

Supporting Information for:

Diazotization of the amino acid [*closo*-1-CB₉H₈-1-COOH-6-NH₃] and reactivity of the [*closo*-1-CB₉H₈-1-COO-6-N₂]⁻ anion

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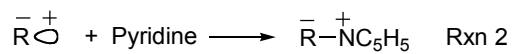
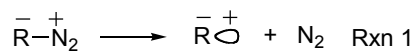
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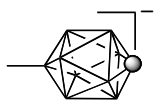
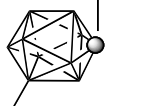
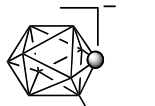
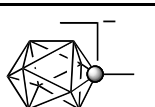
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Table S1. Calculated reaction energies for selected dinitrogen derivatives of the {*closo*-1-CB₉} in MeCN solutions.^a



	Rxn 1	Rxn 2	Rxns 1+2
	$\Delta\text{H} / \text{kcal mol}^{-1}$ $\Delta\text{G}_{298} / \text{kcal mol}^{-1}$	$\Delta\text{H} / \text{kcal mol}^{-1}$ $\Delta\text{G}_{298} / \text{kcal mol}^{-1}$	$\Delta\text{H} / \text{kcal mol}^{-1}$ $\Delta\text{G}_{298} / \text{kcal mol}^{-1}$
	41.9 30.9	-91.6 -79.4	-49.8 -48.5
	28.8 18.1	-77.1 -64.9	-48.3 -46.8
	33.9 23.2	-86.6 -74.6	-52.7 -51.4
	35.8 22.8	-103.5 -88.7	-67.7 -65.9

^a MP2/6-31G(d,p)//MP2/6-31G(d,p) level with DFT thermodynamic corrections in MeCN dielectric medium ($\epsilon = 36.64$, IPCM model).

2. Crystallographic data [*closo*-1-CB₉H₈-1-COOH-6-(1-NC₅H₅)] (4[6]a)

Data collection

A crystal (approximate dimensions 0.40x 0.34 x 0.08mm³) was placed onto the tip of a 0.1 mm diameter glass capillary and mounted on a CCD area detector diffractometer for a data collection at 123(2) K.¹ A preliminary set of cell constants was calculated from reflections harvested from four sets of 30 frames. These initial sets of frames were oriented such that orthogonal wedges of reciprocal space were surveyed. This produced initial orientation matrices determined from 165 reflections. The data collection was carried out using MoK α radiation (graphite monochromator) with a frame time of 45 seconds and a detector distance of 4.8 cm. A randomly oriented region of reciprocal space was surveyed to the extent of one sphere and to a resolution of 0.80 Å. Four major sections of frames were collected with 0.30° steps in ω at four different ϕ settings and a detector position of -28° in 2θ . The intensity data were corrected for absorption and decay (SADABS).² Final cell constants were calculated from 2997 strong reflections from the actual data collection after integration (SAINT).³ Please refer to Table 1 for additional crystal and refinement information.

Structure solution and refinement

The structure was solved using Bruker SHELXTL⁴ and refined using Bruker SHELXTL.⁴ The space group P2₁/n was determined based on systematic absences and intensity statistics. A direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Full-matrix least squares / difference Fourier cycles were performed which located the remaining non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters. The final full matrix least squares refinement converged to $R1 = 0.0387$ and $wR2 = 0.1086$ (F^2 , obs. data).

Structure description

The structure is the one suggested. The molecules form dimers through synergetic hydrogen bonds. It appears these are not disordered since a weak C-H hydrogen bond through H5B forms to O1.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 192 Kolthoff Hall, Department of Chemistry, University of Minnesota. All calculations were performed using Pentium computers using the current SHELXTL suite of programs. All publications arising from this report MUST either 1) include Victor G. Young, Jr. as a coauthor or 2) acknowledge Victor G. Young, Jr. and the X-Ray Crystallographic Laboratory.

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- ¹ SMART V5.054, Bruker Analytical X-ray Systems, Madison, WI (2001).
 - ² An empirical correction for absorption anisotropy, R. Blessing, *Acta Cryst.* **A51**, 33-38(1995).
 - ³ SAINT+ V7.34A, Bruker Analytical X-Ray Systems, Madison, WI (2003).
 - ⁴ SHELXTL V6.14, Bruker Analytical X-Ray Systems, Madison, WI (2000).

Some equations of interest:

$$R_{\text{int}} = \Sigma |F_o^2 - \langle F_o^2 \rangle| / \Sigma |F_o^2|$$

$$R_1 = \Sigma ||F_o| - |F_c|| / \Sigma |F_o|$$

$$wR2 = [\Sigma [w(F_o^2 - F_c^2)^2] / \Sigma [w(F_o^2)^2]]^{1/2}$$

$$\text{where } w = q / [\sigma^2(F_o^2) + (a^*P)^2 + b^*P + d + e^*\sin(\theta)]$$

$$\text{GooF} = S = [\Sigma [w(F_o^2 - F_c^2)^2] / (n-p)]^{1/2}$$

Table 1. Crystal data and structure refinement for 09177a.

