$p^{1.00}$	90.8	$p^{1.00}$	
	N_1 -0.737	B_1-N_2(α) (σ)	0.961	33.0	$sp^{1.03}$	67.0	$sp^{2.96}$	0.281
	N_2 -0.737	B_2-N_1(α) (σ)	0.961	33.0	$sp^{1.03}$	67.0	$sp^{2.96}$	0.281
		B_2-N_2(α) (σ)	0.961	33.0	$sp^{1.03}$	67.0	$sp^{2.96}$	0.281
		B_2-N_2 (α) (π)	0.907	9.2	$p^{1.00}$	90.8	$p^{1.00}$	
		B_1-B_2 (α) (σ)	0.795	50.0	$sp^{16.32}$	50.0	$sp^{16.32}$	0.177
		N_1 (α) (LP)	0.982	-	$sp^{1.00}$	-	-	-
		N_2 (α) (LP)	0.982	-	$sp^{1.00}$	-	-	-
		B-N (β) (σ)**	0.949	28.2	$sp^{1.06}$	71.8	$sp^{2.71}$	0.290
		N_1 (β) (LP) (1)	0.962	-	$sp^{1.14}$	-	-	-
		N_1 (β) (LP) (2)	0.262	-	$p^{1.00}$	-	-	-
		N_2 (β) (LP) (1)	0.962	-	$sp^{1.14}$	-	-	-
$ImMe_2 \cdot B_2N_2$								
C_{2v}	B_1 0.654	B_1-N_1 (σ)	1.789	31.2	$sp^{2.06}$	68.8	$sp^{2.48}$	0.998
	B_2 0.901	B_1-N_1 (π)	1.747	12.2	$p^{1.00}$	87.8	$p^{1.00}$	
	N_1 -1.102	B_1-N_2 (σ)	1.789	31.2	$sp^{2.06}$	68.8	$sp^{2.48}$	0.998
	N_2 -1.102	B_2-N_1 (σ)	1.957	30.8	$sp^{1.18}$	69.2	$sp^{2.60}$	1.320
	N_3 -0.270	B_2-N_2 (σ)	1.957	30.8	$sp^{1.18}$	69.2	$sp^{2.60}$	1.320
	N_4 -0.270	B_2-N_2 (π)	1.751	12.3	$p^{1.00}$	87.7	$p^{1.00}$	
	C 0.235	B_1-C (σ)	1.960	34.1	$sp^{1.87}$	65.9	$sp^{1.46}$	0.861
		C-N_3 (σ)	1.982	38.1	$sp^{2.35}$	61.9	$sp^{1.89}$	1.304
		C-N_4 (σ)	1.982	38.1	$sp^{2.35}$	61.9	$sp^{1.89}$	1.304
		C-N_4 (π)	1.871	28.2	$p^{1.00}$	71.8	$p^{1.00}$	
		N_1 (LP)	1.929	-	$sp^{1.27}$	-	-	-
		N_2 (LP)	1.929	-	$sp^{1.27}$	-	-	-
		N_3 (LP)	1.486	-	$p^{1.00}$	-	-	-

**B-N represents B_1-N_1, B_1-N_2, B_2-N_1, and B_2-N_2.

Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
$ImMe_2CH_2 \cdot B_2N_2$								
C_s	B_1 0.783	B_1-N_1 (σ)	1.784	29.3	$sp^{2.12}$	70.7	$sp^{2.35}$	0.969
	B_2 0.853	B_1-N_2 (σ)	1.784	29.3	$sp^{2.16}$	70.7	$sp^{2.38}$	0.969
	N_1 -1.129	B_1-N_2 (π)	1.739	11.6	$sp^{99.99}$	88.4	$sp^{99.99}$	
	N_2 -1.129	B_2-N_1 (σ)	1.956	31.1	$sp^{1.21}$	68.9	$sp^{2.64}$	1.344
	N_3 -0.301	B_2-N_1 (π)	1.761	12.8	$sp^{99.99}$	87.2	$sp^{99.99}$	
	N_4 -0.301	B_2-N_2 (σ)	1.956	31.1	$sp^{1.20}$	68.9	$sp^{2.62}$	1.344
	$C(H_2)$ -0.738	B_1-$C(H_2)$ (σ)	1.910	32.6	$sp^{1.76}$	67.4	$sp^{2.69}$	0.801
	C 0.509	C-$C(H_2)$ (σ)	1.966	51.9	$sp^{1.55}$	48.1	$sp^{2.96}$	1.059
		C-N_3 (σ)	1.981	38.4	$sp^{2.29}$	61.6	$sp^{1.89}$	1.284
		C-N_3 (π)	1.880	26.6	$p^{1.00}$	73.4	$sp^{99.99}$	
		C-N_4 (σ)	1.981	38.4	$sp^{2.29}$	61.6	$sp^{1.89}$	1.284
		N_1 (LP)	1.928	-	$sp^{1.33}$	-	-	-
		N_2 (LP)	1.928	-	$sp^{1.33}$	-	-	-
		N_4 (LP)	1.517	-	$p^{1.00}$	-	-	-
$Me_3PCH_2 \cdot B_2N_2$								
C_s	B_1 0.769	B_1-N_1 (σ)	1.806	30.1	$sp^{1.87}$	69.9	$sp^{2.07}$	1.096
	B_2 0.860	B_1-N_2 (σ)	1.757	29.1	$sp^{2.48}$	70.9	$sp^{2.90}$	0.846
	N_1 -1.051	B_1-N_2 (π)	1.743	8.3	$p^{1.00}$	91.7	$p^{1.00}$	
	N_2 -1.202	B_2-N_1 (σ)	1.948	31.8	$sp^{1.17}$	68.2	$sp^{2.91}$	1.316
	P 1.637	B_2-N_1 (π)	1.708	13.5	$p^{1.00}$	86.5	$p^{1.00}$	
	$C(H_2)$ -1.037	B_2-N_2 (σ)	1.966	30.1	$sp^{1.21}$	69.9	$sp^{2.24}$	1.372
		B_1-$C(H_2)$ (σ)	1.956	32.1	$sp^{1.74}$	67.9	$sp^{2.36}$	0.840
		P-$C(H_2)$ (σ)	1.975	41.4	$sp^{2.69}$	58.6	$sp^{3.06}$	0.964
		N_1 (LP)	1.928	-	$sp^{1.35}$	-	-	-
		N_2 (LP)	1.932	-	$sp^{1.28}$	-	-	-

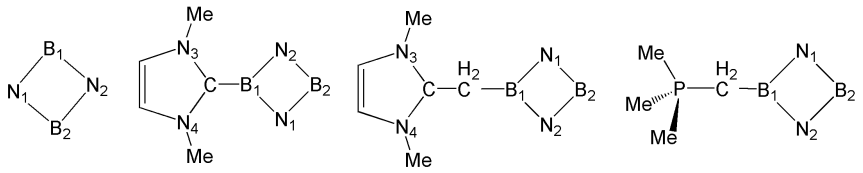


Table S6: NBO Analysis for the Di-substituted B_2N_2 Complexes at the M05-2X/cc-pVTZ Level of Theory

Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
$(ImMe_2)_2 \cdot B_2N_2$								
C_{2v}	B_1 0.676	B_1-N_1 (σ)	1.880	25.6	$sp^{1.61}$	74.4	$sp^{2.44}$	1.068
	B_2 0.676	B_1-N_1 (π)	1.643	8.8	$sp^{24.07}$	91.2	$sp^{46.22}$	
	N_1 -1.233	B_2-N_1 (σ)	1.926	28.5	$sp^{2.14}$	71.5	$sp^{2.20}$	1.068
	N_2 -1.233	B_1-C (σ)	1.962	32.0	$sp^{3.05}$	68.0	$sp^{1.38}$	0.817
	N_3 -0.291	B_2-C (σ)	1.966	32.0	$sp^{2.69}$	68.0	$sp^{1.38}$	0.817
	C 0.268	C-N_2 (σ)	1.982	37.4	$sp^{2.43}$	62.6	$sp^{1.86}$	1.300
		C-N_2 (π)	1.870	26.1	$p^{1.00}$	73.9	$p^{1.00}$	
		C-N_3 (σ)	1.982	37.4	$sp^{2.43}$	62.6	$sp^{1.86}$	1.300
		N_1 (LP)	1.917	-	$sp^{1.64}$	-	-	-
		N_3 (LP)	1.504	-	$p^{1.00}$	-	-	-

Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
$(ImMe_2CH_2)_2 \cdot B_2N_2$								
C_2	B 0.826	B-N_1 (σ)	1.927	26.7	$sp^{1.85}$	73.3	$sp^{2.06}$	1.079
	N_1 -1.300	B-N_1 (π)	1.744	13.2	$sp^{40.36}$	86.8	$sp^{67.34}$	
	N_2 -1.300	B-N_2 (σ)	1.914	26.8	$sp^{1.64}$	73.2	$sp^{2.20}$	1.028
	N_3 -0.326	B-C(H_2) (σ)	1.865	29.0	$sp^{3.05}$	71.0	$sp^{2.90}$	0.685
	N_4 -0.320	C-N_3 (σ)	1.980	38.0	$sp^{2.38}$	62.0	$sp^{1.89}$	1.246
	C(H_2) -0.756	C-N_4 (σ)	1.980	38.2	$sp^{2.34}$	61.8	$sp^{1.89}$	1.254
	C 0.527	C-N_4 (π)	1.874	24.6	$sp^{99.99}$	75.4	$sp^{99.99}$	
		C-C(H_2) (σ)	1.971	52.4	$sp^{1.46}$	47.6	$sp^{2.80}$	1.126
		N_1 (LP)	1.914	-	$sp^{1.84}$	-	-	-
		N_2 (LP)	1.914	-	$sp^{1.84}$	-	-	-
		N_3 (LP)	1.548	-	$p^{1.00}$	-	-	-
$(Me_3PCH_2)_2 \cdot B_2N_2$								
C_2	B 0.820	B-N_1 (σ)	1.932	27.0	$sp^{1.58}$	73.0	$sp^{1.88}$	1.062
	N_1 -1.328	B-N_2 (σ)	1.925	26.6	$sp^{2.02}$	73.4	$sp^{2.34}$	1.031
	N_2 -1.328	B-N_2 (π)	1.745	12.2	$sp^{46.16}$	87.8	$sp^{99.99}$	
	C(H_2) -1.058	B-C(H_2) (σ)	1.956	29.0	$sp^{2.86}$	71.0	$sp^{2.27}$	0.763
	P 1.647	P-C(H_2) (σ)	1.977	42.4	$sp^{2.51}$	57.6	$sp^{3.18}$	0.988
		N_1 (LP)	1.918	-	$sp^{1.85}$	-	-	-
		N_2 (LP)	1.918	-	$sp^{1.85}$	-	-	-

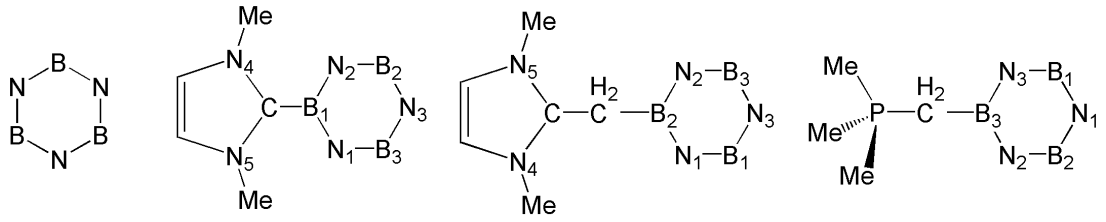
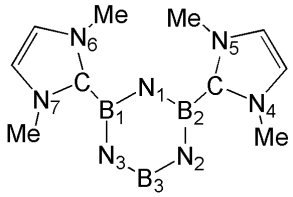


Table S7: NBO Analysis for B_3N_3 and Its Mono-substituted Complexes at the M05-2X/cc-pVTZ Level of Theory

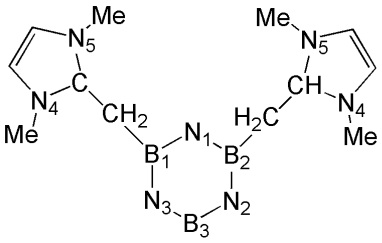
Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
B_3N_3								
D_{3h}	B 1.058	B-N (σ)	1.919	27.6	$sp^{1.01}$	72.4	$sp^{2.08}$	1.326
	N -1.508	B-N (π)	1.761	17.6	$p^{1.00}$	82.4	$p^{1.00}$	
		N (LP)	1.773	-	$sp^{1.79}$	-	-	-

Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
$ImMe_2{\cdot}B_3N_3$								
C_1	B_1 1.041	B_1-N_1 (σ)	1.981	27.6	$sp^{1.00}$	72.4	$sp^{1.51}$	1.405
	B_2 0.749	B_1-N_3 (σ)	1.917	27.4	$sp^{1.05}$	72.6	$sp^{2.04}$	1.314
	B_3 1.046	B_1-N_3 (π)	1.758	17.4	$p^{1.00}$	82.6	$p^{1.00}$	
	C 0.251	B_2-N_1 (σ)	1.902	27.3	$sp^{1.82}$	72.7	$sp^{1.91}$	1.082
	N_1 -1.171	B_2-N_1 (π)	1.738	16.2	$p^{1.00}$	83.8	$sp^{99.99}$	
	N_2 -1.178	B_2-N_2 (σ)	1.905	27.2	$sp^{1.79}$	72.8	$sp^{1.89}$	1.082
	N_3 -1.081	B_3-N_2 (σ)	1.981	27.5	$sp^{1.00}$	72.5	$sp^{1.49}$	1.398
	N_4 -0.288	B_3-N_2 (π)	1.782	18.1	$p^{1.00}$	81.9	$p^{1.00}$	
	N_5-0.289	B_3-N_3 (σ)	1.918	27.4	$sp^{1.05}$	72.6	$sp^{2.03}$	1.316
		B_2-C (σ)	1.962	31.8	$sp^{2.47}$	68.2	$sp^{1.39}$	0.837
		C-N_4 (σ)	1.982	37.5	$sp^{2.42}$	62.5	$sp^{1.85}$	1.298
		C-N_4 (π)	1.872	26.7	$p^{1.00}$	73.3	$p^{1.00}$	
		C-N_5 (σ)	1.982	37.5	$sp^{2.42}$	62.5	$sp^{1.85}$	1.297
		N_1 (LP)	1.842	-	$sp^{2.82}$	-	-	-
		N_2 (LP)	1.840	-	$sp^{2.89}$	-	-	-
		N_3 (LP)	1.789	-	$sp^{1.88}$	-	-	-
		N_5 (LP)	1.503	-	$p^{1.00}$	-	-	-
$ImMe_2CH_2 \cdot B_3N_3$								
C_1	B_1 1.031	B_1-N_1 (σ)	1.979	27.5	$sp^{1.01}$	72.5	$sp^{1.45}$	1.415
	B_2 0.863	B_1-N_1 (π)	1.806	18.0	$p^{1.00}$	82.0	$sp^{99.99}$	
	B_3 1.023	B_1-N_3 (σ)	1.919	27.4	$sp^{1.06}$	72.6	$sp^{1.99}$	1.315
	C 0.551	B_2-N_1 (σ)	1.894	25.6	$sp^{1.93}$	74.4	$sp^{1.93}$	1.022
	$C(H_2)$ -0.763	B_2-N_2(σ)	1.899	26.3	$sp^{1.77}$	73.7	$sp^{1.83}$	1.096
	N_1 -1.232	B_2-N_2 (π)	1.735	16.3	$sp^{99.99}$	83.7	$p^{1.00}$	
	N_2 -1.157	B_3-N_2 (σ)	1.977	28.0	$sp^{0.99}$	72.0	$sp^{1.56}$	1.436
	N_3 -1.097	B_3-N_3 (σ)	1.917	27.4	$sp^{1.07}$	72.6	$sp^{2.03}$	1.295
	N_4 -0.310	B_3-N_3 (π)	1.763	16.9	$p^{1.00}$	83.1	$p^{1.00}$	
	N_5 -0.318	B_2-$C(H_2)$ (σ)	1.901	29.8	$sp^{2.38}$	70.2	$sp^{2.65}$	0.749
		C-$C(H_2)$(σ)	1.975	52.2	$sp^{1.49}$	47.8	$sp^{2.78}$	1.088
		C-N_4 (σ)	1.981	37.9	$sp^{2.30}$	62.1	$sp^{1.85}$	1.275
		C-N_4 (π)	1.881	25.2	$p^{1.00}$	74.8	$sp^{99.99}$	
		C-N_5 (σ)	1.980	37.8	$sp^{2.38}$	62.2	$sp^{1.86}$	1.263
		N_1 (LP)	1.846	-	$sp^{2.91}$	-	-	-
		N_2 (LP)	1.830	-	$sp^{2.82}$	-	-	-
		N_3 (LP)	1.790	-	$sp^{1.92}$	-	-	-
		N_5 (LP)	1.539	-	$p^{1.00}$	-	-	-

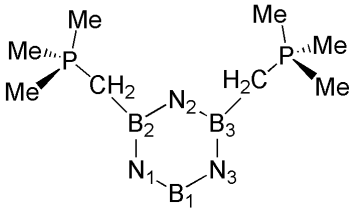
Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
$Me_3PCH_2 \cdot B_3N_3$								
C_1	B_1 1.007	B_1-N_1 (σ)	1.922	27.6	$sp^{1.11}$	72.4	$sp^{1.98}$	1.302
	B_2 1.007	B_1-N_1 (π)	1.770	17.1	$p^{1.00}$	82.9	$p^{1.00}$	
	B_3 0.690	B_1-N_3 (σ)	1.966	28.9	$sp^{1.00}$	71.1	$sp^{2.28}$	1.378
	$C(H_2)$ -1.062	B_2-N_1 (σ)	1.922	27.6	$sp^{1.11}$	72.4	$sp^{1.98}$	1.301
	P 1.658	B_2-N_2 (σ)	1.965	28.9	$sp^{1.00}$	71.1	$sp^{2.29}$	1.379
	N_1 -1.097	B_2-N_2 (π)	1.746	18.1	$p^{1.00}$	81.9	$p^{1.00}$	
	N_2 -1.076	B_3-N_2 (σ)	1.866	28.0	$sp^{1.47}$	72.0	$sp^{1.68}$	1.145
	N_3 -1.080	B_3-N_3 (σ)	1.865	28.0	$sp^{1.48}$	72.0	$sp^{1.68}$	1.143
		B_3-N_3 (π)	1.751	18.7	$sp^{99.99}$	81.3	$p^{1.00}$	
		B_3-$C(H_2)$ (σ)	1.903	28.8	$sp^{4.22}$	71.2	$sp^{2.38}$	0.689
		P-$C(H_2)$ (σ)	1.980	41.3	$sp^{2.03}$	58.7	$sp^{2.72}$	1.046
		N_1 (LP)	1.789	-	$sp^{1.99}$	-	-	-
		N_2 (LP)	1.841	-	$sp^{2.03}$	-	-	-
		N_3 (LP)	1.842	-	$sp^{2.05}$	-	-	-



$(ImMe_2)_2.B_3N_3$

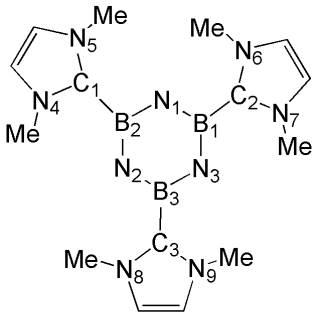


$(ImMe_2CH_2)_2.B_3N_3$

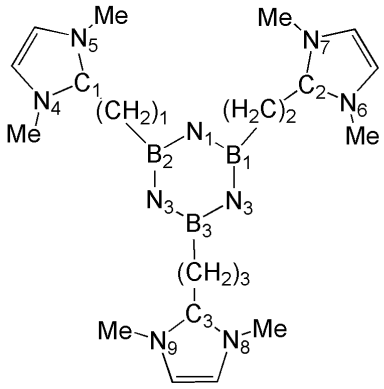


$(Me_3PCH_2)_2.B_3N_3$

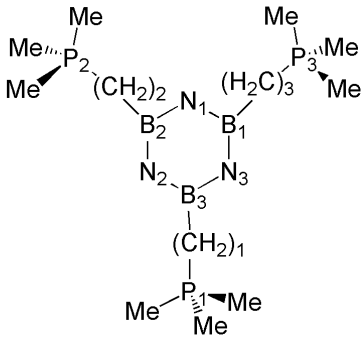
Di-substituted B_3N_3 Complexes



$(ImMe_2)_3.B_3N_3$



$(ImMe_2CH_2)_3.B_3N_3$



$(Me_3PCH_2)_3.B_3N_3$

Tri-substituted B_3N_3 Complexes

Table S8: NBO Analysis for the Di-substituted B_3N_3 Complexes at the M05-2X/cc-pVTZ Level of Theory

Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
$(ImMe_2)_2 \cdot B_3N_3$								
C_2	B_1 0.720	B_1-N_1 (σ)	1.975	27.4	$sp^{1.65}$	72.6	$sp^{1.44}$	1.163
	B_2 0.720	B_1-N_3 (σ)	1.904	27.2	$sp^{1.83}$	72.8	$sp^{1.90}$	1.088
	B_3 1.058	B_1-N_3 (π)	1.731	17.2	$p^{1.00}$	82.8	$sp^{99.99}$	
	C 0.279	B_2-N_1 (σ)	1.975	27.4	$sp^{1.65}$	72.6	$sp^{1.44}$	1.163
	N_1 -1.237	B_2-N_1 (π)	1.745	17.4	$p^{1.00}$	82.6	$p^{1.00}$	
	N_2 -1.175	B_2-N_2 (σ)	1.904	27.2	$sp^{1.83}$	72.8	$sp^{1.89}$	1.088
	N_3 -1.175	B_3-N_2 (σ)	1.978	27.0	$sp^{1.07}$	73.0	$sp^{1.46}$	1.375
	N_4 -0.301	B_3-N_2 (π)	1.753	18.1	$p^{1.00}$	81.9	$p^{1.00}$	
	N_5 -0.300	B_3-N_3 (σ)	1.978	27.0	$sp^{1.07}$	73.0	$sp^{1.46}$	1.375
	N_6 -0.300	B_1-C (σ)	1.962	30.9	$sp^{2.73}$	69.1	$sp^{1.34}$	0.823
	N_7 -0.301	C-N_4 (σ)	1.982	37.1	$sp^{2.48}$	62.9	$sp^{1.84}$	1.290
		C-N_4 (π)	1.869	25.4	$p^{1.00}$	74.6	$p^{1.00}$	
		C-N_5 (σ)	1.982	37.1	$sp^{2.46}$	62.9	$sp^{1.83}$	1.293
		C-N_6 (σ)	1.982	37.1	$sp^{2.46}$	62.9	$sp^{1.83}$	1.293
		C-N_6 (π)	1.872	25.4	$p^{1.00}$	74.6	$p^{1.00}$	
		C-N_7 (σ)	1.982	37.1	$sp^{2.48}$	62.9	$sp^{1.84}$	1.290
		N_1 (LP)	1.867	-	$sp^{4.44}$	-	-	-
		N_2 (LP)	1.852	-	$sp^{2.97}$	-	-	-
		N_3 (LP)	1.852	-	$sp^{2.97}$	-	-	-
		N_5 (LP)	1.515	-	$p^{1.00}$	-	-	-
		N_7 (LP)	1.513	-	$p^{1.00}$	-	-	-

Species	NBO Charge	Bond (A-B)	Occ	(A) %	Hyb (A)	B (%)	Hyb (B)	WBI
$(ImMe_2CH_2)_2 \cdot B_3N_3$								
C_2	B_1 0.861	B_1-N_1 (σ)	1.971	26.2	$sp^{1.65}$	73.8	$sp^{1.41}$	1.153
	B_2 0.861	B_1-N_1 (π)	1.762	16.2	$sp^{99.99}$	83.8	$p^{1.00}$	
	B_3 1.058	B_1-N_3 (σ)	1.902	25.7	$sp^{1.83}$	74.3	$sp^{1.86}$	1.053
	$C(H_2)$ -0.749	B_2-N_1 (σ)	1.971	26.2	$sp^{1.65}$	73.8	$sp^{1.41}$	1.153
	C 0.525	B_2-N_2 (σ)	1.902	25.7	$sp^{1.83}$	74.3	$sp^{1.86}$	1.053
	N_1 -1.308	B_2-N_2 (π)	1.745	15.4	$sp^{99.99}$	84.6	$p^{1.00}$	
	N_2 -1.235	B_3-N_2 (σ)	1.974	27.0	$sp^{1.09}$	73.0	$sp^{1.45}$	1.373
	N_3 -1.235	B_3-N_3 (σ)	1.974	27.0	$sp^{1.09}$	73.0	$sp^{1.45}$	1.373
	N_4 -0.318	B_3-N_3 (π)	1.784	17.4	$p^{1.00}$	82.6	$p^{1.00}$	
	N_5 -0.320	B_1-$C(H_2)$ (σ)	1.875	28.4	$sp^{2.73}$	71.6	$sp^{2.70}$	0.702
		C-$C(H_2)$ (σ)	1.972	52.6	$sp^{1.46}$	47.4	$sp^{2.89}$	1.111
		C-N_4 (σ)	1.981	38.1	$sp^{2.35}$	61.9	$sp^{1.88}$	1.259
		C-N_4 (π)	1.877	24.8	$sp^{99.99}$	75.2	$p^{1.00}$	
		C-N_5 (σ)	1.981	38.1	$sp^{2.37}$	61.9	$sp^{1.88}$	1.256
		N_1 (LP)	1.867	-	$sp^{4.74}$	-	-	-
		N_2 (LP)	1.848	-	$sp^{3.05}$	-	-	-
		N_3 (LP)	1.848	-	$sp^{3.05}$	-	-	-
		N_5 (LP)	1.544	-	$sp^{1.00}$	-	-	-
$(Me_3PCH_2)_2 \cdot B_3N_3$								
C_1	B_1 1.055	B_1-N_1 (σ)	1.976	27.5	$sp^{1.07}$	72.5	$sp^{1.30}$	1.443
	B_2 0.839	B_1-N_1 (π)	1.781	18.9	$p^{1.00}$	81.1	$p^{1.00}$	
	B_3 0.849	B_1-N_3 (σ)	1.976	26.5	$sp^{1.10}$	73.5	$sp^{1.42}$	1.309
	$C(H_2)_1$ -1.051	B_2-N_1 (σ)	1.895	26.6	$sp^{1.79}$	73.4	$sp^{1.89}$	1.075
	$C(H_2)_2$ -1.053	B_2-N_2 (σ)	1.973	26.4	$sp^{1.74}$	73.6	$sp^{1.51}$	1.126
	P_1 1.644	B_2-N_2 (π)	1.764	15.5	$p^{1.00}$	84.4	$p^{1.00}$	
	P_2 1.646	B_3-N_2 (σ)	1.974	26.5	$sp^{1.62}$	73.5	$sp^{1.31}$	1.173
	N_1 -1.165	B_3-N_3 (σ)	1.908	25.6	$sp^{1.90}$	74.4	$sp^{1.87}$	1.035
	N_2 -1.318	B_3-N_3 (π)	1.772	14.6	$p^{1.00}$	85.4	$p^{1.00}$	
	N_3 -1.298	B_2-$C(H_2)_1$ (σ)	1.951	28.1	$sp^{2.62}$	71.9	$sp^{2.18}$	0.763
		B_3-$C(H_2)_2$ (σ)	1.953	27.9	$sp^{2.67}$	72.1	$sp^{2.13}$	0.762
		P_1-$C(H_2)_1$ (σ)	1.979	42.7	$sp^{2.43}$	57.3	$sp^{3.19}$	0.995
		P_2-$C(H_2)_2$ (σ)	1.980	38.4	$sp^{3.68}$	61.6	$sp^{2.59}$	1.000
		N_1 (LP)	1.839	-	$sp^{2.96}$	-	-	-
		N_2 (LP)	1.870	-	$sp^{4.87}$	-	-	-
		N_3 (LP)	1.858	-	$sp^{3.12}$	-	-	-

Table S9: NBO Analysis for the Tri-substituted B_3N_3 Complexes at the M05-2X/cc-pVTZ Level of Theory

Species	NBO Charge	Bond (A-B)	Occ	(A) %	Hyb (A)	B (%)	Hyb (B)	WBI
$(ImMe_2)_3 \cdot B_3N_3$								
C_2	B_1 0.757	B_1-N_1 (σ)	1.972	26.7	$sp^{1.64}$	73.3	$sp^{1.43}$	1.141
	B_2 0.757	B_1-N_3 (σ)	1.971	26.9	$sp^{1.63}$	73.1	$sp^{1.46}$	1.144
	B_3 0.748	B_1-N_3 (π)	1.722	17.7	$p^{1.00}$	82.3	$sp^{99.99}$	
	C_1 0.292	B_2-N_1 (σ)	1.972	26.7	$sp^{1.64}$	73.3	$sp^{1.43}$	1.141
	C_2 0.292	B_2-N_1 (π)	1.731	17.5	$sp^{99.99}$	82.5	$p^{1.00}$	
	C_3 0.311	B_2-N_2 (σ)	1.971	26.8	$sp^{1.63}$	73.2	$sp^{1.46}$	1.144
	N_1 -1.248	B_3-N_2 (σ)	1.970	26.7	$sp^{1.62}$	73.3	$sp^{1.42}$	1.148
	N_2 -1.238	B_3-N_2 (π)	1.729	18.1	$sp^{99.99}$	81.9	$sp^{99.99}$	
	N_3 -1.238	B_3-N_3 (σ)	1.970	26.7	$sp^{1.62}$	73.3	$sp^{1.42}$	1.148
	N_4 -0.310	B_1-C_2 (σ)	1.958	29.4	$sp^{3.15}$	70.6	$sp^{1.30}$	0.797
	N_5 -0.310	B_2-C_1 (σ)	1.959	29.4	$sp^{3.14}$	70.6	$sp^{1.30}$	0.797
	N_6 -0.310	B_3-C_3 (σ)	1.957	29.5	$sp^{3.20}$	70.5	$sp^{1.30}$	0.792
	N_7 -0.310	C_1-N_4 (σ)	1.981	36.8	$sp^{2.51}$	63.2	$sp^{1.81}$	1.286
	N_8 -0.316	C_1-N_5 (σ)	1.982	36.8	$sp^{2.52}$	63.2	$sp^{1.80}$	1.286
	N_9 -0.316	C_1-N_5 (π)	1.870	24.5	$p^{1.00}$	75.5	$p^{1.00}$	
		C_2-N_6 (σ)	1.982	36.8	$sp^{2.52}$	63.2	$sp^{1.80}$	1.286
		C_2-N_6 (π)	1.870	24.5	$p^{1.00}$	75.5	$p^{1.00}$	
		C_2-N_7 (σ)	1.981	36.8	$sp^{2.51}$	63.2	$sp^{1.81}$	1.286
		C_3-N_8 (σ)	1.981	36.7	$sp^{2.51}$	63.3	$sp^{1.81}$	1.286
		C_3-N_8 (π)	1.871	23.9	$p^{1.00}$	76.1	$p^{1.00}$	
		C_3-N_9 (σ)	1.982	36.7	$sp^{2.51}$	63.3	$sp^{1.81}$	1.286
		N_1 (LP)	1.867	-	$sp^{4.56}$	-	-	-
		N_2 (LP)	1.873	-	$sp^{4.48}$	-	-	-
		N_3 (LP)	1.873	-	$sp^{4.48}$	-	-	-
		N_4 (LP)	1.523	-	$p^{1.00}$	-	-	-
		N_7 (LP)	1.523	-	$p^{1.00}$	-	-	-
		N_9 (LP)	1.529	-	$p^{1.00}$	-	-	-

Species	NBO Charge	Bond (A-B)	Occ	(A) %	Hyb (A)	B (%)	Hyb (B)	WBI
$(ImMe_2CH_2)_3 \cdot B_3N_3$								
C_1	B_1 0.904	B_1-N_1 (σ)	1.967	25.3	$sp^{1.60}$	74.7	$sp^{1.38}$	1.135
	B_2 0.909	B_1-N_1 (π)	1.761	16.4	$sp^{99.99}$	83.6	$sp^{99.99}$	
	B_3 0.909	B_1-N_3 (σ)	1.964	25.5	$sp^{1.60}$	74.5	$sp^{1.43}$	1.121
	$C(H_2)_1$ -0.750	B_2-N_1 (σ)	1.966	25.4	$sp^{1.59}$	74.6	$sp^{1.41}$	1.124
	$C(H_2)_2$ -0.750	B_2-N_2 (σ)	1.966	25.3	$sp^{1.58}$	74.7	$sp^{1.38}$	1.137
	$C(H_2)_3$ -0.751	B_2-N_2 (π)	1.758	16.4	$sp^{99.99}$	83.6	$sp^{99.99}$	
	C_1 0.525	B_3-N_2 (σ)	1.966	25.3	$sp^{1.57}$	74.7	$sp^{1.41}$	1.126
	C_2 0.524	B_3-N_3 (σ)	1.966	25.3	$sp^{1.57}$	74.7	$sp^{1.37}$	1.145
	C_3 0.527	B_3-N_3 (π)	1.760	16.7	$sp^{99.99}$	83.3	$sp^{99.99}$	
	N_1 -1.332	B_1-$C(H_2)_2$ (σ)	1.842	26.4	$sp^{3.36}$	73.6	$sp^{2.89}$	0.642
	N_2 -1.331	B_2-$C(H_2)_1$ (σ)	1.835	26.2	$sp^{3.44}$	73.8	$sp^{2.96}$	0.633
	N_3 -1.326	B_3-$C(H_2)_3$ (σ)	1.824	25.9	$sp^{3.54}$	74.1	$sp^{3.06}$	0.620
	N_4 -0.331	C_1-$C(H_2)_1$ (σ)	1.973	52.8	$sp^{1.42}$	47.2	$sp^{2.78}$	1.154
	N_5 -0.327	C_2-$C(H_2)_2$ (σ)	1.973	52.8	$sp^{1.43}$	47.2	$sp^{2.81}$	1.145
	N_6 -0.325	C_3-$C(H_2)_3$ (σ)	1.974	52.8	$sp^{1.41}$	47.2	$sp^{2.72}$	1.167
	N_7 -0.328	C_1-N_4 (σ)	1.980	38.0	$sp^{2.42}$	62.0	$sp^{1.88}$	1.232
	N_8 -0.334	C_1-N_5 (σ)	1.980	38.1	$sp^{2.39}$	61.9	$sp^{1.88}$	1.238
	N_9 -0.333	C_1-N_5 (π)	1.873	23.8	$sp^{99.99}$	76.2	$sp^{99.99}$	
		C_2-N_6 (σ)	1.980	38.1	$sp^{2.39}$	61.9	$sp^{1.88}$	1.242
		C_2-N_6 (π)	1.874	24.0	$sp^{99.99}$	76.0	$sp^{99.99}$	
		C_2-N_7 (σ)	1.980	38.1	$sp^{2.40}$	61.9	$sp^{1.88}$	1.238
		C_3-N_8 (σ)	1.980	38.0	$sp^{2.41}$	62.0	$sp^{1.88}$	1.230
		C_3-N_8 (π)	1.873	23.3	$sp^{99.99}$	76.7	$sp^{99.99}$	
		C_3-N_9 (σ)	1.980	38.0	$sp^{2.42}$	62.0	$sp^{1.88}$	1.230
		N_1 (LP)	1.866	-	$sp^{4.96}$	-	-	-
		N_2 (LP)	1.867	-	$sp^{4.97}$	-	-	-
		N_3 (LP)	1.869	-	$sp^{4.91}$	-	-	-
		N_4 (LP)	1.561	-	$p^{1.00}$	-	-	-
		N_7 (LP)	1.556	-	$p^{1.00}$	-	-	-
		N_9 (LP)	1.561	-	$p^{1.00}$	-	-	-

Species	NBO Charge	Bond A-B	Occ	(A) %	Hyb (A)	(B) %	Hyb (B)	WBI
$(Me_3PCH_2)_3 \cdot B_3N_3$								
C_1	B_1 0.871	B_1-N_1 (σ)	1.968	25.3	$sp^{1.61}$	74.7	$sp^{1.32}$	1.149
	B_2 0.854	B_1-N_3 (σ)	1.969	24.8	$sp^{1.66}$	75.2	$sp^{1.29}$	1.118
	B_3 0.869	B_1-N_3 (π)	1.781	16.3	$sp^{99.99}$	83.7	$sp^{99.99}$	
	$C(H_2)_1$ -1.070	B_2-N_1 (σ)	1.966	25.2	$sp^{1.69}$	74.8	$sp^{1.43}$	1.099
	$C(H_2)_2$ -1.051	B_2-N_1 (π)	1.745	16.0	$sp^{99.99}$	84.0	$sp^{99.99}$	
	$C(H_2)_3$ -1.052	B_2-N_2 (σ)	1.966	25.7	$sp^{1.62}$	74.3	$sp^{1.38}$	1.164
	P_1 1.645	B_3-N_2 (σ)	1.966	26.0	$sp^{1.57}$	74.0	$sp^{1.36}$	1.201
	P_2 1.645	B_3-N_2 (π)	1.740	18.7	$sp^{99.99}$	81.3	$sp^{99.99}$	
	P_3 1.643	B_3-N_3 (σ)	1.967	25.0	$sp^{1.66}$	75.0	$sp^{1.47}$	1.072
	N_1 -1.341	B_1-$C(H_2)_3$ (σ)	1.924	26.0	$sp^{3.21}$	74.0	$sp^{2.22}$	0.704
	N_2 -1.260	B_2-$C(H_2)_2$ (σ)	1.928	26.4	$sp^{3.12}$	73.6	$sp^{2.21}$	0.713
	N_3 -1.381	B_3-$C(H_2)_1$ (σ)	1.931	25.7	$sp^{3.29}$	74.3	$sp^{2.22}$	0.700
		P_1-$C(H_2)_1$ (σ)	1.978	43.5	$sp^{2.32}$	56.5	$sp^{3.24}$	1.024
		P_2-$C(H_2)_2$ (σ)	1.971	43.1	$sp^{2.37}$	56.9	$sp^{3.51}$	1.014
		P_3-$C(H_2)_3$ (σ)	1.972	43.3	$sp^{2.34}$	56.7	$sp^{3.54}$	1.019
		N_1 (LP)	1.872	-	$sp^{5.24}$	-	-	-
		N_2 (LP)	1.871	-	$sp^{5.22}$	-	-	-
		N_3 (LP)	1.870	-	$sp^{5.17}$	-	-	-

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.

ImMe$_2$ C_{2v} **M05-2X**= -304.8704604			
C	-0.00000500	-0.97321900	0.00000000
C	-0.00000300	1.20631500	0.67382200
C	-0.00000300	1.20631500	-0.67382200
H	-0.00001300	2.01808300	1.37515700
H	-0.00001300	2.01808300	-1.37515700
N	-0.00000300	-0.12043200	1.05485000
N	-0.00000300	-0.12043200	-1.05485000
C	0.00000600	-0.56932200	2.42963000
H	-0.00004300	-1.65192800	2.41233400
H	0.88655000	-0.21276100	2.94804100
H	-0.88648300	-0.21267500	2.94807500
C	0.00000600	-0.56932200	-2.42963000
H	0.88655000	-0.21276100	-2.94804100
H	-0.00004300	-1.65192800	-2.41233400
H	-0.88648300	-0.21267500	-2.94807500

ImMe$_2$CH$_2$ C_{2v} **M05-2X** = -344.2017065			
C	-0.00001100	-1.54125200	0.66984000
C	-0.00001100	-1.54125200	-0.66984000
H	-0.00001300	-2.35639200	1.36532200
H	-0.00001300	-2.35639200	-1.36532200
N	-0.00001100	-0.21756400	1.09248300
N	-0.00001100	-0.21756400	-1.09248300
C	0.00001000	0.26987000	2.44048000
H	-0.88401000	0.87981500	2.62573300
H	0.00000900	-0.57440300	3.12134800
H	0.88404200	0.87980500	2.62571600
C	0.00001000	0.26987000	-2.44048000
H	0.00000900	-0.57440300	-3.12134800
H	-0.88401000	0.87981500	-2.62573300
H	0.88404200	0.87980500	-2.62571600
C	-0.00000300	0.62366700	0.00000000
C	0.00001900	1.97674100	0.00000000
H	0.00000000	2.52119400	-0.92585200
H	0.00000000	2.52119400	0.92585200

$\mathbf{Me_3PCH_2}$ C_s **M05-2X** =-500.4034220			
P	-0.12512900	0.00001100	-0.08571600
C	0.05849300	-1.46477200	0.97233500
H	1.04079500	-1.48946400	1.43597000
H	-0.06850900	-2.34987600	0.35415700
H	-0.71935900	-1.44939500	1.72826400
C	1.47600300	-0.00013100	-1.00670300
H	1.50643600	-0.88196800	-1.64151800
H	2.33494900	-0.00017300	-0.33817300
H	1.50656500	0.88166000	-1.64157500
C	0.05874300	1.46477500	0.97232000
H	-0.71911100	1.44953300	1.72825000
H	1.04104900	1.48931400	1.43595400
C	-1.60776400	0.00013000	-0.85889300
H	-1.94522000	0.92302400	-1.30207400
H	-1.94539400	-0.92273200	-1.30200800
H	-0.06811800	2.34989300	0.35413300

BN (singlet) $C_{\infty v}$ **M05-2X** = -79.3899541			
B	0.00000000	0.00000000	-0.73565100
N	0.00000000	0.00000000	0.52546500

BN (triplet) $C_{\infty v}$ **M05-2X** = -79.4244890			
B	0.00000000	0.00000000	-0.76690500
N	0.00000000	0.00000000	0.54779000

ImMe$_2$·BN C_{2v} **M05-2X** = -384.4901216			
B	0.00112600	-1.83909100	-0.00001300
N	0.00190400	-3.08769800	0.00000200
C	0.00019200	-0.32251300	-0.00000200
C	-0.67697700	1.79593700	-0.00001400
C	0.67478000	1.79675900	0.00001100
H	-1.37785900	2.60660300	-0.00003200
H	1.37467900	2.60827400	0.00001900
N	-1.07578800	0.48169800	-0.00001000
N	1.07519300	0.48300900	0.00000300
C	-2.44686300	-0.00266100	0.00001300
H	-2.40819600	-1.08728300	-0.00005500
H	-2.95843800	0.34967300	0.88956400
H	-2.95850200	0.34978100	-0.88945900
C	2.44685800	0.00031700	0.00000200
H	2.95804300	0.35335200	0.88950000
H	2.40951200	-1.08435200	0.00002400
H	2.9580300	0.35330600	-0.88952200

ImMe$_2$CH$_2$· BN C_1 **M05-2X** = -423.7965637			
B	2.15726600	-0.92697300	-0.10734500
N	3.44042800	-0.86090200	-1.02777200
C	-1.27615300	1.65111600	-0.41468200
C	-2.09949400	0.59464500	-0.54020600
H	-1.49477100	2.66473300	-0.67877500
H	-3.09850500	0.60697700	-0.92327100
N	-0.02100500	1.14712300	0.15367600
N	-1.36515000	-0.57763400	-0.05114800
C	1.16774100	1.95474500	0.46289600
H	2.04561500	1.35205400	0.35755400
H	1.22105800	2.78370400	-0.21156800
H	1.10184000	2.31628200	1.46784200
C	-1.87879100	-1.95414900	-0.00127700
H	-2.58523000	-2.10017500	-0.79158900
H	-1.06733700	-2.64206100	-0.11657700
H	-2.35770100	-2.12220800	0.94069700
C	-0.14172400	-0.17968800	0.34423600
C	0.81866100	-0.98830100	0.85454700
H	0.45426000	-1.99354300	0.89498100
H	1.07309100	-0.66120400	1.84105400

$\mathbf{Me_3PCH_2}\cdot$ **BN** C_s **M05-2X** = -580.0255700			
B	1.94523500	-0.67611700	-0.00000400
N	2.70518000	0.31769000	0.00000200
P	-0.51565000	-0.01320300	0.00000000
C	-0.22888600	0.98888400	-1.46541600
H	-0.88513800	1.85473200	-1.44564200
H	-0.42741100	0.39559000	-2.35402300
H	0.82058400	1.27806900	-1.43241900
C	-2.26284800	-0.50602300	-0.00000900
H	-2.46904400	-1.10075300	-0.88552000
H	-2.90025700	0.37369200	0.00000100
H	-2.46904700	-1.10077500	0.88548700
C	-0.22889200	0.98885600	1.46543600
H	-0.88515000	1.85470000	1.44567800
H	-0.42741400	0.39554400	2.35403100
C	0.57592100	-1.43812700	-0.00001100
H	0.38142300	-2.03780800	0.88704600
H	0.38142600	-2.03779100	-0.88708000
H	0.82057500	1.27805000	1.43244500

BNBN (singlet) C_s **M05-2X** = -159.03113210			
B	-0.14875900	-2.00519200	0.00000000
N	0.33418800	-0.76360800	0.00000000
B	0.00000000	0.51117300	0.00000000
N	-0.22793100	1.83076400	0.00000000

BNBN (triplet) C_s **M05-2X** =-159.10314930			
B	-0.00676900	-2.05607100	0.00000000
N	0.02585800	-0.80231300	0.00000000
B	0.00000000	0.56028900	0.00000000
N	-0.02102400	1.87072900	0.00000000

ImMe$_2$· BNBN C_{2v} **M05-2X** = -464.1080049			
B	-1.01100900	0.00001500	0.00000000
N	-2.25066600	0.00001500	0.00000000
B	-3.65379400	0.00001000	0.00000000
N	-4.91314000	0.00000100	-0.00000100
C	0.49864600	0.00000200	-0.00000200
C	2.60953600	0.67684000	0.00002200
C	2.60952500	-0.6768680	-0.00002500
H	3.42154200	1.37641800	0.00003600
H	3.42152000	-1.37645900	-0.00004200
N	1.29950400	1.07936200	0.00004400
N	1.29948700	-1.07937000	-0.00004900
C	0.82588200	2.45717000	-0.00001600
H	-0.25862400	2.44163900	0.00075500
H	1.18450200	2.96345600	0.88944700
H	1.18322900	2.96298500	-0.89026300
C	0.82584100	-2.45717000	0.00002500
H	1.18307000	-2.96294700	0.89034100
H	-0.25866400	-2.44161900	-0.00087800
H	1.18456200	-2.96350500	-0.88936900

ImMe$_2$CH$_2$· BNBN C_1 **M05-2X** = -503.4346098			
B	-0.66374500	-1.96084900	0.08929300
N	-1.54969300	-1.64144300	-0.72417900
B	-2.19058000	-0.45533900	-1.20035400
N	-2.54569700	0.74557400	-1.34587900
C	0.26166900	1.87690500	0.06276300
C	1.38566900	1.51376100	-0.58749000
H	-0.33418000	2.76471800	0.00494300
H	1.99348300	2.03996700	-1.29459600
N	-0.12405700	0.81168500	0.83487000
N	1.65665500	0.21271700	-0.22008800
C	-1.39102100	0.78155500	1.56458200
H	-1.45364400	-0.13794000	2.13258900
H	-1.41736900	1.63098300	2.23837500
H	-2.17625000	0.82924400	0.79713400
C	2.69728600	-0.62303700	-0.79304300
H	3.31438900	0.00077800	-1.42730800
H	3.31333400	-1.05156800	-0.00975800
H	2.24939900	-1.40971200	-1.39326400
C	0.71858300	-0.19950200	1.05985600
C	0.50892800	-1.61734200	1.05985600
H	1.41407900	-2.19658600	0.91687000
H	0.22124500	-1.68271500	2.10520800

$\mathbf{Me_3PCH_2}\cdot$ **BNBN** C_s **M05-2X** = -659.6660397			
B	-0.90537200	-1.69545700	-0.00002100
N	-2.04402200	-1.19040900	-0.00000800
B	-2.57585400	0.13201900	0.00000300
N	-2.60779200	1.39322600	0.00001000
P	0.97135100	0.09612400	-0.00000500
C	2.76795600	0.32084300	0.00000200
H	2.98683200	1.38515600	0.00004900
H	3.19588800	-0.13495800	-0.88833000
H	3.19588500	-0.13503300	0.88829700
C	0.24118900	0.85693800	-1.44925600
H	0.33514200	0.20707100	-2.31426600
H	0.74846600	1.80054500	-1.63552300
H	-0.82098700	1.05756700	-1.19486900
C	0.24119200	0.85689300	1.44927500
H	0.33506600	0.20694600	2.31423500
H	0.74852700	1.80044800	1.63564000
C	0.63726900	-1.70204400	-0.00001300
H	1.08455600	-2.14275300	-0.88777500
H	1.08452500	-2.14273800	0.88777300
H	-0.82096500	1.05759000	1.19487400

$\mathbf{B_2N_2}$ **(singlet)** D_{2h} **M05-2X**=-159.0836566			
N	0.00000000	0.00000000	1.17746900
N	0.00000000	0.00000000	-1.17746900
B	0.00000000	0.74170900	0.00000000
B	0.00000000	-0.74170900	0.00000000

$\mathbf{B_2N_2}$ **(triplet)** D_{2h} **M05-2X**=-159.1046768			
N	1.17737800	-0.00000300	0.00000200
N	-1.17737900	-0.00000100	0.00000200
B	0.00000300	0.79744800	-0.00000300
B	-0.00000100	-0.79744100	-0.00000300

$\mathbf{ImMe_2{\cdot}B_2N_2}$ C_{2v} **M05-2X** = -464.1424308			
N	2.31469300	-1.20050300	-0.00045100
N	2.31509500	1.20010800	0.00038400
B	1.43148000	-0.00011600	0.00003500
B	2.97635500	-0.00028500	-0.00005900
C	-0.12882500	-0.00000200	0.00007900
C	-2.23460000	-0.67771900	-0.00001200
C	-2.23446400	0.67818100	-0.00011300
H	-3.04411500	-1.38016500	0.00001300
H	-3.04380500	1.38082800	-0.00024700
N	-0.92709500	-1.07557500	0.00009200
N	-0.92686000	1.07573200	-0.00004700
C	-0.46955300	-2.46497700	0.00015400
H	0.61768800	-2.45250500	0.00003700
H	-0.85024700	-2.95659300	0.88919400
H	-0.85042200	-2.95671900	-0.88873900
C	-0.46893400	2.46502100	-0.00007300
H	-0.84952600	2.95679100	0.88893300
H	0.61832500	2.45220100	-0.00011400
H	-0.84965200	2.95680200	-0.88901600

$\mathbf{ImMe_2CH_2{\cdot}B_2N_2}$ C_s **M05-2X**= -503.4583931			
N	2.26958100	-1.20178900	0.51897800
N	2.26956200	1.20179400	0.51897400
B	1.81790400	0.00000900	-0.24832100
B	2.61608200	0.00000200	1.07907100
C	-2.12170400	-0.67544900	0.73444500
C	-2.12170200	0.67543500	0.73445800
H	-2.74150000	-1.37884300	1.25228300
H	-2.74149900	1.37882400	1.25230100
N	-1.10556500	-1.07824700	-0.09979900
N	-1.10556200	1.07824100	-0.09978000
C	-0.61789200	-2.44393700	-0.28025400
H	0.43243900	-2.46317700	0.01256900
H	-1.20459200	-3.09040100	0.36089900
H	-0.74666200	-2.74628800	-1.31474100
C	-0.61790800	2.44393600	-0.28025300
H	-1.20464500	3.09040700	0.36085800
H	0.43241500	2.46320200	0.01259900
H	-0.74664900	2.74625300	-1.31475500
C	-0.49886700	0.00000100	-0.59964800
C	0.72637400	0.00000700	-1.40918000
H	0.78241500	0.89354200	-2.02089000
H	0.78242300	-0.89352300	-2.02089600

$\mathbf{Me_3PCH_2}\cdot\ \mathbf{B_2N_2}$ C_s **M05-2X** = -659.6811466			
N	-3.04025700	-0.90284600	-0.00000400
N	-1.71941700	1.10989700	0.00000300
B	-1.65993800	-0.43900400	-0.00000200
B	-2.91804000	0.46821800	0.00000100
P	1.05778100	-0.04490500	-0.00000100
C	2.64881700	-0.91137900	-0.00000200
H	3.46238300	-0.19125300	0.00001400
H	2.72021800	-1.53668600	-0.88551200
H	2.72020500	-1.53668600	0.88549100
C	0.98957200	0.98605500	-1.47003100
H	1.04995300	0.35609500	-2.35357000
H	1.81824800	1.68889100	-1.46092100
H	0.02706900	1.49523100	-1.42461200
C	0.98957200	0.98604900	1.47003400
H	1.04995500	0.35608400	2.35357100
H	1.81824800	1.68888500	1.46092600
C	-0.28344800	-1.22886700	0.00000000
H	-0.20977200	-1.86438900	-0.88082800
H	-0.20977300	-1.86437900	0.88083600
H	0.02706900	1.49522500	1.42461800

$(ImMe_2)_2 \cdot B_2N_2$ C_{2v} **M05-2X** = -769.0983332			
N	-0.00012100	1.17474800	0.82521300
N	0.00012100	-1.17474300	0.82521800
B	0.83288500	0.00007600	0.67676200
B	-0.83288400	-0.00007200	0.67675900
C	2.33791800	0.00018300	0.11821500
C	4.34045600	0.67737700	-0.56790900
C	4.34085100	-0.67675600	-0.56700700
H	5.10460300	1.38064500	-0.83327700
H	5.10541500	-1.37992900	-0.83142500
N	3.09905000	1.07199000	-0.14201400
N	3.09967100	-1.07152500	-0.14060300
C	2.65060400	2.45175800	0.01821600
H	1.59744700	2.40783500	0.30280000
H	3.24552500	2.93201400	0.78913200
H	2.77867700	2.97397100	-0.92510800
C	2.65204700	-2.45134400	0.02148800
H	3.24732800	-2.93022400	0.79298300
H	1.59888000	-2.40768900	0.30604800
H	2.78034300	-2.97473100	-0.92115400
C	-2.33791800	-0.00018200	0.11821300
C	-4.34085300	0.67675300	-0.56700500
C	-4.34045700	-0.67738000	-0.56790400
H	-5.10541900	1.37992400	-0.83142100
H	-5.10460400	-1.38064900	-0.83326900
N	-3.09967300	1.07152400	-0.14060500
N	-3.09904900	-1.07199100	-0.14201300
C	-2.65205100	2.45134300	0.02148500
H	-1.59888300	2.40769100	0.30604000
H	-2.78035200	2.97473100	-0.92115700
H	-3.24733000	2.93022200	0.79298300
C	-2.65059800	-2.45175700	0.01821300
H	-2.77865800	-2.97396600	-0.92511600
H	-1.59744400	-2.40783200	0.30280800
H	-3.24552700	-2.93202200	0.78911900

$(\mathbf{ImMe_2CH_2})_2 \cdot \mathbf{B_2N_2}$ C_2			
M05-2X = -847.7155778			
N	-0.56020900	-2.04895100	-1.03785800
N	0.56019500	-2.04903600	1.03777400
B	0.73249000	-1.98315500	-0.40715700
B	-0.73250020	-1.98316700	0.40707800
C	1.68926500	2.03364900	-0.55347600
C	2.41333700	1.69536600	0.53427400
H	1.26985300	2.97147300	-0.85645100
H	2.74653400	2.28157600	1.36685100
N	1.55595000	0.89536400	-1.31895200
N	2.71873400	0.35688200	0.41909800
C	0.72079400	0.71783100	-2.50045100
H	0.08793500	-0.15869000	-2.33140800
H	0.11241800	1.60830300	-2.61298900
H	1.34271000	0.58749300	-3.38183800
C	3.29727700	-0.50048100	1.44828700
H	3.51233300	0.11779700	2.31260600
H	2.54958000	-1.26258000	1.68587400
H	4.21996800	-0.94150700	1.08244500
C	2.19079000	-0.12039100	-0.71517100
C	2.15139200	-1.49938100	-1.13262600
H	2.97781900	-2.06697400	-0.72062200
H	2.08357000	-1.60307700	-2.20901800
C	-2.41334200	1.69538900	-0.53421200
C	-1.68924800	2.03363200	0.55353500
H	-2.74654900	2.28162700	-1.36676500
H	-1.26982400	2.97144400	0.85653300
N	-2.71875400	0.35690500	-0.41906900
N	-1.55593200	0.89532300	1.31897600
C	-3.29730500	-0.50042400	-1.44828200
H	-4.21997100	-0.94149500	-1.08243000
H	-3.51241100	0.11789000	-2.31256200
H	-2.54959500	-1.26249200	-1.68592700
C	-0.72075500	0.71774900	2.50045300
H	-0.11235700	1.60820500	2.61299400
H	-1.34265400	0.58740600	3.38185200
H	-0.08791800	-0.15878200	2.33138100
C	-2.19079200	-0.12040800	0.71517500
C	-2.15139300	-1.49941100	1.13258500
H	-2.97782700	-2.06699000	0.72057600
H	-2.08354900	-1.60314500	2.20897100

$(Me_3PCH_2)_2 \cdot B_2N_2$ C_2			
M05-2X = -1160.1654385			
N	0.63123900	-0.98919900	-0.35818800
N	-0.63123800	0.98918700	-0.35820700
B	-0.71011400	-0.46418500	-0.26669200
B	0.71011300	0.46417500	-0.26670400
P	-3.38803100	-0.04315200	0.07223200
C	-5.03133200	-0.77955700	0.32320200
H	-5.79208800	-0.00309800	0.32733500
H	-5.04936200	-1.30852300	1.27199100
H	-5.23732300	-1.48276700	-0.47896300
C	-3.12352400	1.13484500	1.40411500
H	-3.09876400	0.60681500	2.35390300
H	-3.92040400	1.87408400	1.40951200
H	-2.14774500	1.57112600	1.16955200
C	-3.43817600	0.84699400	-1.48939500
H	-3.59429400	0.14073000	-2.30077900
H	-4.24270200	1.57763100	-1.47304600
C	-2.10545000	-1.27146000	0.05230200
H	-2.05661100	-1.77324100	1.01733100
H	-2.31304000	-2.01235600	-0.71845900
H	-2.45125300	1.31193700	-1.56237000
P	3.38803100	0.04315600	0.07223000
C	5.03133700	0.77955900	0.32317400
H	5.79209000	0.00309700	0.32730300
H	5.04938500	1.30853500	1.27195600
H	5.23731800	1.48276000	-0.47900200
C	3.12350300	-1.13477300	1.40417000
H	3.09868400	-0.60668300	2.35392500
H	3.92040200	-1.87398900	1.40965100
H	2.14774300	-1.57109100	1.16959800
C	3.43818500	-0.84706700	-1.48935200
H	3.59437600	-0.14085400	-2.30076700
H	4.24267400	-1.57774500	-1.47293300
C	2.10545600	1.27146800	0.05224000
H	2.05663000	1.77330400	1.01724200
H	2.31303700	2.01231700	-0.71856700
H	2.45124400	-1.31196900	-1.56233600

$\mathbf{B_3N_3}$ D_{3h}			
M05-2X= -238.9225916			
B	0.00000000	1.10276700	0.00000000
B	0.95502400	-0.55138300	0.00000000
B	-0.95502400	-0.55138300	0.00000000
N	1.30833000	0.75536500	0.00000000
N	0.00000000	-1.51072900	0.00000000
N	-1.30833000	0.75536500	0.00000000

$\mathbf{ImMe_2}\cdot\ \mathbf{B_3N_3}\ C_1$ **M05-2X** = -543.9069996			
B	2.87899000	0.90586600	0.06433100
B	0.96258600	-0.03828100	-0.00159400
B	2.89284700	-0.95780200	-0.06171200
N	1.59585000	1.26584800	0.08631700
N	1.61444400	-1.33387300	-0.08795100
N	3.86703900	-0.01895400	0.00287300
C	-0.64905100	-0.01660200	-0.00267000
N	-1.50065200	-1.05691100	0.01205800
N	-1.41991400	1.08690300	-0.01603300
C	-2.79495500	-0.61223700	0.01001200
C	-1.15114900	-2.47519300	0.03929600
C	-2.74351300	0.73786100	-0.00873800
C	-0.96674300	2.47686000	-0.03728300
H	-3.62794900	-1.28644100	0.02077200
H	-0.07281200	-2.55381400	-0.02355800
H	-1.51536000	-2.90719600	0.96611500
H	-1.62451900	-2.96399500	-0.80614900
H	-3.52473100	1.47105700	-0.01940000
H	-0.40272100	2.69239900	0.85972700
H	-0.31553300	2.63593100	-0.88527900
H	-1.85339000	3.09791200	-0.10190100

$\mathbf{ImMe_2CH_2}\cdot\ \mathbf{B_3N_3}\ C_1$ **M05-2X** = -583.2215575			
B	3.13834300	-0.05473400	1.06073100
B	1.43181700	-0.72624600	-0.06490300
B	3.35266400	-0.11946800	-0.80516900
N	1.87970900	-0.45363400	1.31105300
N	2.19500300	-0.53920700	-1.30608200
N	4.17197400	0.24547300	0.22930100
C	-0.10295300	-1.25065000	-0.23428600
C	-1.15315900	-0.21321600	-0.08326300
H	-0.20550800	-1.70177400	-1.25597200
N	-2.47105900	-0.48821300	0.04816800
N	-1.04538800	1.12044800	-0.08654900
C	-3.19887300	0.67751900	0.13303800
C	-3.01680500	-1.83370400	0.08438300
C	-2.30164700	1.68546600	0.04641300
C	0.19261000	1.90669300	-0.19506400
H	-4.27193100	0.68636800	0.23529000
H	-2.78987300	-2.31157600	1.03868600
H	-4.09548200	-1.76217600	-0.04421200
H	-2.58337100	-2.41947500	-0.72700900
H	-2.44149200	2.74775900	0.07212000
H	-0.09414600	2.94925300	-0.34158700
H	0.77287800	1.78552500	0.71942400
H	0.77109200	1.54412000	-1.04499700
H	-0.30300300	-2.04251000	0.51639800

$\mathbf{Me_3PCH_2{\cdot}B_3N_3}$ C_1 **M05-2X** = -739.4419961			
B	2.52776900	-1.07349800	-0.00000200
B	3.27844400	0.63768700	0.00000700
B	1.14569500	0.56984800	-0.00001300
N	3.80033800	-0.61933300	0.00001100
N	2.26091000	1.49168700	-0.00000100
N	1.20186800	-0.90504700	-0.00001500
C	-0.34150000	1.24020300	-0.00002500
P	-1.62742700	0.01310800	0.00000100
H	-0.46251100	1.87296600	-0.87879600
C	-3.25899400	0.80382200	0.00000800
C	-1.55731100	-1.02160000	-1.47130500
C	-1.55728500	-1.02157000	1.47132700
H	-4.04119900	0.04953200	0.00006100
H	-3.35645200	1.42668300	-0.88470800
H	-3.35640800	1.42675900	0.88467500
H	-1.63257300	-0.38856500	-2.35155100
H	-2.38082700	-1.73031100	-1.45843000
H	-0.59680700	-1.52718900	-1.45341000
H	-1.63256300	-0.38852300	2.35156300
H	-2.38078300	-1.73030300	1.458463000
H	-0.59676900	-1.52713800	1.45344100
H	-0.46251000	1.87300600	0.87871800