Identification code	09177a	
Empirical formula	C7 H14 B9 N O2	
Formula weight	241.48	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2 ₁ /n	
Unit cell dimensions	$a = 6.6504(7)$ Å	$\alpha = 90^\circ$
	$b = 18.4803(18)$ Å	$\beta = 96.833(1)^\circ$
	$c = 10.8552(11)$ Å	$\gamma = 90^\circ$
Volume	1324.6(2) Å ³	
<i>Z</i>	4	
Density (calculated)	1.211 Mg/m ³	
Absorption coefficient	0.070 mm ⁻¹	
<i>F</i> (000)	496	
Crystal color, morphology	Colorless, Plate	
Crystal size	0.40 x 0.34 x 0.08 mm ³	
Theta range for data collection	2.19 to 26.36°	
Index ranges	-8 ≤ <i>h</i> ≤ 8, 0 ≤ <i>k</i> ≤ 23, 0 ≤ <i>l</i> ≤ 13	
Reflections collected	15107	
Independent reflections	2715 [<i>R</i> (int) = 0.0346]	
Observed reflections	2252	
Completeness to theta = 26.36°	99.8%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.9944 and 0.9724	
Refinement method	Full-matrix least-squares on <i>F</i> ²	
Data / restraints / parameters	2715 / 0 / 173	
Goodness-of-fit on <i>F</i> ²	1.080	
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> 1 = 0.0387, <i>wR</i> 2 = 0.0999	
<i>R</i> indices (all data)	<i>R</i> 1 = 0.0509, <i>wR</i> 2 = 0.1093	
Largest diff. peak and hole	0.267 and -0.210 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 09177a. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U_{eq}
B1	7514(2)	1768(1)	3839(1)	20(1)
B2	5334(2)	1381(1)	4184(1)	17(1)
B3	7264(2)	872(1)	3480(1)	20(1)
B4	7278(2)	1594(1)	2295(1)	21(1)
B5	5360(2)	2104(1)	3030(1)	19(1)
B6	4637(2)	587(1)	3267(1)	18(1)
B7	6015(2)	738(1)	1915(1)	21(1)
B8	4674(2)	1610(1)	1607(1)	20(1)
B9	3286(2)	1463(1)	2945(1)	18(1)
C1	3621(2)	859(1)	1928(1)	18(1)
C2	2005(2)	488(1)	1101(1)	19(1)
O1	1229(2)	774(1)	136(1)	28(1)
O2	1511(2)	-150(1)	1462(1)	35(1)
N1	4733(2)	1392(1)	5518(1)	19(1)
C3	6029(2)	1653(1)	6470(1)	23(1)
C4	5544(2)	1649(1)	7667(1)	28(1)
C5	3694(2)	1380(1)	7909(1)	27(1)
C6	2369(2)	1117(1)	6933(1)	26(1)
C7	2921(2)	1128(1)	5752(1)	23(1)

Table 3. Bond lengths [Å] and angles [°] for 09177a.

B(1)-B(4)	1.696(2)	B(6)-H(6A)	1.1200
B(1)-B(2)	1.697(2)	B(7)-C(1)	1.610(2)
B(1)-B(3)	1.704(2)	B(7)-B(8)	1.853(2)
B(1)-B(5)	1.706(2)	B(7)-H(7A)	1.1200
B(1)-H(1A)	1.1200	B(8)-C(1)	1.612(2)
B(2)-N(1)	1.5470(18)	B(8)-B(9)	1.831(2)
B(2)-B(6)	1.802(2)	B(8)-H(8A)	1.1200
B(2)-B(9)	1.803(2)	B(9)-C(1)	1.605(2)
B(2)-B(3)	1.831(2)	B(9)-H(9A)	1.1200
B(2)-B(5)	1.832(2)	C(1)-C(2)	1.4835(18)
B(3)-B(6)	1.813(2)	C(2)-O(1)	1.2308(17)
B(3)-B(7)	1.817(2)	C(2)-O(2)	1.2958(17)
B(3)-B(4)	1.855(2)	O(2)-H(2B)	0.8400
B(3)-H(3A)	1.1200	N(1)-C(3)	1.3537(17)
B(4)-B(8)	1.803(2)	N(1)-C(7)	1.3514(18)
B(4)-B(7)	1.816(2)	C(3)-C(4)	1.376(2)
B(4)-B(5)	1.842(2)	C(3)-H(3B)	0.9500
B(4)-H(4A)	1.1200	C(4)-C(5)	1.381(2)
B(5)-B(8)	1.806(2)	C(4)-H(4B)	0.9500
B(5)-B(9)	1.812(2)	C(5)-C(6)	1.384(2)
B(5)-H(5A)	1.1200	C(5)-H(5B)	0.9500
B(6)-C(1)	1.6087(19)	C(6)-C(7)	1.375(2)
B(6)-B(7)	1.842(2)	C(6)-H(6B)	0.9500
B(6)-B(9)	1.864(2)	C(7)-H(7B)	0.9500
B(4)-B(1)-B(2)	99.06(10)	B(5)-B(1)-H(1A)	129.8
B(4)-B(1)-B(3)	66.11(9)	N(1)-B(2)-B(1)	121.59(11)
B(2)-B(1)-B(3)	65.14(9)	N(1)-B(2)-B(6)	116.64(11)
B(4)-B(1)-B(5)	65.58(9)	B(1)-B(2)-B(6)	113.01(11)
B(2)-B(1)-B(5)	65.14(9)	N(1)-B(2)-B(9)	116.13(11)
B(3)-B(1)-B(5)	100.55(11)	B(1)-B(2)-B(9)	112.94(11)
B(4)-B(1)-H(1A)	130.1	B(6)-B(2)-B(9)	62.27(8)
B(2)-B(1)-H(1A)	130.8	N(1)-B(2)-B(3)	131.99(11)
B(3)-B(1)-H(1A)	129.6	B(1)-B(2)-B(3)	57.62(9)