$(ImMe_2)_2 \cdot B_3N_3$ C_2			
M05-2X = -848.8593821			
B	-1.18830300	-0.71761000	-0.01390700
B	1.18830100	-0.71761500	0.01394000
B	-0.00000300	-2.41957000	0.00004200
N	0.00000100	0.06042000	0.00000600
N	1.30821900	-2.16210100	-0.00142600
N	-1.30822400	-2.16209600	0.00150100
C	2.61637100	0.05063500	0.06424800
N	3.81068400	-0.47625500	-0.25902700
N	2.87209500	1.31067900	0.45635300
C	4.80651700	0.44722300	-0.06925000
C	4.05148100	-1.83368300	-0.73968700
C	4.21598900	1.57419300	0.38470600
C	1.87536600	2.26155300	0.92939000
H	5.83461700	0.22586600	-0.27489100
H	3.87739800	-2.54144200	0.05988000
H	3.35571200	-2.06338200	-1.53460400
H	5.07742900	-1.87316800	-1.09097700
H	4.62762200	2.52504900	0.65852000
H	1.91382700	3.15311600	0.30993000
H	0.90806300	1.77126400	0.83637900
H	2.09266300	2.52214800	1.96109900
C	-2.61637000	0.05064300	-0.06424600
N	-2.87208100	1.31069100	-0.45634700
N	-3.81069400	-0.47624900	0.25898800
C	-4.21597700	1.57420600	-0.38473800
C	-1.87533800	2.26157500	-0.92933200
C	-4.80652000	0.44723100	0.06918800
C	-4.05151300	-1.83368200	0.73962400
H	-4.62760000	2.52506600	-0.65855400
H	-0.90805000	1.77123500	-0.83642400
H	-2.09268500	2.52229400	-1.96099900
H	-1.91372000	3.15307000	-0.30977100
H	-5.83462700	0.22587200	0.27479300
H	-3.87741700	-2.54143200	-0.05994900
H	-3.35576300	-2.06339800	1.53455300
H	-5.07747000	-1.87316400	1.09088900

$(ImMe_2CH_2)_2 \cdot B_3N_3$ C_2 M05-2X =-927.4820433			
B	-0.94826600	-0.29780000	0.71758800
B	0.94828200	-0.29779900	-0.71761400
B	0.00001100	-2.00187500	-0.00001100
N	0.00000500	0.48227600	-0.00001600
N	1.05555800	-1.75024700	-0.77755800
N	-1.05553400	-1.75025000	0.77753800
C	2.20529400	0.50675900	-1.47358900
C	3.25881200	0.38224100	-0.48732800
H	2.47347100	0.00562000	-2.39657100
N	4.14858900	-0.61341100	-0.38745300
N	3.42882100	1.17180500	0.58224900
C	4.88556700	-0.45480200	0.76581300
C	4.20492600	-1.74695700	-1.30157700
C	4.43709600	0.66309700	1.37163400
C	2.57044900	2.30827100	0.88815700
H	5.64693100	-1.15192900	1.05106200
H	4.58948300	-1.42495600	-2.26529500
H	4.87343800	-2.48482500	-0.87353700
H	3.19763700	-2.15046200	-1.39143300
H	4.73167000	1.13365300	2.28753900
H	2.71527100	2.56355800	1.93167200
H	2.84107800	3.15680200	0.26520100
H	1.53601000	2.00446200	0.71237400
H	1.94453800	1.54532700	-1.64261400
C	-2.20527500	0.50674700	1.47357500
C	-3.25881100	0.38223100	0.48733100
H	-2.47343500	0.00560300	2.39655900
N	-4.14858400	-0.61342400	0.38745900
N	-3.42883900	1.17180600	-0.58223500
C	-4.88558600	-0.45480300	-0.76579000
C	-4.20490700	-1.74697900	1.30157600
C	-4.43712800	0.66310300	-1.37160700
C	-2.57047300	2.30827100	-0.88815200
H	-5.64695800	-1.15192600	-1.05103000
H	-4.58953100	-1.42500400	2.26527600
H	-4.87335700	-2.48488000	0.87349600
H	-3.19760300	-2.15043700	1.39146700
H	-4.73171600	1.13366600	-2.28750400
H	-2.71536000	2.56360500	-1.93164500
H	-2.84104900	3.15678000	-0.26514200
H	-1.53602500	2.00444900	-0.71243600
H	-1.94452600	1.54531700	1.64260000

$(Me_3PCH_2)_2{\cdot}B_3N_3$ C_1 **M05-2X** = –1239.9224708				
	B	0.40891296	2.41675797	0.01937519
	B	-1.37454800	1.37225691	-0.03369784
	B	0.79179803	0.35852799	-0.03499592
	N	-0.87806405	2.73485293	0.01074123
	N	-0.60952296	0.16216994	-0.05493891
	N	1.50294199	1.63809401	0.01325614
	C	1.77072908	-0.97561698	-0.07119100
	P	3.47439706	-0.48902892	0.00113300
	H	1.61329608	-1.54290394	-0.98842503
	C	4.56343311	-1.94675189	-0.02194109
	C	3.96598401	0.50323617	-1.42021496
	C	3.86956305	0.38333401	1.52617204
	H	5.60485110	-1.63938685	0.02859691
	H	4.39621112	-2.50662884	-0.93783812
	H	4.33287114	-2.58229994	0.82858688
	H	3.75414501	-0.05650179	-2.32760098
	H	5.02977700	0.71824420	-1.36219996
	H	3.36543598	1.40716214	-1.38440090
	H	3.60411909	-0.24908804	2.36955301
	H	4.93369504	0.60268805	1.55386704
	H	3.26879602	1.28777899	1.52714509
	H	1.56430811	-1.63412803	0.77235997
	C	-3.02293600	1.23858085	-0.05912982
	P	-3.49416394	-0.46477916	0.00281610
	H	-3.42271403	1.68309889	-0.96999379
	C	-5.30342793	-0.65659023	0.03135211
	C	-2.92348593	-1.37046007	-1.44488096
	C	-2.88765089	-1.26757622	1.49562705
	H	-5.57123790	-1.70967324	0.06516006
	H	-5.72643896	-0.20420120	-0.86114086
	H	-5.70475894	-0.15313729	0.90637414
	H	-3.34702596	-0.91483304	-2.33612893
	H	-3.23570089	-2.40936009	-1.37771001
	H	-1.84065593	-1.26315103	-1.43337397
	H	-3.27473490	-0.73851628	2.36262508
	H	-3.21551186	-2.30349623	1.51884800
	H	-1.80463790	-1.17809818	1.44365704
	H	-3.45913601	1.76108680	0.79122621

$(ImMe_2CH_2)_3{\cdot}B_3N_3$ C_1			
M05-2X = -1271.7042346			
B	-1.43559600	0.03283800	0.54323100
B	0.09907700	0.98757900	-0.90150700
B	0.11392100	-1.28625600	-0.54079500
N	-1.01543200	1.24337200	-0.06085400
N	0.77188800	-0.22085400	-1.20587800
N	-0.94578900	-1.29189700	0.39364800
C	0.81673300	2.41099000	-1.55881800
C	1.58269100	2.86349900	-0.43313100
H	1.44146900	2.14255200	-2.40171800
N	2.81107300	2.43743400	-0.08989200
N	1.16695100	3.67675300	0.55156600
C	3.16342700	2.97666900	1.12970900
C	3.53907100	1.43200600	-0.84498600
C	2.13486100	3.74895300	1.53056200
C	-0.17639200	4.23118000	0.61603400
H	4.10188400	2.75688400	1.59669200
H	3.97476600	1.87462400	-1.73810600
H	4.32678700	1.04140000	-0.20940000
H	2.82789600	0.64154800	-1.10250800
H	1.99919600	4.33310300	2.41795300
H	-0.30874000	4.67169500	1.59807300
H	-0.29749000	4.99823800	-0.14500800
H	-0.86892500	3.39883800	0.46394100
H	0.03645000	3.11253500	-1.82679700
C	-2.85173200	0.15650000	1.50678600
C	-3.85375200	-0.19726700	0.53834800
H	-2.80545000	-0.55973500	2.31815800
N	-4.28472500	-1.43492800	0.24701400
N	-4.43226400	0.63359500	-0.34507100
C	-5.13101800	-1.38427200	-0.83981500
C	-3.77879500	-2.63273500	0.90034800
C	-5.22458400	-0.09186900	-1.20934400
C	-4.11801400	2.05097900	-0.43390000
H	-5.57582500	-2.26705400	-1.25198100
H	-4.17423000	-2.69877100	1.91115900
H	-4.11009900	-3.49049700	0.32551000
H	-2.68736200	-2.56162300	0.89786700
H	-5.76750800	0.37461100	-2.00601200
H	-4.50002000	2.41917900	-2.00601200

$(ImMe_2CH_2)_3 \cdot B_3N_3$ (cont'd.)			
H	-4.59189800	2.58962200	0.38342700
H	-3.02944900	2.14847200	-0.39443300
H	-2.96818600	1.17459800	1.85836500
C	0.78750300	-2.85053500	-0.85727700
C	2.07238600	-2.71550600	-0.24701600
H	0.16331000	-3.58655900	-0.36748900
N	3.20807500	-2.31310600	-0.84098900
N	2.33647300	-2.82021100	1.06782200
C	4.19318800	-2.14985300	0.11156000
C	3.28161300	-1.95699100	-2.24877400
C	3.64902900	-2.46810800	1.30284000
C	1.31326400	-3.11134000	2.06027500
H	5.18326800	-1.83150100	-0.14575400
H	2.46361200	-1.26215300	-2.44686600
H	4.24119200	-1.48280300	-2.42616600
H	3.20254100	-2.84960900	-2.86397900
H	4.07063100	-2.47864900	2.28753200
H	1.68101900	-2.78823900	3.02778900
H	0.41139800	-2.55420100	1.79323100
H	1.10976400	-4.17915200	2.08660700
H	0.85236000	-3.00304000	-1.92711700

$(Me_3PCH_2)_3 \cdot B_3N_3$ C_1			
M05-2X = -1740.3584081			
B	-0.13805400	0.87058900	-0.59184700
B	-1.60659900	-0.33461100	0.75397400
B	0.39837400	-1.28965500	0.10537600
N	-1.40778400	0.87951200	0.03136100
N	-0.77901600	-1.47562800	0.84809600
N	0.87758400	-0.12835100	-0.59083300
C	1.36567800	-2.68739600	0.02395300
P	3.05715100	-2.22583100	-0.03013700
H	1.12322500	-3.23772200	-0.88457200
C	4.23249300	-3.59986400	0.18470800
C	3.45726500	-1.44771500	-1.60274400
C	3.41090500	-1.08979300	1.32788300
H	5.25607000	-3.23389100	0.15578200
H	4.08371800	-4.32197500	-0.61309100
H	4.04614400	-4.08433500	1.13918000
H	3.42629300	-2.20369300	-2.38364800
H	4.44375400	-0.99247000	-1.56774800
H	2.65535900	-0.71289400	-1.73595700
H	3.26951600	-1.62052300	2.26593400
H	4.42828700	-0.71368500	1.26379300
H	2.68173600	-0.28871400	1.24734600
H	1.16245200	-3.30397100	0.89577900
C	-3.14199200	-0.52920300	1.42664600
P	-4.13607000	-0.66858200	-0.01982500
H	-3.48388500	0.33184800	1.99751900
C	-5.76240500	-1.44003800	0.25615500
C	-4.42384400	0.96541100	-0.71574200
C	-3.31843200	-1.68913200	-1.26347300
H	-6.33402100	-1.46469200	-0.66828600
H	-6.30463600	-0.86997100	1.00515300
H	-5.61528100	-2.45351500	0.61943500
H	-5.10403400	1.51651600	-0.07140200
H	-4.83710200	0.88750400	-1.71767400
H	-3.42617000	1.42087600	-0.71007800
H	-2.93702400	-2.58110000	-0.77360400
H	-4.01515900	-1.93526900	-2.06087300
H	-2.46501900	-1.12670700	-1.63376000
H	-3.17920200	-1.44855100	2.00374200
C	0.27327700	2.36873900	-1.26776800

$(Me_3PCH_2)_3 \cdot B_3N_3$ (cont'd.)			
P	1.30553500	3.03992300	-0.01333400
H	-0.62622800	2.96608400	-1.38054300
C	2.94911000	2.32564600	-0.20912800
C	1.49658900	4.84981200	-0.04633800
C	0.69616600	2.64384300	1.63740900
H	3.55339400	2.47799200	0.68076600
H	3.43541400	2.77049100	-1.07322100
H	2.74233800	1.26737800	-0.38858500
H	1.86419000	5.15266800	-1.02254200
H	2.19162700	5.17440900	0.72401800
H	0.52626200	5.30770600	0.12549000
H	0.77461500	1.56810000	1.77689400
H	1.26477500	3.19375400	2.38362900
H	-0.36223800	2.88707800	1.67267900
H	0.84864300	2.30643000	-2.18936000

$(ImMe_2)_3 \cdot B_3N_3$ C_2			
M05-2X = -1153.7788135			
B	0.66115700	-1.16633200	0.02445000
B	0.66081500	1.16654400	-0.02452800
B	-1.33925500	-0.00021800	0.00003200
N	1.46270100	0.00022100	-0.00006300
N	-0.74842500	1.28407100	0.05606800
N	-0.74805500	-1.28431100	-0.05608900
C	1.49082100	2.58869300	-0.18949400
N	1.03966500	3.83683000	0.04345000
N	2.76079300	2.75348300	-0.61083400
C	2.01311200	4.76728300	-0.21951800
C	3.09886200	4.08344300	-0.63659500
H	1.84579900	5.81806700	-0.09088300
H	4.06656600	4.41881200	-0.95240300
C	1.49156400	-2.58825600	0.18945200
N	2.76152200	-2.75272800	0.61096500
N	1.04078000	-3.83651300	-0.04363400
C	3.09995000	-4.08260100	0.63669800
C	2.01443400	-4.76670900	0.21946300
H	4.06767500	-4.41772000	0.95270700
H	1.84742800	-5.81753800	0.09077800
C	-2.98382600	-0.00043900	0.00008700
N	-3.79989600	0.82407300	0.67850900
N	-3.79967700	-0.82517900	-0.67834400
C	-5.11703600	0.51869200	0.43086500
C	-5.11690300	-0.52009400	-0.43075700
H	-5.92503800	1.05618800	0.88590900
H	-5.92476700	-1.05780500	-0.88578100
C	-0.29258200	-4.17521400	-0.52021100
H	-0.91246400	-3.29721300	-0.33128700
H	-0.25467000	-4.39927900	-1.58339100
H	-0.64218900	-5.04673700	0.02545800
C	3.66080700	-1.69098700	1.04142400
H	4.55357200	-1.70811000	0.42145600
H	3.11782900	-0.75489400	0.90657200
H	3.93395200	-1.85712700	2.07991400
C	-3.34953800	-1.86530000	-1.58913200
H	-2.26716100	-1.90637300	-1.49864900
H	-3.78404800	-2.81539800	-1.29105500
H	-3.65869500	-1.62058100	-2.60146400
C	-3.34999100	1.86436800	1.58923900
H	-2.26769500	1.90628300	1.49803500
H	-3.78556400	2.81413600	1.29168000
H	-3.65819900	1.61916000	2.60174600
C	3.66045000	1.69198000	-1.04111900
H	4.55300100	1.70922000	-0.42085500
H	3.11762300	0.75575000	-0.90655900
H	3.93390800	1.85831000	-2.07949400
C	-0.29392500	4.17519600	0.51964300
H	-0.91351500	3.29699300	0.33068000
H	-0.25634800	4.39934200	1.58282300
H	-0.64363500	5.04658100	-0.02617700

$(ImMe_2)_3 \cdot BN \cdot BH_3$ (C_1) M05-2X = -411.1686683			
B	-1.30978013	-0.02280891	-0.00039906
N	-2.54265213	-0.02056791	-0.00105807
C	0.20503187	-0.00566692	0.00002695
C	2.32688187	-0.65134393	0.00060701
C	2.30717088	0.70148307	0.00056990
H	3.14807787	-1.33994693	0.00088306
H	3.10809188	1.41357307	0.00082785
N	1.02069487	-1.07067792	0.00027803
N	0.98945088	1.08264208	0.00018987
C	0.56139387	-2.45283492	-0.00070086
H	-0.52331613	-2.44254391	0.00362913
H	0.92101387	-2.95374299	-0.89290182
H	0.92830586	-2.95721685	0.88654218
C	0.48924088	2.45073008	-0.00067124
H	0.83560989	2.96251101	-0.89193128
H	-0.59478812	2.40822609	0.00173776
H	0.83962988	2.96499415	0.88757372
B	-4.07280913	-0.01515890	-0.00045908
H	-4.45592412	1.11853308	-0.22208316
H	-4.45648312	-0.78664397	-0.86177202
H	-4.44804313	-0.39188181	1.09692595

$(ImMe_2)_3$·BNBN·BH_3 (C_1) **M05-2X** = -490.796326			
B	0.38975896	0.00280498	-0.00176798
N	1.62853896	0.00386898	-0.00261496
B	3.02519396	0.00429598	-0.00319293
N	4.26542296	0.00363798	-0.00285091
C	-1.12327304	0.00044898	-0.00050801
C	-3.23055404	0.67425898	0.00034903
C	-3.22819904	-0.68067802	0.00252988
H	-4.04380704	1.37255998	0.00033810
H	-4.03902804	-1.38179002	0.00399178
N	-1.92264504	1.07870598	-0.00193390
N	-1.91889304	-1.08058302	0.00236086
C	-1.45361504	2.46000998	0.00095526
H	-0.36997704	2.45194698	-0.03974672
H	-1.84786102	2.97497807	-0.86782168
H	-1.78095405	2.95075187	0.91076731
C	-1.44506804	-2.46025902	-0.00102029
H	-1.77491102	-2.95317192	-0.90874535
H	-0.36128804	-2.44837503	0.03464973
H	-1.83348505	-2.97559212	0.87016864
B	5.78621196	0.00013798	0.00091812
H	6.17292594	-0.28666315	1.12913709
H	6.18865198	-0.84922093	-0.78262397
H	6.20119697	1.10628701	-0.30846375

$(ImMe_2)_3{\cdot}B_2N_2{\cdot}BH_3$ (C_1) **M05-2X** = -490.8127653			
N	2.33759599	0.01319495	-0.17312680
N	1.34143884	-2.11050847	-0.53169570
B	1.00044028	-0.71366158	-0.27785386
B	2.44450553	-1.33447003	-0.36603567
C	-0.40487799	-0.06320711	-0.12883704
C	-2.04508457	1.40767427	-0.01091132
C	-2.57272411	0.18016308	0.22185574
H	-2.50506594	2.37504609	-0.04453945
H	-3.57816002	-0.12459729	0.43354267
N	-0.70863148	1.23558777	-0.22737419
N	-1.54514476	-0.71495853	0.13659391
C	0.23122012	2.32450910	-0.49741920
H	1.13403732	1.90844042	-0.92433308
H	-0.24591908	3.01440386	-1.18467030
H	0.49277785	2.80714829	0.43643878
C	-1.67354222	-2.15774356	0.33415203
H	-2.48011802	-2.52099793	-0.29296702
H	-0.73434202	-2.62068322	0.05314315
H	-1.89541924	-2.35329255	1.37793102
B	2.65760449	0.99586318	1.06434614
H	3.52756462	0.50228258	1.74315327
H	2.97376311	2.09023427	0.64511108
H	1.61137240	1.07177283	1.71108504

(ImMe$_2$)$_3$·B$_3$N$_3$·BH$_3$·*ortho* (C_1) **M05-2X** = -570.5681327			
B	2.88562006	0.39997071	0.23397014
B	0.82966401	-0.24999409	-0.18486390
B	2.68418793	-1.19013424	-0.74471691
N	1.61199310	0.80115982	0.47204714
N	1.37755092	-1.38949612	-0.87039194
N	3.74569399	-0.47176735	-0.29770988
C	-0.76221898	-0.12466195	-0.11472792
N	-1.60503807	-1.10258388	0.24026204
N	-1.51671088	0.92984013	-0.43529889
C	-2.89843003	-0.65358977	0.16569804
C	-1.21041920	-2.42919593	0.69897700
C	-2.84200291	0.62630324	-0.26516292
C	-1.02336976	2.22883410	-0.87349585
H	-3.73327109	-1.27615070	0.41795001
H	-0.26598321	-2.67990300	0.23251800
H	-1.11252621	-2.42823798	1.77986500
H	-1.97543526	-3.13554586	0.39766697
H	-3.61876784	1.33600732	-0.46798591
H	-1.16368470	2.95044509	-0.07778382
H	0.03702524	2.14879401	-1.07072484
H	-1.55872172	2.51852418	-1.77160484
B	1.10875419	1.96745083	1.48882717
H	1.83954118	1.94794173	2.45224318
H	1.17030829	3.03275384	0.91042621
H	-0.03539384	1.69269892	1.80125815

(ImMe$_2$)$_3$·B$_3$N$_3$·BH$_3$·*para* (C_1) **M05-2X** = -570.5472887			
B	2.41748493	0.88757502	0.09622814
B	0.48771594	-0.05892700	-0.00378891
B	2.40644095	-1.04030597	-0.10306395
N	1.14695092	1.22865300	0.12870416
N	1.12908896	-1.35626799	-0.13638797
N	3.38484694	-0.08349197	-0.00300890
C	-1.11823906	-0.01399502	-0.00393691
N	-1.98396105	-1.04210104	0.01654704
N	-1.87089908	1.10157897	-0.02273386
C	-3.27023106	-0.57737105	0.01408006
C	-1.66114503	-2.46703504	0.06476797
C	-3.19845307	0.77222495	-0.01270987
C	-1.39839109	2.48593497	-0.05508179
H	-4.11360405	-1.23847907	0.02924003
H	-0.59866203	-2.58008801	-0.10097203
H	-1.93491803	-2.85710209	1.03989395
H	-2.23066302	-2.97213400	-0.70800506
H	-3.96888308	1.51665894	-0.02899884
H	-0.84184710	2.70498394	0.84576623
H	-0.74138410	2.62885002	-0.90158978
H	-2.27546310	3.11795297	-0.13452476
B	5.05454994	0.06188905	0.00979111
H	5.42844194	-0.57350399	0.96283407
H	5.42696994	-0.38327189	-1.04611092
H	5.25562292	1.24782805	0.12207516

$(ImMe_2)_3$·BN·$W(CO)_5$ (C_1) M05-2X = -1018.8598516			
B	0.00000000	-0.00000000	-1.98744396
N	0.00000000	-0.00000000	-0.74698196
C	0.00000000	-0.00000000	-3.50454296
C	0.00000000	0.67655700	-5.61638996
C	0.00000000	-0.67655700	-5.61638996
H	0.00000000	1.37692900	-6.42762796
H	0.00000000	-1.37692900	-6.42762796
N	0.00000000	1.07703500	-4.30472696
N	0.00000000	-1.07703500	-4.30472696
C	0.00000000	2.45374800	-3.82842296
H	0.00000000	2.43141000	-2.74401796
H	0.88969288	2.96067004	-4.18563496
H	-0.88969288	2.96067004	-4.18563496
C	0.00000000	-2.45374800	-3.82842296
H	0.88969288	-2.96067004	-4.18563496
H	0.00000000	-2.43141000	-2.74401796
H	-0.88969288	-2.96067004	-4.18563496
W	0.00000000	-0.00000000	1.42790704
C	0.00000000	-2.05087400	1.39442304
C	0.00000000	-0.00000000	3.41224604
C	2.05191500	-0.00000000	1.49269404
C	-0.00000000	2.05087400	1.39442304
C	-2.05191500	-0.00000000	1.49269404
O	-3.18737200	0.00000000	1.59206004
O	0.00000000	-3.19088600	1.38277104
O	0.00000000	-0.00000000	4.56272704
O	3.18737200	0.00000000	1.59206004
O	-0.00000000	3.19088600	1.38277104

$(ImMe_2)_3$·BNBN·$W(CO)_5$ (C_1) M05-2X = -1098.4921553			
B	0.00000000	0.00000000	3.79210627
N	0.00000000	0.00000000	2.55225627
B	0.00000000	0.00000000	1.15664527
N	0.00000000	0.00000000	-0.09242373
C	0.00000000	0.00000000	5.30473727
C	-0.00086012	0.67753800	7.41096726
C	0.00086012	-0.67753800	7.41096726
H	-0.00112441	1.37700601	8.22326425
H	0.00112441	-1.37700601	8.22326425
N	-0.00204428	1.08019498	6.10280425
N	0.00204428	-1.08019498	6.10280425
C	0.00471616	2.46112597	5.63303923
H	-0.05680783	2.45383193	4.55043123
H	-0.85187306	2.98378463	6.04343621
H	0.92475096	2.94435735	5.94270522
C	-0.00471616	-2.46112597	5.63303923
H	-0.92475096	-2.94435735	5.94270522
H	0.05680783	-2.45383193	4.55043123
H	0.85187306	-2.98378463	6.04343621
W	0.00000000	0.00000000	-2.24710873
C	1.33703357	1.55843038	-2.27791575
C	1.55021176	-1.34642353	-2.29284270
C	-1.33703357	-1.55843038	-2.27791575
C	-1.55021176	1.34642353	-2.29284270
C	0.00000000	0.00000000	-4.23006173
O	-2.40650665	2.09455884	-2.38042278
O	2.07570721	2.42418768	-2.35050676
O	0.00000000	0.00000000	-5.38345373
O	2.40650665	-2.09455884	-2.38042278
O	-2.07570721	-2.42418768	-2.35050676

$(ImMe_2)_3{\cdot}B_2N_2{\cdot}W(CO)_5$ (C_1) **M05-2X** = -1098.4998056			
N	0.26539289	0.64371056	-1.61514919
N	1.87634583	2.40666962	-1.60792263
B	1.69421989	1.02291470	-1.18793033
B	0.63983084	1.92590651	-1.91472648
C	2.71057395	0.09625489	-0.45740717
C	3.80374504	-1.67529192	0.27822317
C	4.34425003	-0.58018977	0.86577391
H	4.04312207	-2.71524789	0.37567539
H	5.14178305	-0.48513159	1.57516786
N	2.79811899	-1.23612412	-0.53438088
N	3.66157497	0.50398510	0.39068171
C	1.94365298	-2.10127233	-1.34316266
H	1.21367094	-1.47894846	-1.84757177
H	2.55809697	-2.63086346	-2.06337657
H	1.43976003	-2.80428220	-0.68872449
C	3.90022895	1.89049620	0.78887440
H	4.96985294	2.06611423	0.79207832
H	3.41014290	2.53610703	0.06883228
H	3.49164298	2.05106340	1.78111638
W	-1.18309303	-0.00621812	0.04948901
C	0.20400705	-0.84729182	1.24133714
C	-0.90040104	1.75994211	1.06747762
C	-2.74700910	0.80552559	-1.07043210
C	-2.50569395	-0.51972687	1.41549118
C	-1.43884700	-1.82995532	-0.84895858
O	-1.57288299	-2.87615842	-1.28192035
O	-3.27565891	-0.81603372	2.21587727
O	-0.76271304	2.69277925	1.70559641
O	0.94280409	-1.35259064	1.96301222
O	-3.64236313	1.22182744	-1.62731615

$(ImMe_2)_3{\cdot}B_3N_3{\cdot}W(CO)_5{\cdot}$***ortho*** (C_1) **M05-2X** = -1178.2522794			
B	-0.15780330	2.66867635	0.75612335
B	-1.87803361	1.38612357	0.37829809
B	-1.79726721	3.52916398	0.47315399
N	-0.42868771	1.35145504	0.64325189
N	-2.68809522	2.56355626	0.25772518
N	-0.53622235	3.95353443	0.73799091
C	-2.61067777	-0.02721343	0.20966211
N	-3.36438744	-0.41312396	-0.82444446
N	-2.62122532	-1.03643799	1.08753768
C	-3.83959622	-1.68264238	-0.60754247
C	-3.61670255	0.38172059	-2.02187348
C	-3.37642820	-2.07232098	0.60075099
C	-1.99501378	-1.00947925	2.40356545
H	-4.45087419	-2.19238690	-1.32490623
H	-3.49155773	1.42575496	-1.76162535
H	-2.92206928	0.09623861	-2.80432140
H	-4.63687321	0.20256252	-2.34153985
H	-3.50556336	-2.98666643	1.14412567
H	-1.59475256	-1.99390355	2.61450388
H	-1.18920876	-0.28549403	2.38135837
H	-2.73107691	-0.73224006	3.15127915
W	1.19752943	-0.14802724	-0.07803385
C	0.27900266	-1.88603028	0.38863734
C	2.01411356	-0.10290715	1.81737282
C	2.62457426	-1.33502297	-0.73085244
C	2.44950998	1.36990500	-0.72840805
C	0.24543393	-0.20048591	-1.88342213
O	2.45500922	-0.11771874	2.86442856
O	-0.13511510	-2.93466565	0.59859799
O	3.45616292	-2.02751246	-1.11448837
O	-0.31641395	-0.26478169	-2.87454587
O	3.22727562	2.08896667	-1.13949427

$(ImMe_2)_3{\cdot}B_3N_3{\cdot}W(CO)_5{\cdot}$***para*** (C_1) **M05-2X** = -1178.2389328			
B	1.14628863	-0.88528988	0.09680199
B	3.07386486	0.05817184	-0.00402560
B	1.15240809	1.01879982	-0.10350478
N	2.41619455	-1.23248157	0.13100608
N	2.42599717	1.35349634	-0.13904749
N	0.16676786	0.07061804	-0.00283058
C	4.67882586	0.01893273	-0.00413147
N	5.54023089	1.05070289	0.01427116
N	5.43570581	-1.09381251	-0.02089148
C	6.82801487	0.59098779	0.01270156
C	5.21269691	2.47485345	0.06150832
C	6.76165982	-0.75910549	-0.01160311
C	4.96907077	-2.48037782	-0.05097140
H	7.66883789	1.25537689	0.02652436
H	4.15328222	2.58662541	-0.12241772
H	5.46747430	2.86250966	1.04270231
H	5.79535220	2.98330971	-0.69903953
H	7.53518380	-1.50036071	-0.02676434
H	4.41328326	-2.70021648	0.85013319
H	4.31357817	-2.62779947	-0.89787780
H	5.84876086	-3.10880977	-0.12874174
W	-2.16404115	0.00224522	0.00026232
C	-2.17887398	-1.53326235	-1.36129613
C	-2.18832480	-1.35230014	1.54142578
C	-4.12304916	-0.04959763	0.00208866
C	-2.25491232	1.53541083	1.36418563
C	-2.26038650	1.35411858	-1.54268630
O	-2.25611278	-2.38281897	-2.11516854
O	-5.27196616	-0.07972654	0.00308409
O	-2.27449327	-2.10145738	2.39440921
O	-2.38475203	2.09654982	-2.39639300
O	-2.37294053	2.37835148	2.11967179

$\mathbf{ImMe_2{\cdot}B_2N_2{\cdot}(BH_3)_2}$ (C_2) **M05-2X** = -517.473553			
N	0.22253853	1.14499445	-1.97064321
N	-0.22253853	-1.14499445	-1.97064321
B	-0.00000000	0.00000000	-1.05377440
B	-0.00000000	0.00000000	-2.66270840
C	-0.00000000	0.00000000	0.49638660
C	-0.25114988	0.62986254	2.59218470
C	0.25114988	-0.62986254	2.59218470
H	-0.51493347	1.28142885	3.40119481
H	0.51493347	-1.28142885	3.40119481
N	-0.39538636	1.00286754	1.28776876
N	0.39538636	-1.00286754	1.28776876
C	-0.91169232	2.30052993	0.85140698
H	-1.04611277	2.28548524	-0.22152003
H	-1.85420478	2.47883573	1.35725200
H	-0.18519210	3.06794618	1.08961511
C	0.91169232	-2.30052993	0.85140698
H	0.18519210	-3.06794618	1.08961511
H	1.04611277	-2.28548524	-0.22152003
H	1.85420478	-2.47883573	1.35725200
B	1.05568162	2.49626557	-1.74160597
H	1.89373280	2.57457505	-2.60409395
H	0.28473476	3.43203767	-1.75665782
H	1.56567116	2.37052584	-0.63714198
B	-1.05568162	-2.49626557	-1.74160597
H	-1.89373280	-2.57457505	-2.60409395
H	-0.28473476	-3.43203767	-1.75665782
H	-1.56567116	-2.37052584	-0.63714198

$(ImMe_2)_2{\cdot}B_2N_2{\cdot}(BH_3)_2$ (C_s) **M05-2X** = -822.4890566			
N	-0.14148669	1.12732236	0.00000000
N	-0.71041884	-1.04557115	0.00000000
B	-0.33150552	0.00632084	0.89354505
B	-0.33150552	0.00632084	-0.89354505
C	-0.05051355	-0.00028541	2.45175405
C	0.17855604	0.70261673	4.53793306
C	0.44370656	-0.62551836	4.51698403
H	0.17820262	1.40729472	5.34539208
H	0.72259625	-1.30032258	5.30143801
N	-0.12425610	1.06805115	3.25609308
N	0.29275027	-1.03932314	3.22236202
C	-0.45473735	2.43038677	2.84282311
H	-0.85265461	2.39911893	1.83709312
H	-1.18231018	2.83041050	3.54119613
H	0.44906837	3.02791964	2.82899511
C	0.50362845	-2.40854479	2.76109798
H	-0.20716071	-3.06257919	3.25361098
H	0.32863208	-2.45327239	1.69371599
H	1.52044812	-2.70349883	2.99922096
C	-0.05051355	-0.00028541	-2.45175405
C	0.17855604	0.70261673	-4.53793306
C	0.44370656	-0.62551836	-4.51698403
H	0.17820262	1.40729472	-5.34539208
H	0.72259625	-1.30032258	-5.30143801
N	-0.12425610	1.06805115	-3.25609308
N	0.29275027	-1.03932314	-3.22236202
C	-0.45473735	2.43038677	-2.84282311
H	-0.85265461	2.39911893	-1.83709312
H	0.44906837	3.02791964	-2.82899511
H	-1.18231018	2.83041050	-3.54119613
C	0.50362845	-2.40854479	-2.76109798
H	1.52044812	-2.70349883	-2.99922096
H	0.32863208	-2.45327239	-1.69371599
H	-0.20716071	-3.06257919	-3.25361098
B	1.02734968	2.18766113	0.00000000
H	0.58326671	3.33174564	0.00000000
H	1.72630937	2.01856159	0.99671706
B	-1.38906702	-2.46111679	0.00000000
H	-0.52942903	-3.34899358	0.00000000
H	-2.06985995	-2.58212844	1.00585103
H	-2.06985995	-2.58212844	-1.00585103
H	1.72630937	2.01856159	-0.99671706

$(ImMe_2)_2{\cdot}B_3N_3{\cdot}(BH_3)_3$ (C_1)			
M05-2X = -928.8776936			
B	1.20746506	0.46461983	-0.20060712
B	-1.23470995	0.42406010	-0.20682913
B	-0.02259477	2.01543075	-1.01548055
N	-0.00236402	-0.19846495	0.13307205
N	-1.31655280	1.71426293	-0.87128748
N	1.27462220	1.75022265	-0.87022347
C	-2.62079603	-0.28696067	0.11630005
N	-3.54629699	0.13755667	0.97560393
N	-3.09425114	-1.39713577	-0.44847566
C	-4.62231408	-0.71104022	0.95502215
C	-3.44272386	1.37450386	1.73702260
C	-4.33605718	-1.68152649	0.05678241
C	-2.35859422	-2.18549311	-1.42565144
H	-5.48496607	-0.55349996	1.57015110
H	-2.50331286	1.38045490	2.27925560
H	-3.48664576	2.21404168	1.04908737
H	-4.26641486	1.41045814	2.43972258
H	-4.89859927	-2.53662352	-0.25901236
H	-2.96216731	-3.04473311	-1.69202321
H	-2.17508615	-1.58167937	-2.30847960
H	-1.42240026	-2.50666909	-0.97782334
C	2.60924798	-0.19764622	0.15817607
N	3.33034400	0.02080299	1.25411901
N	3.29383390	-1.05071050	-0.59882670
C	4.49196492	-0.70541115	1.19612622
C	2.89744209	0.89755433	2.33008178
C	4.47076186	-1.38038446	0.02368440
C	2.84133186	-1.49408580	-1.90740358
H	5.22123892	-0.67956002	1.98019922
H	1.98695504	0.49513854	2.76374388
H	3.67968508	0.93613344	3.07828377
H	2.72977920	1.88955424	1.92186551
H	5.17955379	-2.05365066	-0.41402941
H	1.83241882	-1.88242667	-1.80826349
H	2.86786196	-0.65296099	-2.59370781
H	3.50227578	-2.27965597	-2.25289037
B	0.10788582	-1.59901975	0.90456242
H	0.55916474	-2.44199101	0.13622665
H	0.86024783	-1.47250458	1.85514540
B	2.69641328	2.45573539	-1.24027264
H	3.31921420	1.64879715	-1.90503442
H	2.46689440	3.46635925	-1.85316292
B	-2.66311372	2.45126192	-1.42765369
H	-3.54455881	1.61346902	-1.41354247
H	-2.90911362	3.37889015	-0.68490294
H	-0.99307121	-1.93301352	1.29872051
H	-2.43550167	2.83303160	-2.54937879
H	3.26289330	2.67940061	-0.18746270

$(ImMe_2)_3{\cdot}B_3N_3{\cdot}(BH_3)_3$ (C_1) **M05-2X** = -1233.872235			
B	-1.36188115	-0.19843015	-0.13063997
B	0.50369974	1.28815373	-0.01096499
B	0.84378332	-1.08353547	0.01658603
N	-0.90302135	1.14054557	-0.11711298
N	1.42548809	0.21188218	0.05220102
N	-0.54210084	-1.35134564	-0.06376496
C	1.09496663	2.77589438	0.06183500
N	0.94876715	3.63962648	1.06656999
N	1.84021599	3.38577992	-0.86005901
C	1.60675585	4.80907908	0.78083798
C	2.17481174	4.64699473	-0.43524202
H	1.61110435	5.64198408	1.45437797
H	2.77804014	5.30765336	-1.02434203
C	-2.94554329	-0.43319021	-0.21836296
N	-3.78705234	-0.51187570	0.81004105
N	-3.67163939	-0.59187278	-1.32215895
C	-5.06510846	-0.72348894	0.35549105
C	-4.99120250	-0.77382199	-0.99388195
H	-5.90058952	-0.81768743	1.01905706
H	-5.75047759	-0.92002755	-1.73511194
C	1.85112158	-2.32779007	0.10692904
N	2.67120730	-2.78028257	-0.84075696
N	2.04230412	-3.09726918	1.17737605
C	3.38956866	-3.85197600	-0.36731995
C	2.99135855	-4.05001575	0.90871205
H	4.11105135	-4.36785544	-0.96805395
H	3.29800212	-4.77324892	1.63707606
C	-3.09184538	-0.57142514	-2.65238896
H	-2.62046881	0.39423557	-2.80953997
H	-2.36352286	-1.37393258	-2.72388895
H	-3.88303748	-0.72110168	-3.37747195
C	-3.35659626	-0.38789194	2.19146004
H	-2.66512174	-1.19483735	2.41466305
H	-2.87705568	0.57812077	2.31827603
H	-4.22763529	-0.45604841	2.83241205
C	1.29945523	-2.92727872	2.41398405
H	0.24030016	-3.04347609	2.19896306
H	1.62577478	-3.68414391	3.11758706
H	1.50440282	-1.93927884	2.81497704
C	2.76797463	-2.22256364	-2.17658496
H	2.24901320	-1.27156833	-2.17817097
H	3.81125273	-2.05078227	-2.41615197
H	2.31627222	-2.90312238	-2.89190795
C	2.30389760	2.73634964	-2.07435701
H	3.01788513	1.96226121	-1.80618700
H	1.45401033	2.29896714	-2.58750600
H	2.76545804	3.48453835	-2.70828102
C	0.13664799	3.37256197	2.24177600
H	-0.90350906	3.29328859	1.93719200
H	0.46678144	2.44386778	2.69550200
H	0.27124748	4.18826090	2.94256099
B	2.98670019	0.37472625	0.30720501
H	3.33627774	-0.38748295	1.19751002
H	3.61731003	0.10390686	-0.71400299
B	-1.95001264	2.32709720	-0.24208199
H	-2.68119776	2.13699862	-1.20356398
H	-2.64253961	2.37774262	0.77521102
B	-1.19682670	-2.79653725	-0.04524694
H	-1.79739980	-2.95953088	1.01755206
H	-1.99186478	-2.90923879	-0.96732894
H	-0.33225022	-3.64990577	-0.15984694
H	-1.36809701	3.38844085	-0.39458200
H	3.23651288	1.52068910	0.64506400

Table S11: Gas Phase Ground State BP86/TZ2P Determined XYZ Coordinates (in Å) for the Mono-substituted Species.