B(6)-B(2)-B(3)	59.85(8)	B(3)-B(4)-H(4A)	131.1
B(9)-B(2)-B(3)	103.69(10)	B(1)-B(5)-B(8)	111.54(11)
N(1)-B(2)-B(5)	130.93(11)	B(1)-B(5)-B(9)	112.06(11)
B(1)-B(2)-B(5)	57.67(8)	B(8)-B(5)-B(9)	60.83(8)
B(6)-B(2)-B(5)	103.82(10)	B(1)-B(5)-B(2)	57.19(8)
B(9)-B(2)-B(5)	59.79(8)	B(8)-B(5)-B(2)	101.20(10)
B(3)-B(2)-B(5)	91.46(10)	B(9)-B(5)-B(2)	59.31(8)
B(1)-B(3)-B(6)	112.15(11)	B(1)-B(5)-B(4)	56.93(8)
B(1)-B(3)-B(7)	111.59(11)	B(8)-B(5)-B(4)	59.21(8)
B(6)-B(3)-B(7)	60.99(8)	B(9)-B(5)-B(4)	101.87(10)
B(1)-B(3)-B(2)	57.24(8)	B(2)-B(5)-B(4)	89.24(10)
B(6)-B(3)-B(2)	59.29(8)	B(1)-B(5)-H(5A)	118.5
B(7)-B(3)-B(2)	101.26(10)	B(8)-B(5)-H(5A)	120.7
B(1)-B(3)-B(4)	56.72(9)	B(9)-B(5)-H(5A)	120.2
B(6)-B(3)-B(4)	101.81(10)	B(2)-B(5)-H(5A)	131.6
B(7)-B(3)-B(4)	59.29(8)	B(4)-B(5)-H(5A)	131.5
B(2)-B(3)-B(4)	88.90(10)	C(1)-B(6)-B(2)	107.34(11)
B(1)-B(3)-H(3A)	118.5	C(1)-B(6)-B(3)	108.63(11)
B(6)-B(3)-H(3A)	120.1	B(2)-B(6)-B(3)	60.86(8)
B(7)-B(3)-H(3A)	120.6	C(1)-B(6)-B(7)	55.12(8)
B(2)-B(3)-H(3A)	131.7	B(2)-B(6)-B(7)	101.40(10)
B(4)-B(3)-H(3A)	131.7	B(3)-B(6)-B(7)	59.61(8)
B(1)-B(4)-B(8)	112.20(11)	C(1)-B(6)-B(9)	54.45(8)
B(1)-B(4)-B(7)	112.03(11)	B(2)-B(6)-B(9)	58.88(8)
B(8)-B(4)-B(7)	61.61(9)	B(3)-B(6)-B(9)	102.00(10)
B(1)-B(4)-B(5)	57.49(8)	B(7)-B(6)-B(9)	89.66(10)
B(8)-B(4)-B(5)	59.38(8)	C(1)-B(6)-H(6A)	122.2
B(7)-B(4)-B(5)	102.64(10)	B(2)-B(6)-H(6A)	121.6
B(1)-B(4)-B(3)	57.17(9)	B(3)-B(6)-H(6A)	120.6
B(8)-B(4)-B(3)	102.42(10)	B(7)-B(6)-H(6A)	130.9
B(7)-B(4)-B(3)	59.32(8)	B(9)-B(6)-H(6A)	131.2
B(5)-B(4)-B(3)	90.39(10)	C(1)-B(7)-B(3)	108.40(11)
B(1)-B(4)-H(4A)	118.4	C(1)-B(7)-B(4)	107.95(11)
B(8)-B(4)-H(4A)	120.0	B(3)-B(7)-B(4)	61.39(9)
B(7)-B(4)-H(4A)	120.0	C(1)-B(7)-B(6)	55.07(8)
B(5)-B(4)-H(4A)	130.8	B(3)-B(7)-B(6)	59.40(8)

B(4)-B(7)-B(6)	102.18(10)	B(2)-B(9)-H(9A)	121.6
C(1)-B(7)-B(8)	54.93(8)	B(5)-B(9)-H(9A)	120.6
B(3)-B(7)-B(8)	101.92(10)	B(8)-B(9)-H(9A)	130.8
B(4)-B(7)-B(8)	58.83(8)	B(6)-B(9)-H(9A)	131.0
B(6)-B(7)-B(8)	90.02(10)	C(2)-C(1)-B(9)	126.00(11)
C(1)-B(7)-H(7A)	122.1	C(2)-C(1)-B(6)	126.82(12)
B(3)-B(7)-H(7A)	120.7	B(9)-C(1)-B(6)	70.91(9)
B(4)-B(7)-H(7A)	121.0	C(2)-C(1)-B(7)	125.23(12)
B(6)-B(7)-H(7A)	130.7	B(9)-C(1)-B(7)	108.74(11)
B(8)-B(7)-H(7A)	131.1	B(6)-C(1)-B(7)	69.82(9)
C(1)-B(8)-B(4)	108.50(11)	C(2)-C(1)-B(8)	124.69(11)
C(1)-B(8)-B(5)	108.83(11)	B(9)-C(1)-B(8)	69.41(9)
B(4)-B(8)-B(5)	61.41(9)	B(6)-C(1)-B(8)	108.49(11)
C(1)-B(8)-B(9)	55.12(8)	B(7)-C(1)-B(8)	70.25(10)
B(4)-B(8)-B(9)	102.67(10)	O(1)-C(2)-O(2)	123.54(12)
B(5)-B(8)-B(9)	59.76(8)	O(1)-C(2)-C(1)	121.10(12)
C(1)-B(8)-B(7)	54.82(8)	O(2)-C(2)-C(1)	115.36(12)
B(4)-B(8)-B(7)	59.55(8)	C(2)-O(2)-H(2B)	109.5
B(5)-B(8)-B(7)	102.62(10)	C(3)-N(1)-C(7)	119.05(12)
B(9)-B(8)-B(7)	90.32(10)	C(3)-N(1)-B(2)	120.46(11)
C(1)-B(8)-H(8A)	122.0	C(7)-N(1)-B(2)	120.49(11)
B(4)-B(8)-H(8A)	120.6	N(1)-C(3)-C(4)	121.33(13)
B(5)-B(8)-H(8A)	120.4	N(1)-C(3)-H(3B)	119.3
B(9)-B(8)-H(8A)	130.5	C(4)-C(3)-H(3B)	119.3
B(7)-B(8)-H(8A)	130.8	C(3)-C(4)-C(5)	119.74(14)
C(1)-B(9)-B(2)	107.47(10)	C(3)-C(4)-H(4B)	120.1
C(1)-B(9)-B(5)	108.84(11)	C(5)-C(4)-H(4B)	120.1
B(2)-B(9)-B(5)	60.90(8)	C(4)-C(5)-C(6)	118.77(13)
C(1)-B(9)-B(8)	55.47(8)	C(4)-C(5)-H(5B)	120.6
B(2)-B(9)-B(8)	101.33(10)	C(6)-C(5)-H(5B)	120.6
B(5)-B(9)-B(8)	59.42(8)	C(7)-C(6)-C(5)	119.50(14)
C(1)-B(9)-B(6)	54.64(8)	C(7)-C(6)-H(6B)	120.2
B(2)-B(9)-B(6)	58.85(8)	C(5)-C(6)-H(6B)	120.2
B(5)-B(9)-B(6)	102.17(10)	N(1)-C(7)-C(6)	121.61(13)
B(8)-B(9)-B(6)	90.00(9)	N(1)-C(7)-H(7B)	119.2
C(1)-B(9)-H(9A)	122.0	C(6)-C(7)-H(7B)	119.2