ImMe$_2$ C_{2v}			
C	0.000000	0.000000	-0.986088
C	-0.680550	0.000000	1.217578
C	0.680550	0.000000	1.217578
H	-1.384266	0.000000	2.041305
H	1.384266	0.000000	2.041305
N	-1.063891	0.000000	-0.120553
N	1.063891	0.000000	-0.120553
C	-2.445208	0.000000	-0.574008
H	-2.429119	0.000000	-1.666982
H	-2.972823	-0.894452	-0.216760
H	-2.972823	0.894452	-0.216760
C	2.445208	0.000000	-0.574008
H	2.972823	-0.894452	-0.216760
H	2.429119	0.000000	-1.666982
H	2.972823	0.894452	-0.216760

$\mathbf{ImMe_2CH_2}$ C_{2v}			
C	-0.677678	0.000000	-1.547475
C	0.677678	0.000000	-1.547475
H	-1.378124	0.000000	-2.371113
H	1.378124	0.000000	-2.371113
N	-1.102842	0.000000	-0.217853
N	1.102842	0.000000	-0.217853
C	-2.462761	0.000000	0.258075
H	-2.663490	0.892342	0.872381
H	-3.144558	0.000000	-0.598602
H	-2.663490	-0.892342	0.872381
C	2.462761	0.000000	0.258075
H	3.144558	0.000000	-0.598602
H	2.663490	0.892342	0.872381
H	2.663490	-0.892342	0.872381
C	0.000000	0.000000	0.636611
C	0.000000	0.000000	2.003407
H	0.932546	0.000000	2.557697
H	-0.932546	0.000000	2.557697

$\mathbf{Me_3PCH_2}$ C_s			
P	0.087154	0.127845	0.000000
C	-0.966605	-0.057479	-1.483377
H	-1.435473	-1.050245	-1.520669
H	-0.335643	0.068320	-2.374442
H	-1.735494	0.724995	-1.487073
C	1.001738	-1.500169	0.000000
H	1.647432	-1.543766	-0.889416
H	0.325922	-2.370108	0.000000
H	1.647432	-1.543766	0.889416
C	-0.966605	-0.057479	1.483377
H	-1.735494	0.724995	1.487073
H	-1.435473	-1.050245	1.520669
C	0.843802	1.630599	0.000000
H	1.319964	1.956026	0.927372
H	1.319964	1.956026	-0.927372
H	-0.335643	0.068320	2.374442

BN (singlet) $C_{\infty v}$			
B	0.000000	0.000000	-0.742953
N	0.000000	0.000000	0.531206

ImMe$_2$·BN C_{2v}			
B	0.000000	0.000000	-1.848388
N	0.000000	0.000000	-3.118818
C	0.000000	0.000000	-0.340532
C	0.000000	0.681922	1.808369
C	0.000000	-0.681922	1.808369
H	0.000000	1.384650	2.630678
H	0.000000	-1.384650	2.630678
N	0.000000	1.088558	0.487312
N	0.000000	-1.088558	0.487312
C	0.000000	2.466640	0.008955
H	0.000000	2.435261	-1.087270
H	-0.897210	2.987926	0.363232
H	0.897210	2.987926	0.363232
C	0.000000	-2.466640	0.008955
H	-0.897210	-2.987926	0.363232
H	0.000000	-2.435261	-1.087270
H	0.897210	-2.987926	0.363232

ImMe$_2$CH$_2$·BN C_1			
B	1.912860	-1.348082	-0.259767
N	2.788159	-1.119008	-1.151961
C	-0.892438	1.804575	-0.318303
C	-1.930891	0.927551	-0.381962
H	-0.839015	2.853032	-0.575255
H	-2.955509	1.063460	-0.697854
N	0.205665	1.115464	0.163832
N	-1.453367	-0.294693	0.066026
C	1.577276	1.628279	0.215237
H	2.208204	0.950526	-0.406030
H	1.570348	2.656201	-0.159059
H	1.947012	1.615181	1.247185
C	-2.227810	-1.531184	0.122574
H	-3.252827	-1.308704	-0.186716
H	-1.800903	-2.276332	-0.558910
H	-2.243160	-1.930485	1.142811
C	-0.137954	-0.177567	0.390768
C	0.768126	-1.265607	0.828646
H	0.195633	-2.195353	0.945535
H	1.185953	-1.023127	1.820675

$\mathbf{Me_3PCH_2{\cdot}BN}$ C_s			
B	1.955249	-0.668240	0.000000
N	2.749475	0.321947	0.000000
P	-0.524976	-0.014926	0.000000
C	-0.235112	0.986765	-1.480132
H	-0.851434	1.895858	-1.443642
H	-0.491052	0.404585	-2.376827
H	0.841004	1.230067	-1.476532
C	-2.290483	-0.503512	0.000000
H	-2.506585	-1.105437	-0.894020
H	-2.938430	0.384010	0.000000
H	-2.506585	-1.105437	0.894020
C	-0.235112	0.986765	1.480132
H	-0.851434	1.895858	1.443642
H	-0.491052	0.404585	2.376827
C	0.589567	-1.441691	0.000000
H	0.385810	-2.055250	0.893339
H	0.385810	-2.055250	-0.893339
H	0.841004	1.230067	1.476532

$\mathbf{B_3N_3}$ **(singlet)** D_{3h}			
B	-0.543937	0.942126	0.000000
B	1.087874	0.000000	0.000000
B	-0.543937	-0.942126	0.000000
N	0.764899	1.324844	0.000000
N	0.764899	-1.324844	0.000000
N	-1.529798	0.000000	0.000000

$\mathbf{ImMe_2{\cdot}B_3N_3}$ C_1			
B	2.892220	0.888542	0.017021
B	0.962475	-0.031202	0.000596
B	2.892782	-0.957399	-0.018066
N	1.608508	1.281412	0.024772
N	1.608101	-1.346404	-0.024369
N	3.897735	-0.034425	-0.000680
C	-0.642224	-0.008542	0.000176
N	-1.504654	-1.064825	0.001029
N	-1.435821	1.102015	-0.003237
C	-2.810586	-0.622043	-0.001229
C	-1.132809	-2.483063	0.008364
C	-2.766626	0.740224	-0.003445
C	-0.984273	2.496318	-0.002841
H	-3.650825	-1.303349	-0.001400
H	-0.036421	-2.534213	-0.020278
H	-1.518410	-2.950963	0.921788
H	-1.570340	-2.972122	-0.869625
H	-3.561962	1.473200	-0.006871
H	-0.408135	2.702026	0.902497
H	-0.326395	2.674587	-0.856021
H	-1.874375	3.131677	-0.052012

$\mathbf{ImMe_2CH_2{\cdot}B_3N_3}$ C_1			
B	2.652787	-1.182279	1.144550
B	1.295568	-0.704573	-0.417526
B	3.124894	0.254606	0.078260
N	1.473485	-1.646867	0.693694
N	2.150130	0.413475	-0.835317
N	3.732112	-0.344413	1.145744
C	-0.128334	-0.858197	-1.253397
C	-1.088984	-0.012858	-0.546249
H	0.003155	-0.513751	-2.284596
N	-1.854358	-0.373882	0.513875
N	-1.298638	1.312041	-0.747830
C	-2.557072	0.729014	0.973597
C	-1.831345	-1.706186	1.123666
C	-2.209701	1.782922	0.184760
C	-0.571082	2.114246	-1.735115
H	-3.227894	0.669887	1.819054
H	-0.781350	-2.018761	1.233385
H	-2.308370	-1.641498	2.105727
H	-2.384033	-2.419420	0.499090
H	-2.519905	2.817952	0.211318
H	-0.950793	1.910626	-2.744439
H	-0.725319	3.170720	-1.498220
H	0.498645	1.863166	-1.664980
H	-0.455438	-1.903258	-1.247461

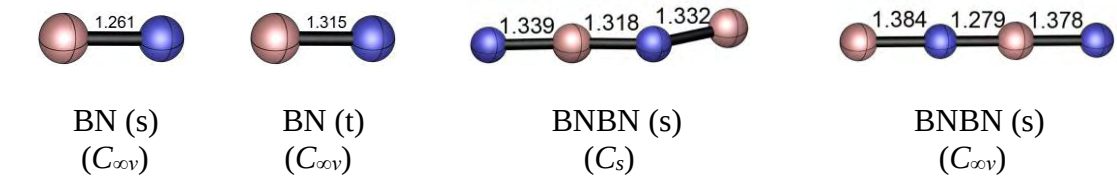
$\mathbf{Me_3PCH_2{\cdot}B_3N_3}$ C_s			
B	2.555023	-1.066334	0.000000
B	3.288014	0.629835	0.000000
B	1.161571	0.560121	0.000000
N	3.842854	-0.623209	0.000000
N	2.269940	1.501911	0.000000
N	1.215147	-0.921039	0.000000
C	-0.340359	1.236981	0.000000
P	-1.652955	0.022007	0.000000
H	-0.464036	1.883086	-0.884506
C	-3.297320	0.815126	0.000000
C	-1.562985	-1.026458	-1.473237
C	-1.562985	-1.026458	1.473237
H	-4.090938	0.054726	0.000000
H	-3.404527	1.446426	-0.892944
H	-3.404527	1.446426	0.892944
H	-1.654350	-0.403903	-2.373863
H	-2.366864	-1.774777	-1.459472
H	-0.571265	-1.502700	-1.443829
H	-1.654350	-0.403903	2.373863
H	-2.366864	-1.774777	1.459472
H	-0.571265	-1.502700	1.443829
H	-0.464036	1.883086	0.884506

Table S12: The M05-2X/cc-pVTZ Computed Complexation Energies[a] (in kcal/mol) for the Attachment of Different $ImMe_2{\cdot}(BN)_x$ Donors to the BH_3 and WCO_5 Acceptor Groups[b]

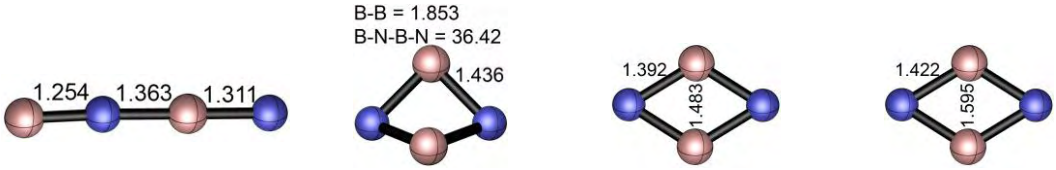
Species	ΔE_{LA}[b]	$(\Delta E + ZPE)_{LA}$[b]	$\Delta G°_{LA}$[b]
$ImMe_2{\cdot}BN{\cdot}BH_3$	–45.7	–42.7	–35.2
$ImMe_2{\cdot}BN{\cdot}WCO_5$	–59.0	–58.0	–46.6
$ImMe_2{\cdot}BNBN{\cdot}BH_3$	–51.9	–49.1	–41.5
$ImMe_2{\cdot}BNBN{\cdot}WCO_5$	–68.1	–67.1	–55.6
$ImMe_2{\cdot}B_2N_2{\cdot}BH_3$	–40.6	–36.8	–27.0
$ImMe_2{\cdot}B_2N_2{\cdot}WCO_5$	–51.3	–49.9	–38.1
$ImMe_2{\cdot}B_3N_3{\cdot}BH_3{\cdot}$*ortho*	–34.8	–31.4	–21.3
$ImMe_2{\cdot}B_3N_3{\cdot}WCO_5{\cdot}$*ortho*	–43.7	–42.8	–30.6
$ImMe_2{\cdot}B_3N_3{\cdot}BH_3{\cdot}$*para*	–21.7	–18.9	–10.7
$ImMe_2{\cdot}B_3N_3{\cdot}WCO_5{\cdot}$*para*	–35.3	–34.8	–26.2

[a]See Table 2 for Definition of Each Term.
[b]For the Reaction: $ImMe_2{\cdot}(BN)_n$ + LA → $ImMe_2{\cdot}(BN)_n{\cdot}$LA ($n$ = 1–3)

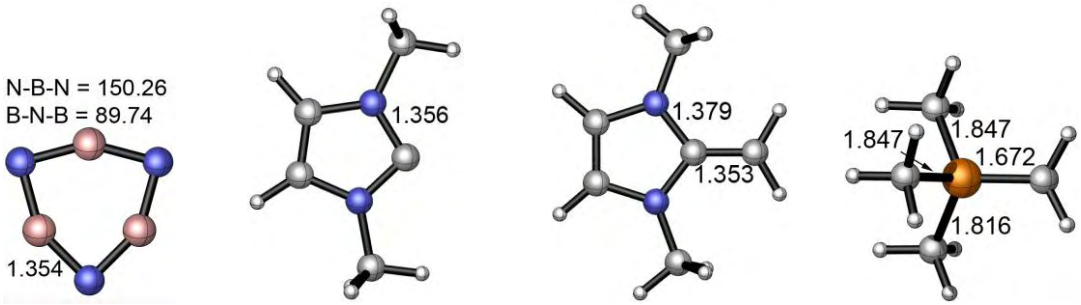
Figure S1: M05-2X/cc-pVTZ Optimized Structures of the Isolated Species in the Gas Phase.



BN (s) ($C_{\infty v}$) BN (t) ($C_{\infty v}$) BNBN (s) (C_s) BNBN (s) ($C_{\infty v}$)



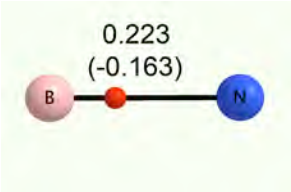
BNBN (t) (C_s) B_2N_2 (s) (C_{2v}) B_2N_2 (s) (D_{2h}) B_2N_2 (t) (D_{2h})

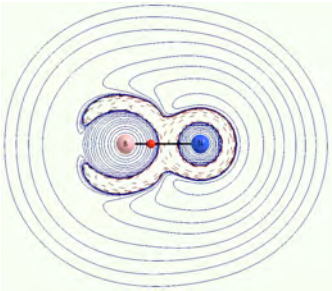


B_3N_3 (D_{3h}) $ImMe_2$ (C_{2v}) $ImMe_2CH_2$ (C_{2v}) Me_3PCH_2 (C_{2v})

Figure S2: M05-2X/cc-pVTZ Calculated AIM Results, i.e., ρ and H(r) (in Parenthesis), for All the Structures in This Study. Average Values of the ρ and H(r) Are Provided for Some of the Two and Three-base Substituted Complexes.

BN (s)





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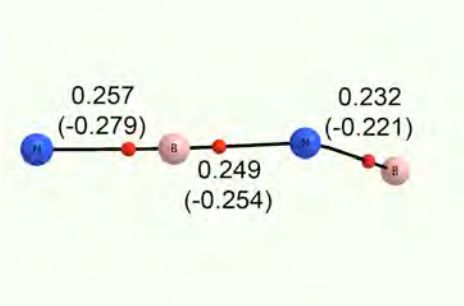
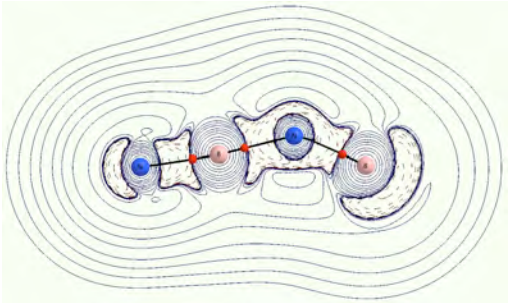
BNBN (s)





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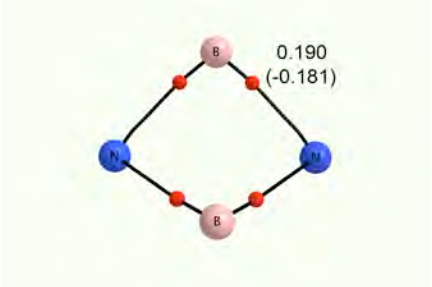
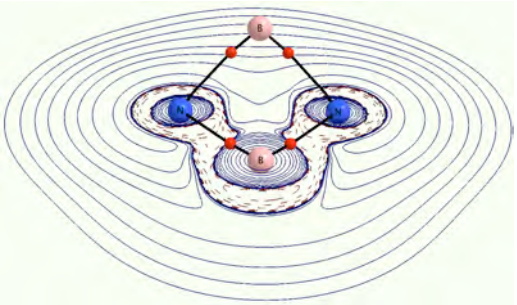
B_2N_2 (s)





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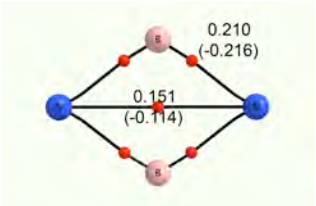
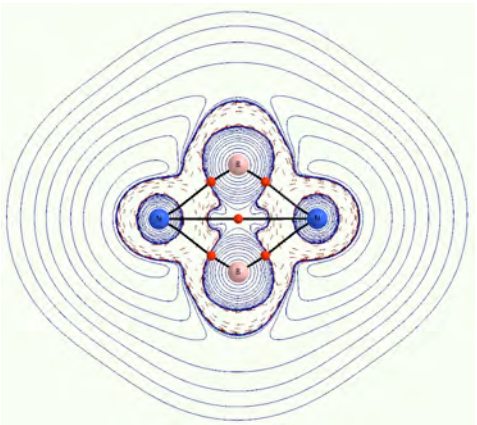
B_2N_2 (t)





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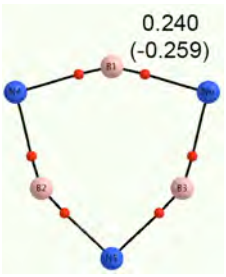
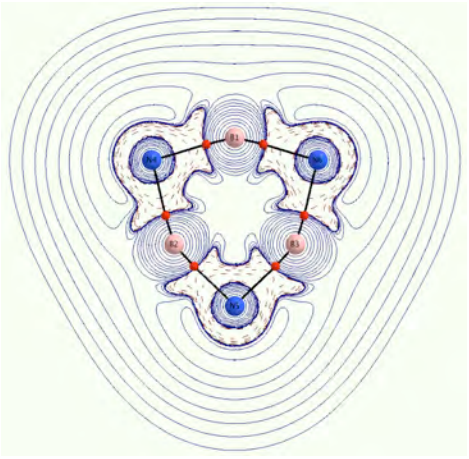
B_3N_3 (s)





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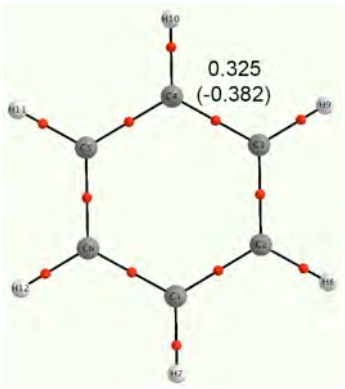
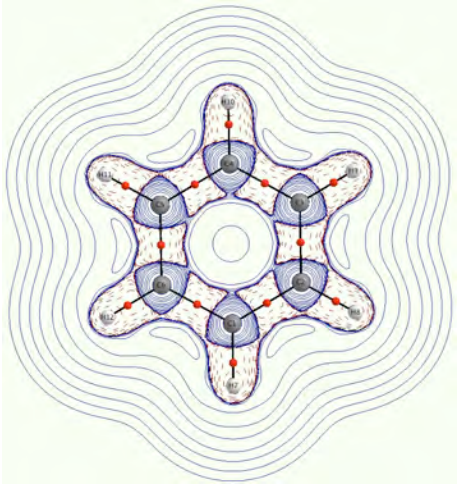
C_6H_6





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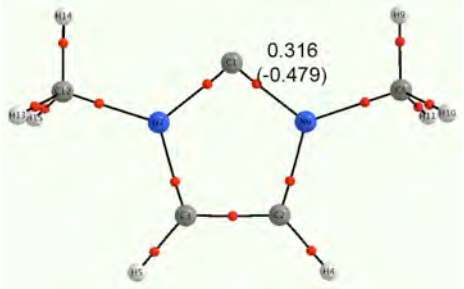
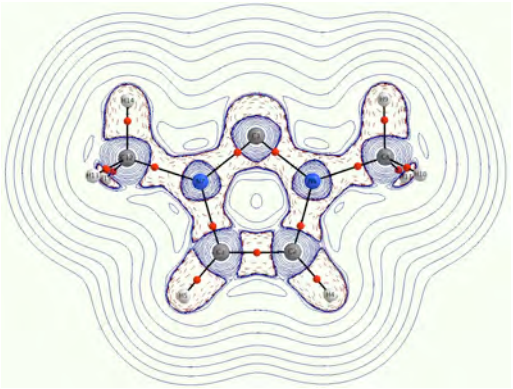
$ImMe_2$





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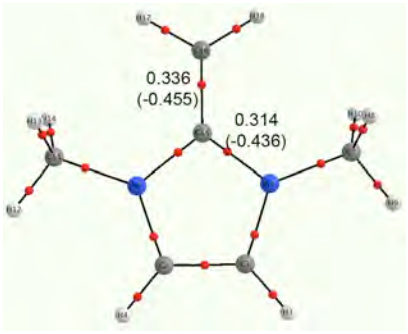
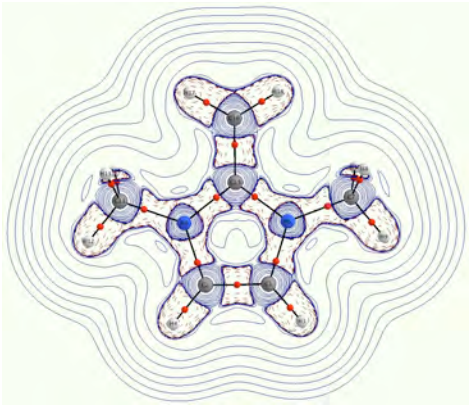
$ImMe_2CH_2$





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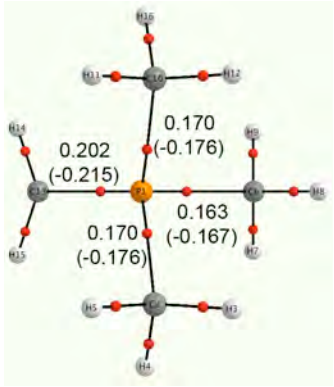
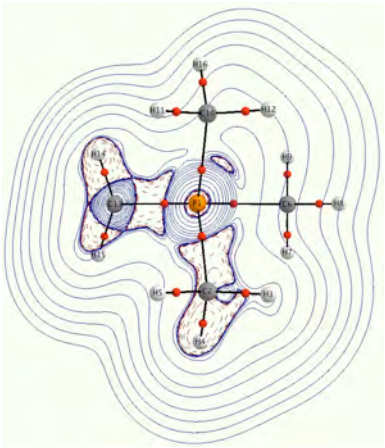
Me_3PCH_2





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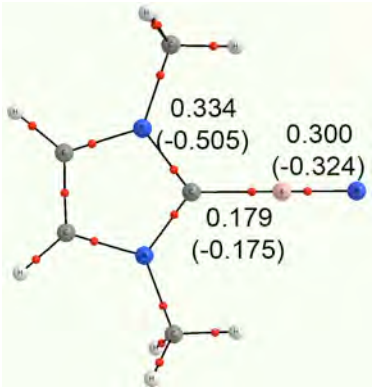

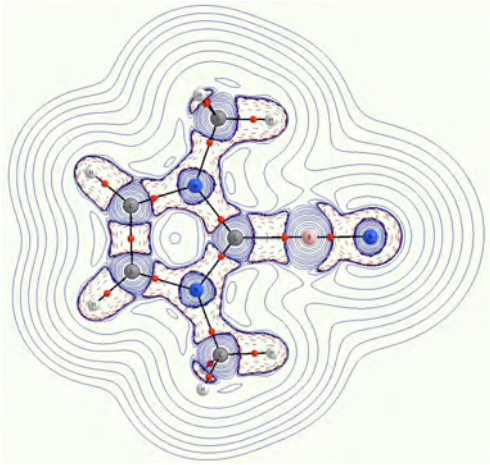

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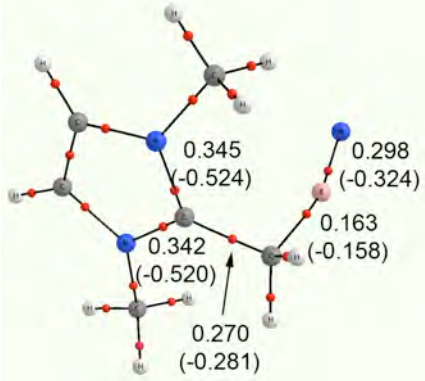
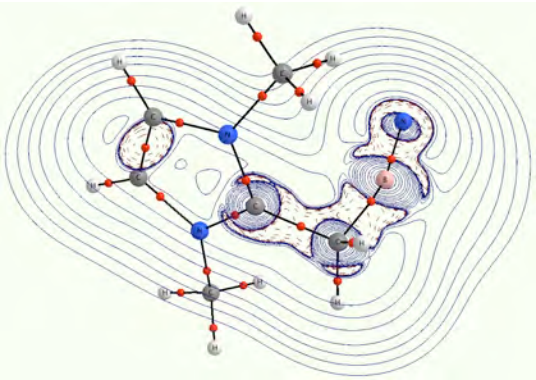
$ImMe_2CH_2$·BN





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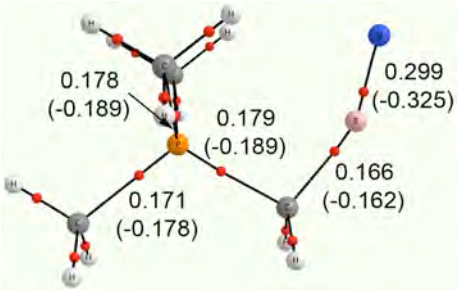

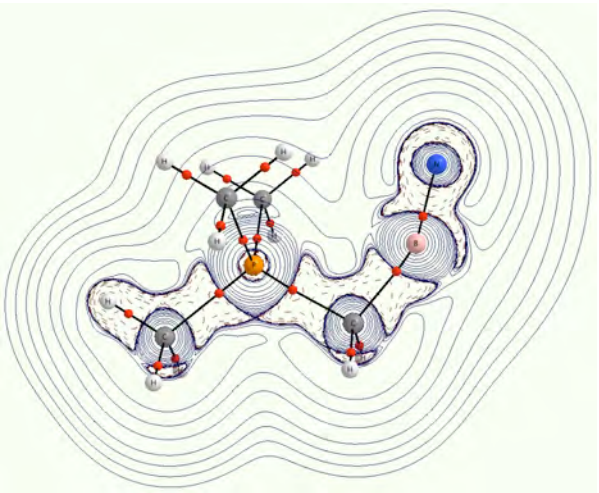

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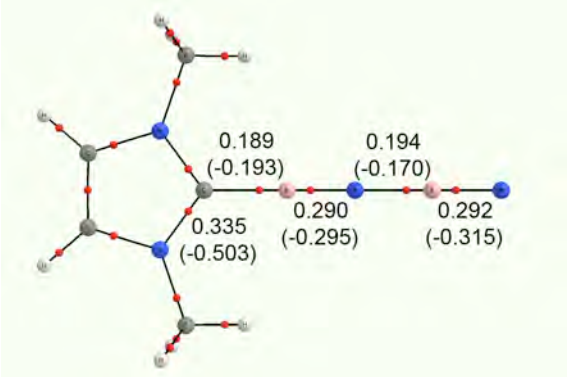

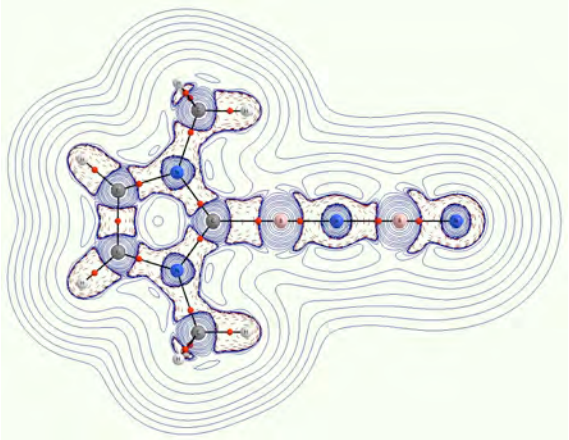

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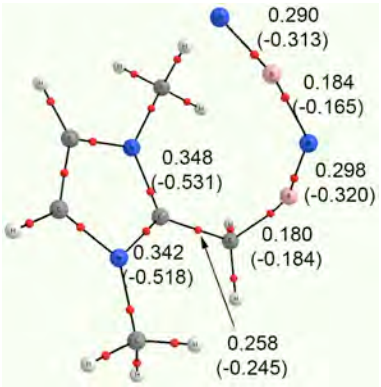

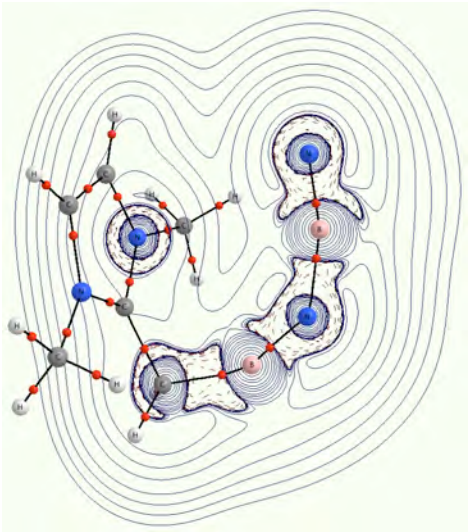

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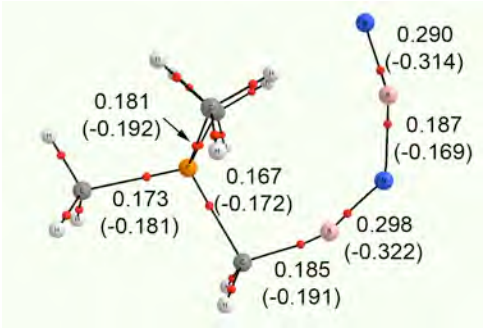
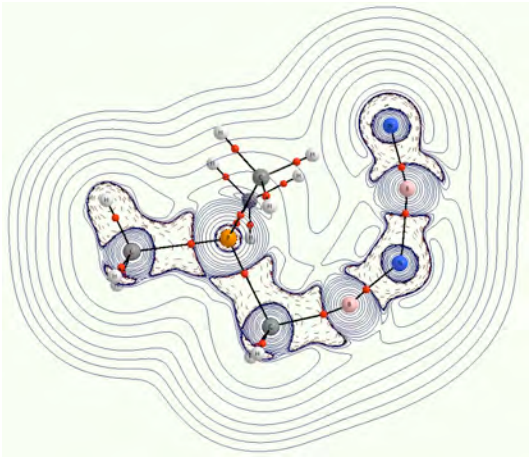
Me_3PCH_2·BNBN





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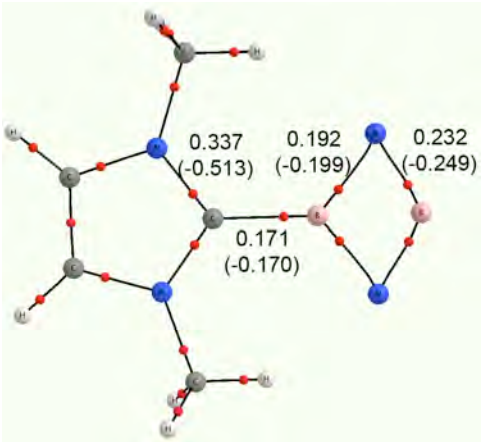
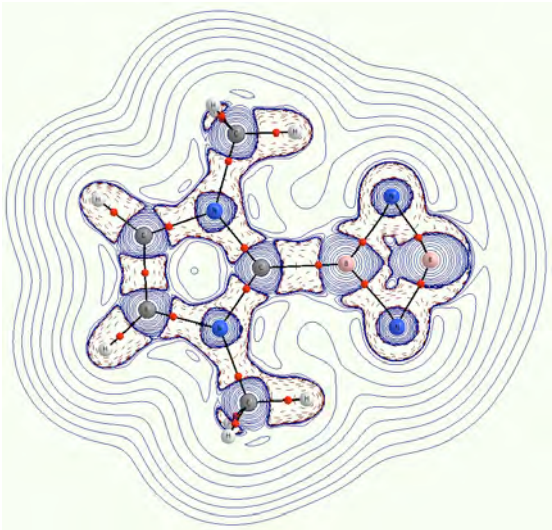
$ImMe_2{\cdot}B_2N_2$





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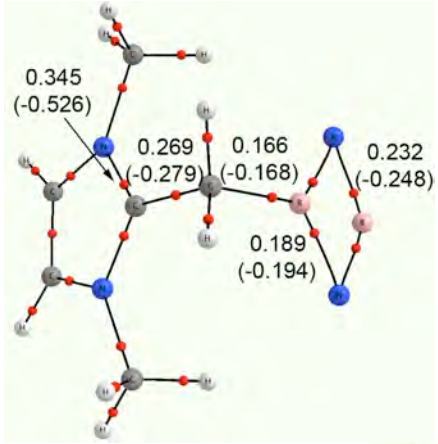

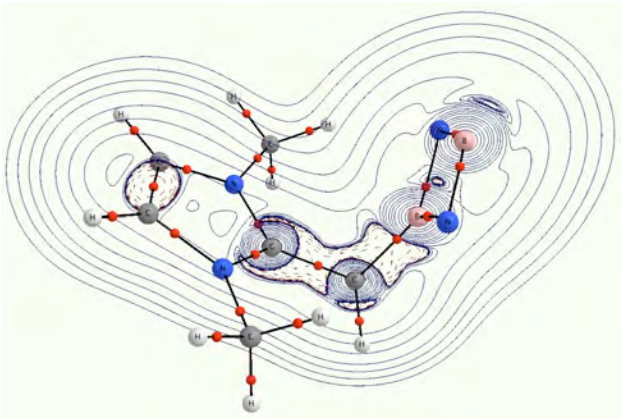

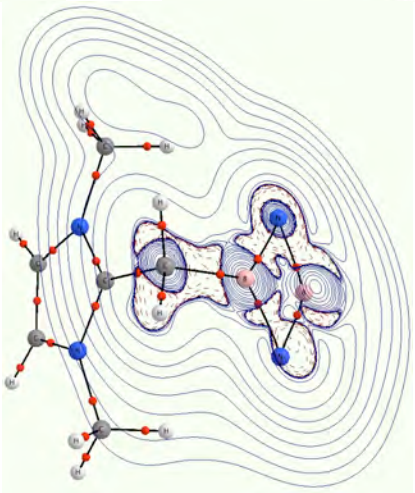

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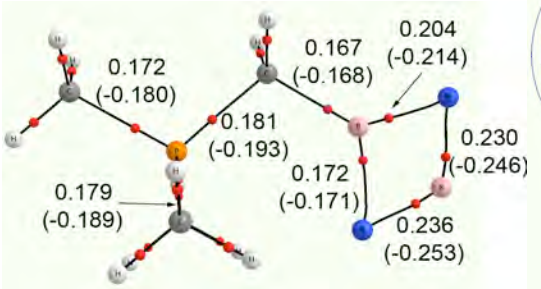

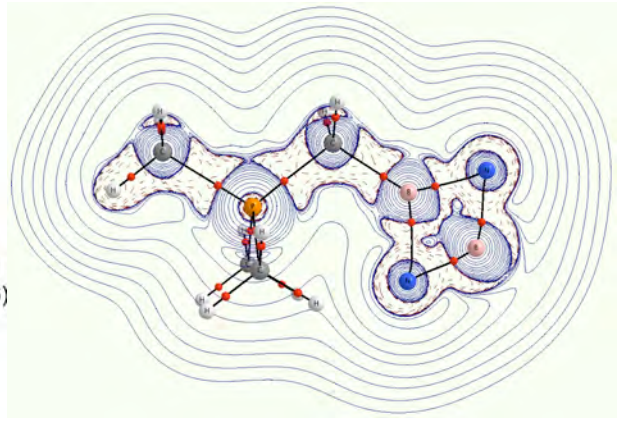

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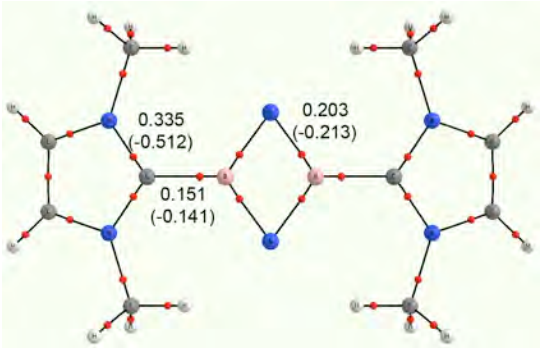
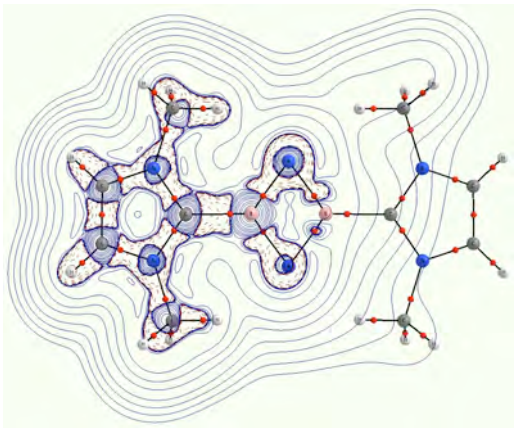
$(ImMe_2)_2 \cdot B_2N_2$





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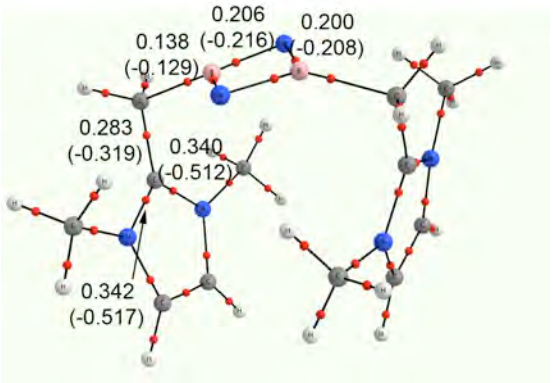

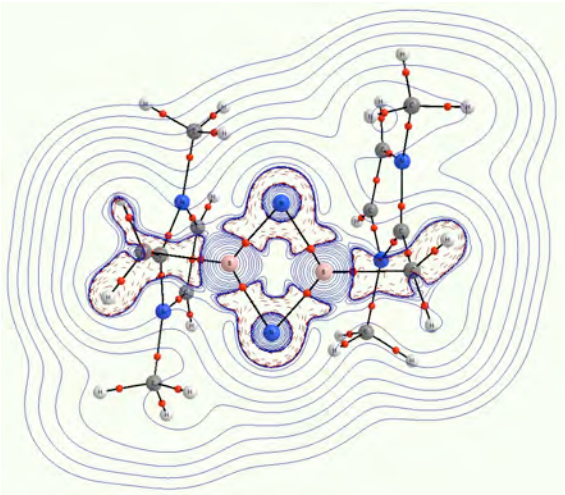

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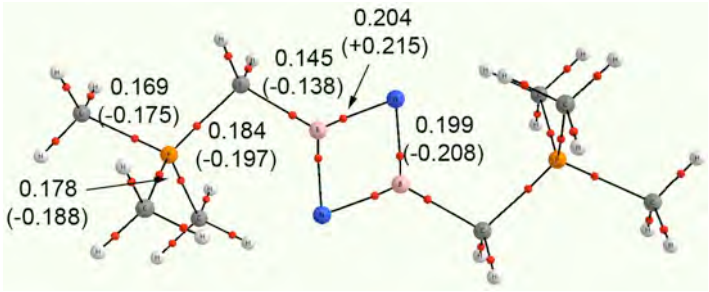

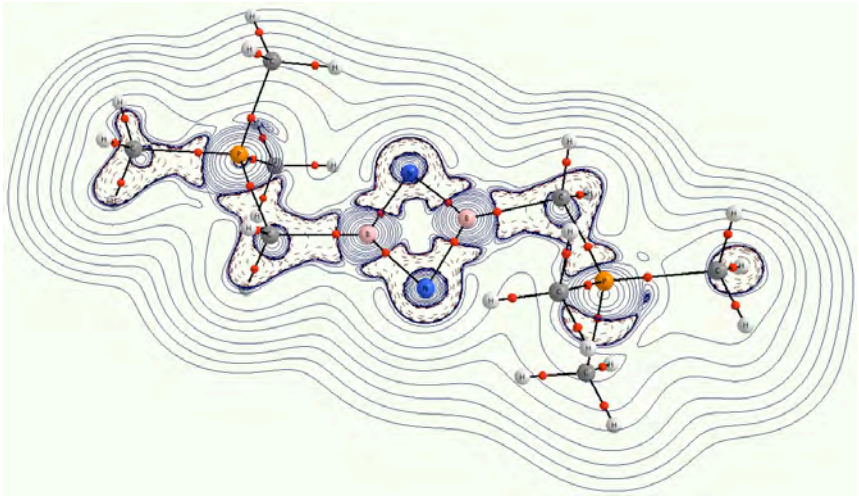

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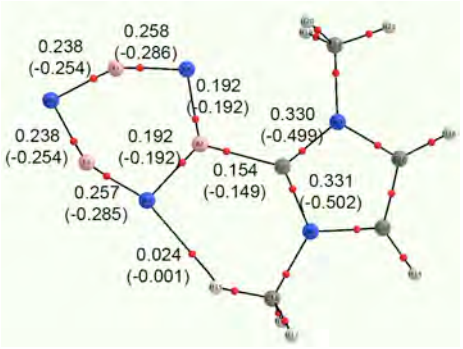
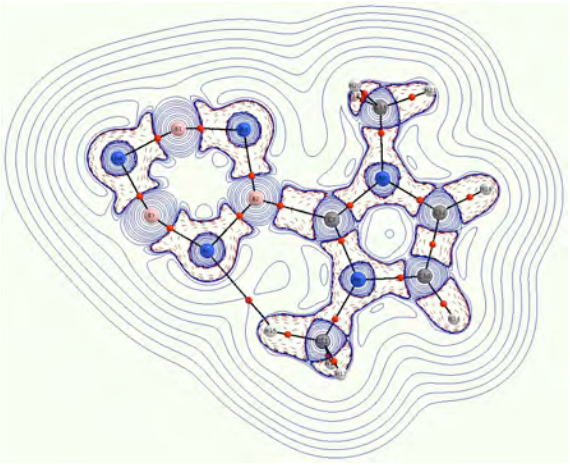
$ImMe_2 \cdot B_3N_3$