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 09177a. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
B1	17(1)	24(1)	18(1)	-2(1)	1(1)	-2(1)
B2	18(1)	20(1)	13(1)	-1(1)	0(1)	0(1)
B3	16(1)	25(1)	19(1)	-3(1)	-1(1)	1(1)
B4	19(1)	26(1)	19(1)	-3(1)	3(1)	-4(1)
B5	20(1)	20(1)	18(1)	0(1)	1(1)	-2(1)
B6	18(1)	19(1)	16(1)	-1(1)	-1(1)	0(1)
B7	20(1)	24(1)	18(1)	-4(1)	1(1)	-1(1)
B8	21(1)	23(1)	17(1)	1(1)	0(1)	-3(1)
B9	17(1)	20(1)	16(1)	0(1)	-1(1)	-1(1)
C1	19(1)	22(1)	14(1)	0(1)	-1(1)	-2(1)
C2	19(1)	23(1)	16(1)	-2(1)	2(1)	-2(1)
O1	29(1)	33(1)	19(1)	4(1)	-7(1)	-9(1)
O2	42(1)	31(1)	27(1)	6(1)	-16(1)	-17(1)
N1	21(1)	18(1)	16(1)	-1(1)	0(1)	1(1)
C3	25(1)	26(1)	19(1)	-2(1)	-1(1)	-3(1)
C4	35(1)	29(1)	18(1)	-4(1)	-1(1)	-3(1)
C5	40(1)	24(1)	18(1)	-1(1)	7(1)	2(1)
C6	29(1)	25(1)	24(1)	-1(1)	8(1)	-1(1)
C7	24(1)	24(1)	21(1)	-2(1)	2(1)	-2(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 09177a.

	x	y	z	U(eq)
H1A	8746	2054	4445	24
H3A	8471	489	3886	24
H4A	8503	1785	1749	25
H5A	5055	2699	3082	23
H6A	4160	75	3701	22
H7A	6631	343	1272	25
H8A	4227	1906	716	24
H9A	1737	1642	3123	21
H2B	630	-329	931	42
H3B	7299	1843	6308	28
H4B	6478	1831	8324	33
H5B	3338	1375	8731	33
H6B	1086	931	7077	31
H7B	2008	946	5085	28

Table 6. Torsion angles [°] for 09177a.

B4-B1-B2-N1	-179.04(12)	B9-B2-B3-B7	0.16(12)
B3-B1-B2-N1	122.68(13)	B5-B2-B3-B7	-59.06(11)
B5-B1-B2-N1	-121.40(13)	N1-B2-B3-B4	-155.48(14)
B4-B1-B2-B6	34.55(14)	B1-B2-B3-B4	-50.19(9)
B3-B1-B2-B6	-23.72(11)	B6-B2-B3-B4	104.45(10)
B5-B1-B2-B6	92.20(11)	B9-B2-B3-B4	58.51(11)
B4-B1-B2-B9	-33.78(14)	B5-B2-B3-B4	-0.70(9)
B3-B1-B2-B9	-92.06(12)	B2-B1-B4-B8	33.18(14)
B5-B1-B2-B9	23.86(11)	B3-B1-B4-B8	90.75(12)
B4-B1-B2-B3	58.28(10)	B5-B1-B4-B8	-24.15(11)
B5-B1-B2-B3	115.92(10)	B2-B1-B4-B7	-33.94(14)
B4-B1-B2-B5	-57.64(10)	B3-B1-B4-B7	23.63(11)
B3-B1-B2-B5	-115.92(10)	B5-B1-B4-B7	-91.27(12)
B4-B1-B3-B6	-89.84(12)	B2-B1-B4-B5	57.32(10)
B2-B1-B3-B6	23.42(11)	B3-B1-B4-B5	114.90(10)
B5-B1-B3-B6	-32.68(14)	B2-B1-B4-B3	-57.58(10)
B4-B1-B3-B7	-23.55(11)	B5-B1-B4-B3	-114.90(10)
B2-B1-B3-B7	89.72(11)	B6-B3-B4-B1	108.87(11)
B5-B1-B3-B7	33.61(13)	B7-B3-B4-B1	154.40(12)
B4-B1-B3-B2	-113.26(10)	B2-B3-B4-B1	50.60(9)
B5-B1-B3-B2	-56.11(9)	B1-B3-B4-B8	-108.56(11)
B2-B1-B3-B4	113.26(10)	B6-B3-B4-B8	0.31(12)
B5-B1-B3-B4	57.16(10)	B7-B3-B4-B8	45.84(10)
N1-B2-B3-B1	-105.29(16)	B2-B3-B4-B8	-57.96(11)
B6-B2-B3-B1	154.64(11)	B1-B3-B4-B7	-154.40(12)
B9-B2-B3-B1	108.70(11)	B6-B3-B4-B7	-45.53(9)
B5-B2-B3-B1	49.48(9)	B2-B3-B4-B7	-103.80(10)
N1-B2-B3-B6	100.07(15)	B1-B3-B4-B5	-49.90(9)
B1-B2-B3-B6	-154.64(11)	B6-B3-B4-B5	58.97(10)
B9-B2-B3-B6	-45.94(10)	B7-B3-B4-B5	104.50(10)
B5-B2-B3-B6	-105.16(10)	B2-B3-B4-B5	0.70(9)
N1-B2-B3-B7	146.17(13)	B4-B1-B5-B8	23.98(11)
B1-B2-B3-B7	-108.54(11)	B2-B1-B5-B8	-89.66(11)
B6-B2-B3-B7	46.10(9)	B3-B1-B5-B8	-33.54(13)

B4-B1-B5-B9	90.06(12)	B8-B4-B5-B2	103.53(10)
B2-B1-B5-B9	-23.58(10)	B7-B4-B5-B2	57.88(10)
B3-B1-B5-B9	32.54(13)	B3-B4-B5-B2	-0.70(9)
B4-B1-B5-B2	113.64(11)	N1-B2-B6-C1	132.89(11)
B3-B1-B5-B2	56.11(10)	B1-B2-B6-C1	-78.94(13)
B2-B1-B5-B4	-113.64(11)	B9-B2-B6-C1	25.85(10)
B3-B1-B5-B4	-57.53(10)	B3-B2-B6-C1	-102.07(12)
N1-B2-B5-B1	105.77(15)	B5-B2-B6-C1	-18.53(13)
B6-B2-B5-B1	-108.70(11)	N1-B2-B6-B3	-125.04(13)
B9-B2-B5-B1	-154.46(12)	B1-B2-B6-B3	23.14(11)
B3-B2-B5-B1	-49.44(9)	B9-B2-B6-B3	127.93(11)
N1-B2-B5-B8	-145.71(13)	B5-B2-B6-B3	83.54(10)
B1-B2-B5-B8	108.52(11)	N1-B2-B6-B7	-170.36(10)
B6-B2-B5-B8	-0.18(12)	B1-B2-B6-B7	-22.19(13)
B9-B2-B5-B8	-45.94(9)	B9-B2-B6-B7	82.60(10)
B3-B2-B5-B8	59.08(10)	B3-B2-B6-B7	-45.32(9)
N1-B2-B5-B9	-99.77(15)	B5-B2-B6-B7	38.22(12)
B1-B2-B5-B9	154.46(12)	N1-B2-B6-B9	107.03(12)
B6-B2-B5-B9	45.76(9)	B1-B2-B6-B9	-104.79(12)
B3-B2-B5-B9	105.02(10)	B3-B2-B6-B9	-127.93(11)
N1-B2-B5-B4	155.92(13)	B5-B2-B6-B9	-44.39(9)
B1-B2-B5-B4	50.15(9)	B1-B3-B6-C1	77.03(14)
B6-B2-B5-B4	-58.55(10)	B7-B3-B6-C1	-26.18(10)
B9-B2-B5-B4	-104.31(10)	B2-B3-B6-C1	99.91(12)
B3-B2-B5-B4	0.71(9)	B4-B3-B6-C1	18.37(13)
B8-B4-B5-B1	153.89(12)	B1-B3-B6-B2	-22.88(10)
B7-B4-B5-B1	108.23(11)	B7-B3-B6-B2	-126.09(10)
B3-B4-B5-B1	49.66(9)	B4-B3-B6-B2	-81.54(10)
B1-B4-B5-B8	-153.89(12)	B1-B3-B6-B7	103.21(12)
B7-B4-B5-B8	-45.66(10)	B2-B3-B6-B7	126.09(10)
B3-B4-B5-B8	-104.23(10)	B4-B3-B6-B7	44.55(9)
B1-B4-B5-B9	-108.73(11)	B1-B3-B6-B9	20.78(14)
B8-B4-B5-B9	45.16(9)	B7-B3-B6-B9	-82.43(10)
B7-B4-B5-B9	-0.49(12)	B2-B3-B6-B9	43.66(9)
B3-B4-B5-B9	-59.07(10)	B4-B3-B6-B9	-37.88(12)
B1-B4-B5-B2	-50.36(9)	B1-B3-B7-C1	-78.00(14)

B6-B3-B7-C1	26.13(10)	B9-B6-B7-B4	58.32(10)
B2-B3-B7-C1	-18.97(13)	C1-B6-B7-B8	45.48(9)
B4-B3-B7-C1	-100.86(12)	B2-B6-B7-B8	-57.82(10)
B1-B3-B7-B4	22.86(11)	B3-B6-B7-B8	-103.87(10)
B6-B3-B7-B4	126.99(11)	B9-B6-B7-B8	0.28(9)
B2-B3-B7-B4	81.89(10)	B1-B4-B8-C1	-78.22(14)
B1-B3-B7-B6	-104.13(12)	B7-B4-B8-C1	25.66(10)
B2-B3-B7-B6	-45.10(9)	B5-B4-B8-C1	-101.85(12)
B4-B3-B7-B6	-126.99(11)	B3-B4-B8-C1	-18.86(13)
B1-B3-B7-B8	-21.28(14)	B1-B4-B8-B5	23.63(11)
B6-B3-B7-B8	82.85(10)	B7-B4-B8-B5	127.51(11)
B2-B3-B7-B8	37.75(12)	B3-B4-B8-B5	82.98(10)
B4-B3-B7-B8	-44.14(9)	B1-B4-B8-B9	-21.10(14)
B1-B4-B7-C1	78.55(14)	B7-B4-B8-B9	82.79(10)
B8-B4-B7-C1	-25.61(10)	B5-B4-B8-B9	-44.73(9)
B5-B4-B7-C1	18.78(13)	B3-B4-B8-B9	38.26(12)
B3-B4-B7-C1	101.61(12)	B1-B4-B8-B7	-103.88(12)
B1-B4-B7-B3	-23.06(11)	B5-B4-B8-B7	-127.51(11)
B8-B4-B7-B3	-127.22(10)	B3-B4-B8-B7	-44.53(9)
B5-B4-B7-B3	-82.83(10)	B1-B5-B8-C1	77.94(13)
B1-B4-B7-B6	21.64(14)	B9-B5-B8-C1	-26.07(10)
B8-B4-B7-B6	-82.53(10)	B2-B5-B8-C1	18.98(13)
B5-B4-B7-B6	-38.13(12)	B4-B5-B8-C1	101.30(12)
B3-B4-B7-B6	44.69(9)	B1-B5-B8-B4	-23.36(10)
B1-B4-B7-B8	104.16(12)	B9-B5-B8-B4	-127.37(11)
B5-B4-B7-B8	44.39(9)	B2-B5-B8-B4	-82.32(10)
B3-B4-B7-B8	127.22(10)	B1-B5-B8-B9	104.01(12)
B2-B6-B7-C1	-103.30(11)	B2-B5-B8-B9	45.05(9)
B3-B6-B7-C1	-149.36(12)	B4-B5-B8-B9	127.37(11)
B9-B6-B7-C1	-45.20(9)	B1-B5-B8-B7	21.13(14)
C1-B6-B7-B3	149.36(12)	B9-B5-B8-B7	-82.88(10)
B2-B6-B7-B3	46.06(9)	B2-B5-B8-B7	-37.83(12)
B9-B6-B7-B3	104.16(10)	B4-B5-B8-B7	44.49(9)
C1-B6-B7-B4	103.52(11)	B3-B7-B8-C1	-104.23(11)
B2-B6-B7-B4	0.22(12)	B4-B7-B8-C1	-149.84(12)
B3-B6-B7-B4	-45.84(10)	B6-B7-B8-C1	-45.58(9)