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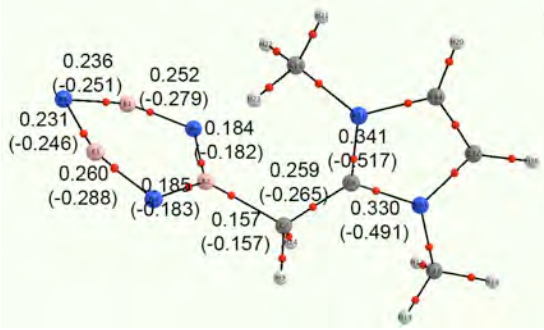
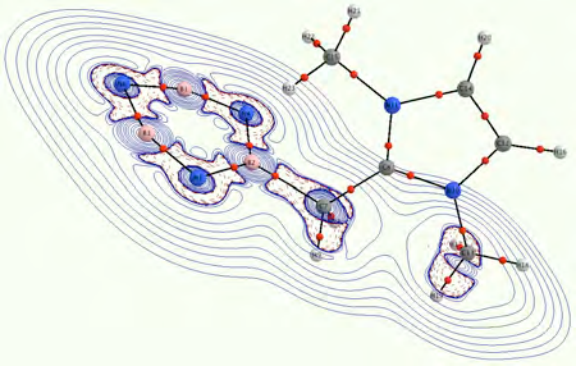
$ImMe_2CH_2 \cdot B_3N_3$





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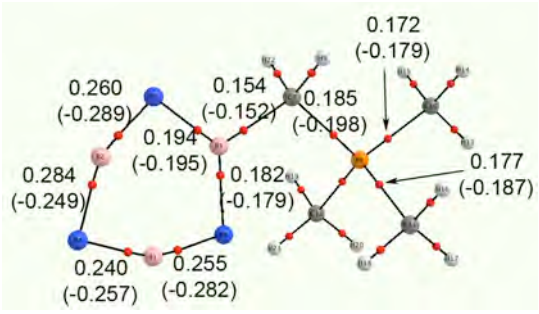
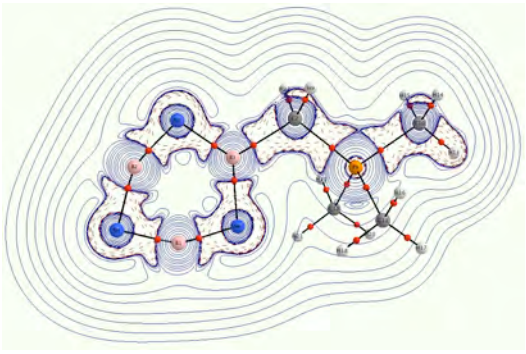
$Me_3PCH_2 \cdot B_3N_3$





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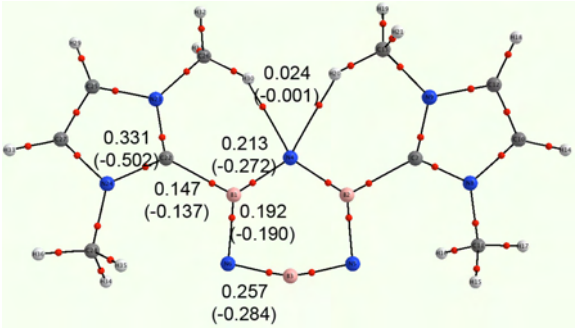
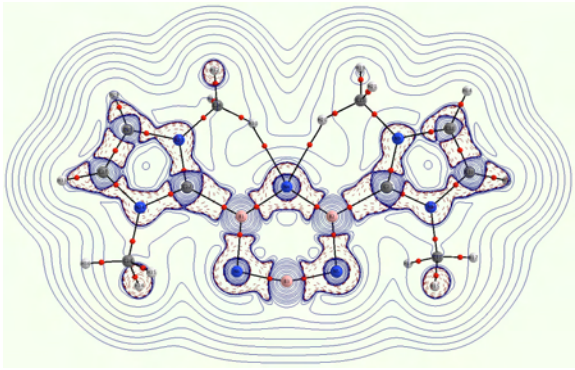
$(ImMe_2)_2 \cdot B_3N_3$





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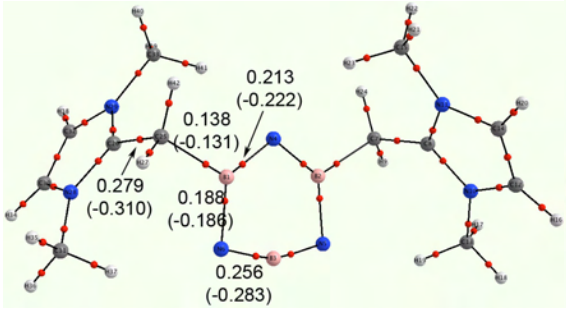
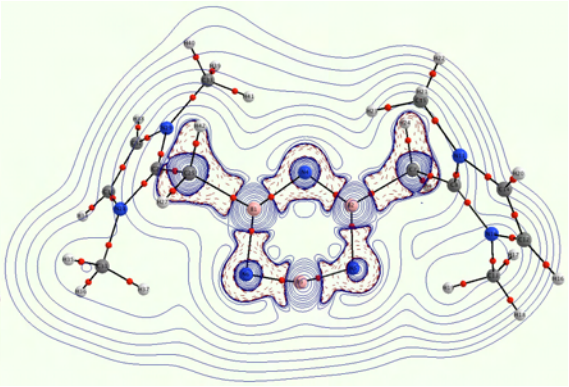
$(ImMe_2CH_2)_2 \cdot B_3N_3$





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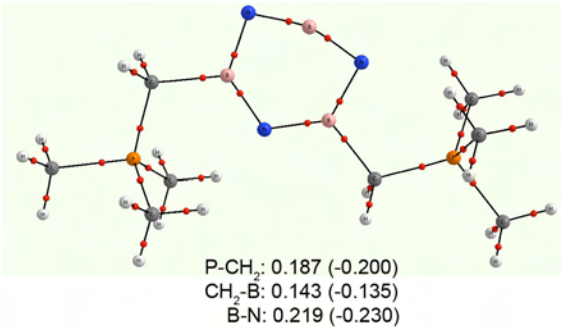
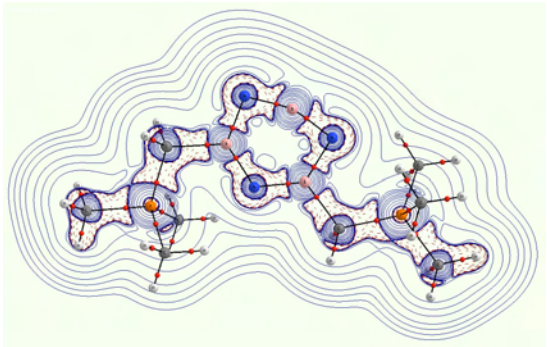
$(Me_3PCH_2)_2 \cdot B_3N_3$





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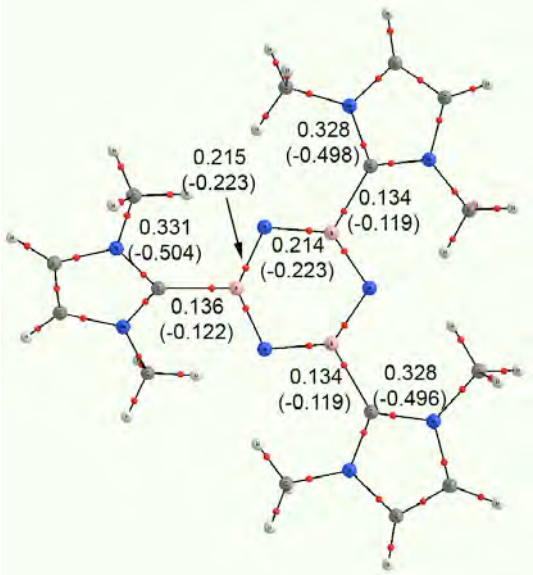
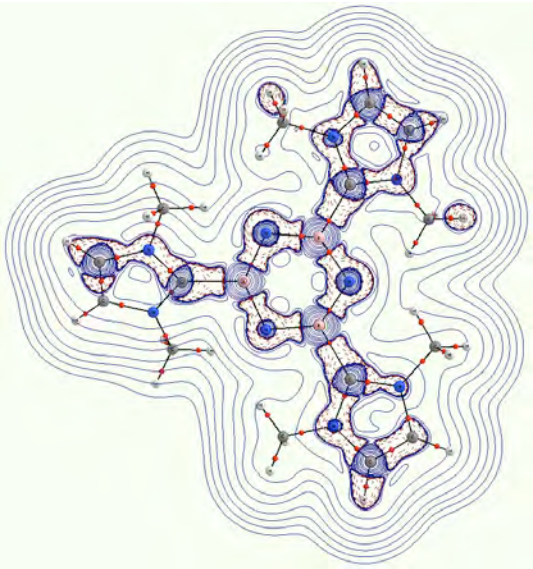
$(ImMe_2)_3 \cdot B_3N_3$





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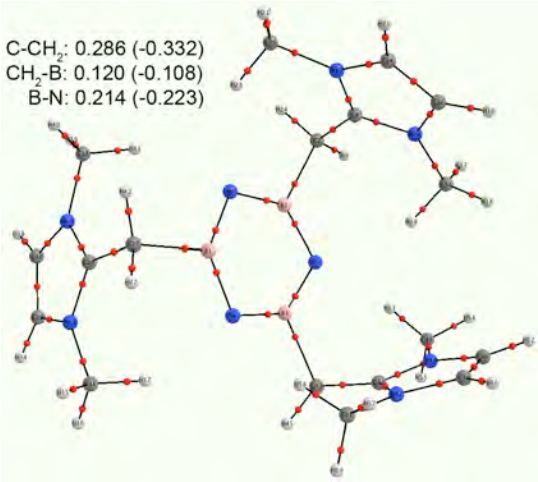
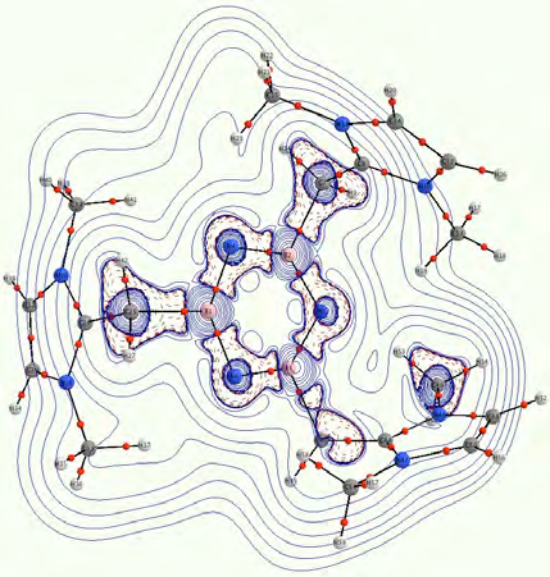
$(ImMe_2CH_2)_3\text{-}B_3N_3$





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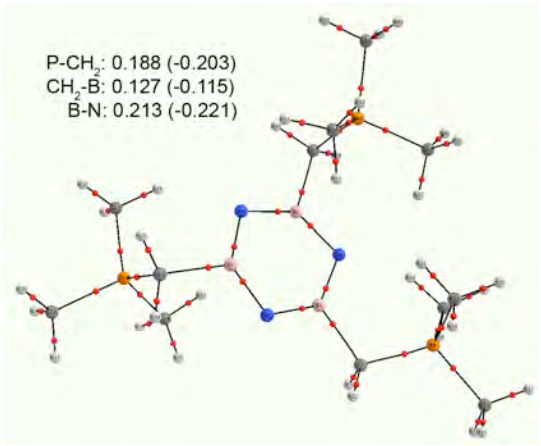
$(Me_3PCH_2)_3 \cdot B_3N_3$



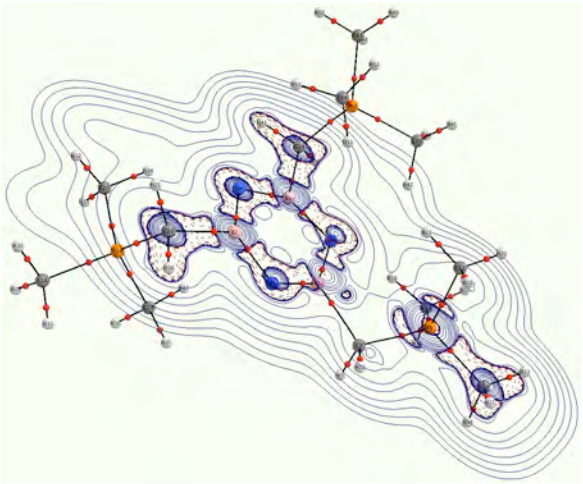


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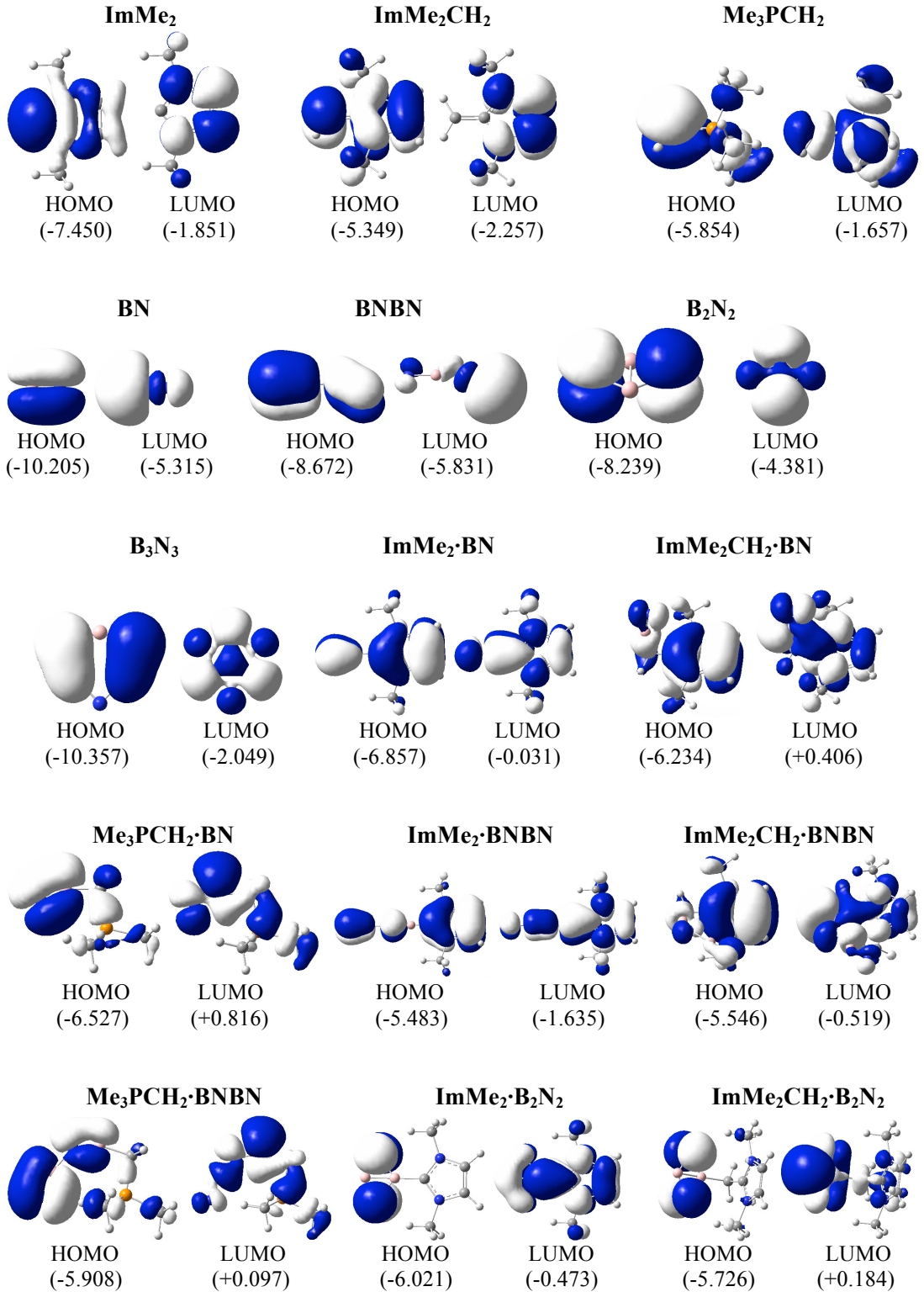
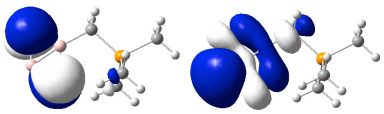
Figure S3: Highest Occupied (HOMO) and Lowest Unoccupied (LUMO) Molecular Orbitals of All the Studied Structures (Isovalue = 0.02) Computed at the M05-2X/cc-pVTZ Level of Theory. Energies (in eV) Are Also Given in Parentheses.

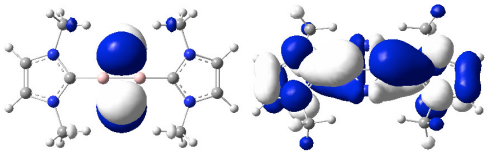


$Me_3PCH_2 \cdot B_2N_2$



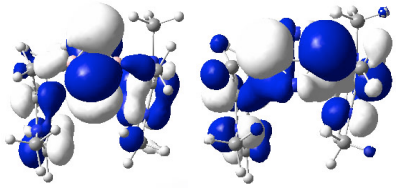
HOMO (-5.783) LUMO (+0.711)

$(ImMe_2)_2 \cdot B_2N_2$



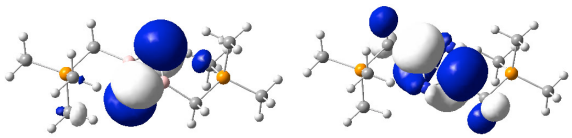
HOMO (-4.320) LUMO (+0.553)

$(ImMe_2CH_2)_2 \cdot B_2N_2$



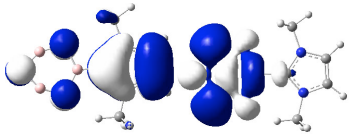
HOMO (-4.110) LUMO (+1.137)

$(Me_3PCH_2)_2 \cdot B_2N_2$



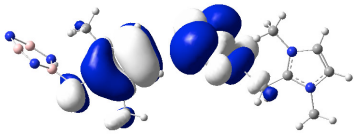
HOMO (-3.968) LUMO (+1.586)

$ImMe_2 \cdot B_3N_3$



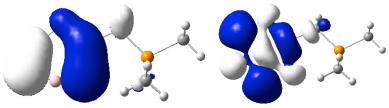
HOMO (-8.073) LUMO (-0.082)

$ImMe_2CH_2 \cdot B_3N_3$



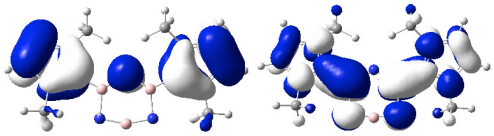
HOMO (-7.833) LUMO (+0.406)

$Me_3PCH_2 \cdot B_3N_3$



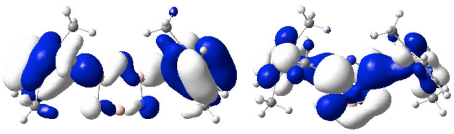
HOMO (-7.760) LUMO (+0.800)

$(ImMe_2)_2 \cdot B_3N_3$



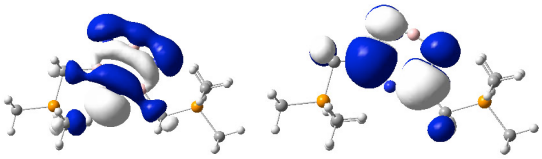
HOMO (-6.392) LUMO (+0.717)

$(ImMe_2CH_2)_2 \cdot B_3N_3$



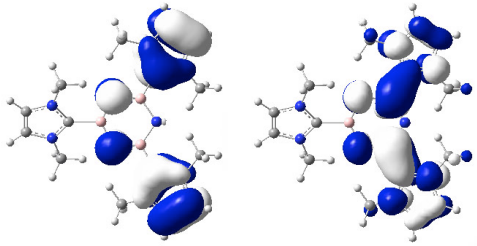
HOMO (-5.932) LUMO (+1.262)

$(Me_3PCH_2)_2 \cdot B_3N_3$



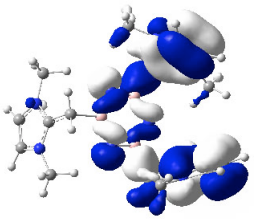
HOMO (-5.460) LUMO (+1.509)

$(ImMe_2)_3 \cdot B_3N_3$

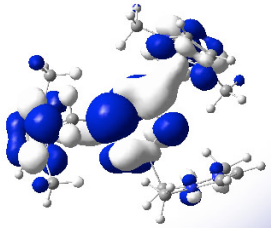


HOMO (-5.340) LUMO (+1.383)

$(ImMe_2CH_2)_3 \cdot B_3N_3$

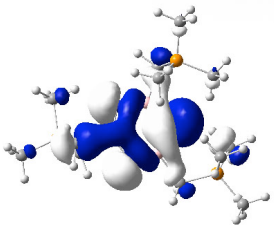


HOMO
(-4.888)

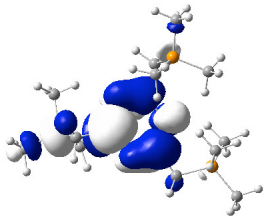


LUMO
(+1.688)

$(Me_3PCH_2)_3 \cdot B_3N_3$



HOMO
(-4.563)



LUMO
(+1.541)

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