C1-B7-B8-B4	149.84(12)	B1-B5-B9-B8	-103.15(12)
B3-B7-B8-B4	45.60(9)	B2-B5-B9-B8	-126.16(10)
B6-B7-B8-B4	104.26(10)	B4-B5-B9-B8	-44.24(9)
C1-B7-B8-B5	104.30(11)	B1-B5-B9-B6	-20.47(13)
B3-B7-B8-B5	0.06(12)	B8-B5-B9-B6	82.68(10)
B4-B7-B8-B5	-45.54(10)	B2-B5-B9-B6	-43.48(9)
B6-B7-B8-B5	58.72(10)	B4-B5-B9-B6	38.44(11)
C1-B7-B8-B9	45.29(9)	B4-B8-B9-C1	-103.87(11)
B3-B7-B8-B9	-58.94(10)	B5-B8-B9-C1	-149.54(12)
B4-B7-B8-B9	-104.55(10)	B7-B8-B9-C1	-45.08(9)
B6-B7-B8-B9	-0.29(9)	C1-B8-B9-B2	103.53(11)
N1-B2-B9-C1	-133.78(11)	B4-B8-B9-B2	-0.35(12)
B1-B2-B9-C1	78.95(13)	B5-B8-B9-B2	-46.01(9)
B6-B2-B9-C1	-25.94(10)	B7-B8-B9-B2	58.44(10)
B3-B2-B9-C1	18.65(13)	C1-B8-B9-B5	149.54(12)
B5-B2-B9-C1	102.25(11)	B4-B8-B9-B5	45.66(10)
N1-B2-B9-B5	123.97(12)	B7-B8-B9-B5	104.46(10)
B1-B2-B9-B5	-23.30(11)	C1-B8-B9-B6	45.37(8)
B6-B2-B9-B5	-128.19(10)	B4-B8-B9-B6	-58.51(11)
B3-B2-B9-B5	-83.60(10)	B5-B8-B9-B6	-104.17(10)
N1-B2-B9-B8	169.11(11)	B7-B8-B9-B6	0.29(9)
B1-B2-B9-B8	21.84(14)	B2-B6-B9-C1	149.23(11)
B6-B2-B9-B8	-83.05(10)	B3-B6-B9-C1	104.45(11)
B3-B2-B9-B8	-38.46(12)	B7-B6-B9-C1	45.67(9)
B5-B2-B9-B8	45.14(9)	C1-B6-B9-B2	-149.23(11)
N1-B2-B9-B6	-107.84(12)	B3-B6-B9-B2	-44.78(9)
B1-B2-B9-B6	104.89(12)	B7-B6-B9-B2	-103.55(10)
B3-B2-B9-B6	44.59(9)	C1-B6-B9-B5	-104.60(11)
B5-B2-B9-B6	128.19(10)	B2-B6-B9-B5	44.63(9)
B1-B5-B9-C1	-76.96(13)	B3-B6-B9-B5	-0.15(12)
B8-B5-B9-C1	26.19(10)	B7-B6-B9-B5	-58.92(10)
B2-B5-B9-C1	-99.97(11)	C1-B6-B9-B8	-45.96(9)
B4-B5-B9-C1	-18.06(13)	B2-B6-B9-B8	103.27(10)
B1-B5-B9-B2	23.01(10)	B3-B6-B9-B8	58.49(10)
B8-B5-B9-B2	126.16(10)	B7-B6-B9-B8	-0.29(9)
B4-B5-B9-B2	81.92(10)	B2-B9-C1-C2	149.49(12)

B5-B9-C1-C2	-146.06(13)	B4-B7-C1-B6	-92.53(11)
B8-B9-C1-C2	-118.59(15)	B8-B7-C1-B6	-119.40(10)
B6-B9-C1-C2	122.17(15)	B3-B7-C1-B8	91.86(11)
B2-B9-C1-B6	27.32(10)	B4-B7-C1-B8	26.87(10)
B5-B9-C1-B6	91.77(11)	B6-B7-C1-B8	119.40(10)
B8-B9-C1-B6	119.24(10)	B4-B8-C1-C2	-146.97(12)
B2-B9-C1-B7	-32.49(14)	B5-B8-C1-C2	147.80(12)
B5-B9-C1-B7	31.96(14)	B9-B8-C1-C2	120.24(15)
B8-B9-C1-B7	59.42(11)	B7-B8-C1-C2	-119.79(15)
B6-B9-C1-B7	-59.81(10)	B4-B8-C1-B9	92.79(11)
B2-B9-C1-B8	-91.91(11)	B5-B8-C1-B9	27.56(10)
B5-B9-C1-B8	-27.46(10)	B7-B8-C1-B9	119.97(10)
B6-B9-C1-B8	-119.24(10)	B4-B8-C1-B6	32.39(14)
B2-B6-C1-C2	-148.50(13)	B5-B8-C1-B6	-32.84(14)
B3-B6-C1-C2	147.16(13)	B9-B8-C1-B6	-60.40(10)
B7-B6-C1-C2	119.51(15)	B7-B8-C1-B6	59.57(10)
B9-B6-C1-C2	-121.19(15)	B4-B8-C1-B7	-27.18(11)
B2-B6-C1-B9	-27.31(10)	B5-B8-C1-B7	-92.40(11)
B3-B6-C1-B9	-91.65(11)	B9-B8-C1-B7	-119.97(10)
B7-B6-C1-B9	-119.30(11)	B9-C1-C2-O1	82.00(18)
B2-B6-C1-B7	91.99(11)	B6-C1-C2-O1	174.23(13)
B3-B6-C1-B7	27.65(11)	B7-C1-C2-O1	-95.70(17)
B9-B6-C1-B7	119.30(11)	B8-C1-C2-O1	-6.5(2)
B2-B6-C1-B8	32.16(14)	B9-C1-C2-O2	-98.85(16)
B3-B6-C1-B8	-32.19(14)	B6-C1-C2-O2	-6.6(2)
B7-B6-C1-B8	-59.83(11)	B7-C1-C2-O2	83.45(17)
B9-B6-C1-B8	59.47(10)	B8-C1-C2-O2	172.63(13)
B3-B7-C1-C2	-149.01(12)	B1-B2-N1-C3	-6.09(19)
B4-B7-C1-C2	145.99(12)	B6-B2-N1-C3	139.18(12)
B6-B7-C1-C2	-121.47(15)	B9-B2-N1-C3	-150.32(12)
B8-B7-C1-C2	119.13(15)	B3-B2-N1-C3	66.91(19)
B3-B7-C1-B9	32.95(14)	B5-B2-N1-C3	-78.76(18)
B4-B7-C1-B9	-32.04(14)	B1-B2-N1-C7	175.12(12)
B6-B7-C1-B9	60.49(10)	B6-B2-N1-C7	-39.62(16)
B8-B7-C1-B9	-58.91(10)	B9-B2-N1-C7	30.89(17)
B3-B7-C1-B6	-27.54(11)	B3-B2-N1-C7	-111.89(16)

B5-B2-N1-C7	102.44(16)	C4-C5-C6-C7	0.2(2)
C7-N1-C3-C4	0.6(2)	C3-N1-C7-C6	-0.2(2)
B2-N1-C3-C4	-178.26(13)	B2-N1-C7-C6	178.63(13)
N1-C3-C4-C5	-0.6(2)	C5-C6-C7-N1	-0.2(2)
C3-C4-C5-C6	0.2(2)		

Symmetry transformations used to generate equivalent atoms:

Table 7. Hydrogen bonds for 09177a [$\text{\AA}$ and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	$\angle(\text{DHA})$
O2-H2B...O1#1	0.84	1.79	2.6288(14)	175.7

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z

3. Archive files for MP2/6-31G(d,p) geometry optimizations.

[*closo*-1-CB₉H₉-1-NH₃]

```
1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C1H12B9N1\PIOTR\31-Aug-2009\0
\\#P MP2/6-31G(d,p) FOpt(tight) geom(noangle, nodistance) fcheck\\1-CB
9-1-NH3, Cs at the DFT geom\\0,1\B,1.4830739869,-0.0993879777,0.\B,-0.
7699504007,1.2501517633,0.\B,1.6882614778,2.7892300175,0.\B,0.35867289
29,0.5740194868,1.3131349614\B,0.3586728929,0.5740194868,-1.3131349614
\B,1.9157578449,1.3752395014,-0.9224553623\B,1.9157578449,1.3752395014
,0.9224553623\B,0.3344898687,2.3252217632,0.9221949513\B,0.3344898687,
2.3252217632,-0.9221949513\C,-0.1094717524,-0.1970447036,0.\N,-0.86147
09729,-1.460288346,0.\H,-0.2178055316,-2.2564130823,0.\H,-1.4553693951
,-1.5237441389,0.8309490253\H,-1.4553693951,-1.5237441389,-0.830949025
3\H,2.2962206297,3.800616126,0.\H,2.0844638241,-1.1247680006,0.\H,-1.9
552993434,1.3194537072,0.\H,0.0686621771,0.0950437678,2.3609071211\H,0
.0686621771,0.0950437678,-2.3609071211\H,2.7951473179,1.301285116,1.71
38799191\H,2.7951473179,1.301285116,-1.7138799191\H,-0.1445536612,3.06
5402754,1.7145747631\H,-0.1445536612,3.065402754,-1.7145747631\\Versio
n=AM64L-G03RevD.01\State=1-A'\HF=-321.4675685\MP2=-322.6856426\RMSD=5.
755e-09\RMSF=1.891e-07\Thermal=0.\Dipole=-2.5036235,-4.172361,0.\PG=CS
[SG(C1H4B3N1),X(H8B6)]\\@
```

[*closo*-1-CB₉H₉-1-NH₂]

```
1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C1H11B9N1(1-)\PIOTR\31-Aug-20
09\0\\#P MP2/6-31G(d,p) FOpt(tight) geom(noangle, nodistance) fcheck\\
1-CB9-1-NH2, Cs, start at the DFT geom\\-1,1\B,-2.9009510509,-0.794956
8681,0.\B,-0.3312766714,-0.3395275715,1.2892073865\B,-0.3312766714,-0.
3395275715,-1.2892073865\B,-0.5800441628,0.9378929029,0.\B,-0.11803156
31,-1.6246852988,0.\B,-1.6568688737,-1.5079513541,0.9151596854\B,-1.98
2950273,0.3050247806,-0.9144931879\B,-1.6568688737,-1.5079513541,-0.91
51596854\B,-1.982950273,0.3050247806,0.9144931879\C,0.5931735209,-0.17
42354757,0.\N,2.0189132579,0.0496403616,0.\H,2.2414580573,0.6191227968
,0.811007838\H,2.2414580573,0.6191227968,-0.811007838\H,0.1787418006,-
0.2403652349,2.3595985054\H,0.1787418006,-0.2403652349,-2.3595985054\H
,-0.2421679714,2.0785113091,0.\H,0.5860838272,-2.5789514033,0.\H,-1.89
83345042,-2.3573008545,1.714287915\H,-4.0677727799,-1.0071312873,0.\H,
-2.4980670618,1.0199188118,-1.7159940284\H,-1.8983345042,-2.3573008545
,-1.714287915\H,-2.4980670618,1.0199188118,1.7159940284\\Version=AM64L
-G03RevD.01\State=1-A'\HF=-320.9751419\MP2=-322.1963579\RMSD=5.047e-09
\RMSF=3.499e-06\Thermal=0.\Dipole=1.6500026,0.8215806,0.\PG=CS [SG(C1H
3B3N1),X(H8B6)]\\@
```

[*closo*-1-CB₉H₉-2-NH₃]

```
1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C1H12B9N1\PIOTR\11-Dec-2010\0
\\#P MP2/6-31G(d,p) FOpt geom(noangle, nodistance) fcheck\\1-CB9-2-NH3
, C1, start at DFT geom\\0,1\B,0.5781573546,-1.2711587808,0.0945416399
\B,-0.2343498214,0.0314848805,-0.8618080966\B,0.5526243422,1.347728516
9,0.0972460164\B,1.3607138064,0.044988051,1.1034678507\B,-0.057145364,
-0.8915691782,1.7288818551\B,-1.1891196115,-0.8992237793,0.2926618709\
B,-1.2070631602,0.9409818932,0.2945611091\B,-0.0751315837,0.9524229982
,1.730784218\C,1.3022818939,0.0460806512,-0.4990728021\B,-1.5011087024
,0.0164719449,1.6919660508\N,-0.6631999142,0.028698702,-2.3694773079\H
,-2.4330270184,0.0066470805,2.4165943805\H,0.9573768116,-2.3381570032,
-0.252860373\H,0.9109906474,2.4226386218,-0.2478860128\H,2.4168339613,
0.0547532974,1.6343207527\H,0.125357495,-1.68401394,2.5910052167\H,-1.
9697395529,-1.6832992753,-0.1472386\H,-2.0028622375,1.7105886413,-0.14
36879945\H,0.0919024745,1.7465007958,2.5945392933\H,2.1481035706,0.055
```

0152357,-1.1682939923\H,-0.3130284784,-0.7947680878,-2.8596036695\H,-1.6815301241,0.0193763815,-2.4310849046\H,-0.3282257886,0.8591393528,-2.8584565008\\Version=EM64L-G09RevA.02\State=1-A\HF=-321.5267894\MP2=-322.7450682\RMSD=8.323e-09\RMSF=1.887e-05\Dipole=0.0766686,0.0049947,-4.2998494\PG=C01 [X(C1H12B9N1)]\\@

[*closo*-1-CB₉H₉-2-NH₂]⁻

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C1H11B9N1(1-)\PIOTR\11-Dec-2010\0\#P MP2/6-31G(d,p) FOpt geom(noangle, nodistance) fcheck\\1-CB9-2-NH2, C1, start at DFT geom\\-1,1\B,-0.0005984443,0.7018946608,-1.2941486826\B,-1.1426902364,-0.120063295,-0.0796351475\B,-0.1392388876,0.6263516501,1.3063085223\B,0.9498803628,1.4338724939,0.0863104527\B,1.6012399756,0.0271555751,-0.8407296923\B,0.1348052577,-1.0600516729,-0.9475709302\B,0.0439351826,-1.1092972797,0.8903173496\B,1.5089035836,-0.0217732336,0.9956364031\C,-0.6526156672,1.3968545162,-0.0066620505\B,1.4726494535,-1.4284830039,0.0356409967\N,-2.5798463879,-0.4415140477,-0.2138603787\H,-0.2362192542,1.1406682826,-2.3730428034\H,-0.5000741168,1.0076505562,2.3742108674\H,1.4965766006,2.4871221276,0.1477746873\H,2.5130806969,0.2065031241,-1.586778229\H,-0.240831611,-1.8265087601,-1.7791761043\H,-0.4253898284,-1.9130848973,1.6369479521\H,2.3383162954,0.1186302749,1.8402347569\H,-1.2926448941,2.2651053044,-0.0184869135\H,2.1813213282,-2.380518163,0.041592745\H,-3.1561233322,0.1159761588,0.4056619454\H,-2.7575580767,-1.4142573715,0.0029532536\\Version=EM64L-G09RevA.02\State=1-A\HF=-321.0148729\MP2=-322.2338038\RMSD=4.951e-09\RMSF=9.120e-06\Dipole=-1.5573772,0.6587566,0.366513\PG=C01 [X(C1H11B9N1)]\\@

[*closo*-1-CB₉H₉-6-NH₃]

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C1H12B9N1\PIOTR\18-Nov-2010\0\#P MP2/6-31G(d,p) FOpt geom(noangle, nodistance) fcheck\\1-CB9-6-NH3, C1, start at DFT geom\\0,1\B,0.5319310269,-1.2960950819,0.1043363828\B,-0.2060761667,0.0244349197,-0.8684207311\B,0.6101521114,1.3159987673,0.0804507285\B,1.3613573743,-0.0043680649,1.1143901333\B,-0.0965697071,-0.8774046077,1.743144054\B,-1.2171148396,-0.8573159624,0.2999676464\B,-1.16190767,0.9863020824,0.2831068972\B,-0.0413760615,0.965675029,1.7262907059\B,1.4483370131,-0.0223946842,-0.5721821238\C,-1.3736714599,0.0817921725,1.5800324647\N,-0.7016202226,0.0255934643,-2.3677722029\H,-2.2247317729,0.1133047145,2.2392314845\H,0.7852049369,-2.4256017835,-0.1550260187\H,0.930401535,2.4234019349,-0.1993739158\H,2.3506651658,-0.0280387571,1.7660147021\H,-0.0502703488,-1.6336416082,2.6507295433\H,-2.0936379591,-1.579285226,-0.046483203\H,-1.993848118,1.7529779586,-0.0769523183\H,0.0505801014,1.7342452462,2.619931362\H,2.338712383,-0.056201757,-1.3528805738\H,0.0864158742,-0.0042393334,-3.0130665111\H,-1.2969889501,-0.7812052171,-2.5546022115\H,-1.2471332454,0.8633927944,-2.5697662947\\Version=EM64L-G09RevA.02\State=1-A\HF=-321.5405144\MP2=-322.7572171\RMSD=7.875e-09\RMSF=2.016e-05\Dipole=-1.687688,0.0240109,-2.9061767\PG=C01 [X(C1H12B9N1)]\\@

[*closo*-1-CB₉H₉-6-NH₂]⁻

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C1H11B9N1(1-)\PIOTR\18-Nov-2010\0\#P MP2/6-31G(d,p) FOpt geom(noangle, nodistance) fcheck\\1-CB9-6-NH2, C1, orientation b start at the DFT geom\\-1,1\B,0.6915186429,1.340647872,0.0729927699\B,0.0006555907,0.0174243739,1.1845485425\B,0.7939413755,-1.2611572183,0.0750023176\B,1.4596679617,0.0649606457,-0.9904954679\B,-0.0296588906,0.9273565652,-1.524541632\B,-1.0540697813,0.8880945202,-0.0082569423\B,-0.9799874465,-0.9434973745,-0.0026513345\B,0.0425572408,-0.9145164841,-1.5221213077\B,1.6308134324,0.0754415897,0.7021570988\C,-1.2844627379,-0.0437060038,-1.2883882417\N,-0.4139369799,

0.059521075,2.6129487433\H,-2.1759085059,-0.0789018824,-1.8925039385\H,
 0.9760736928,2.4810022637,0.2698359663\H,1.1637777812,-2.376263709,0.
 2814686866\H,2.4188615742,0.1007650501,-1.6958359934\H,-0.0595750433,1.
 6870023859,-2.4385999289\H,-1.9256215612,1.6102914086,0.3522501583\H,
 -1.7933605284,-1.7301313901,0.3666853203\H,0.0717405823,-1.678862419,-
 2.4325827386\H,2.6073139323,0.1107737586,1.3791550788\H,0.2961569373,-
 0.3192496246,3.2264845063\H,-1.2743692692,-0.4444414027,2.7867333365\\
 Version=EM64L-G09RevA.02\State=1-A\HF=-321.011266\MP2=-322.2304281\RMS
 D=6.920e-09\RMSF=5.653e-05\Dipole=-1.1123446,-0.4704704,0.1774534\PG=C
 01 [X(C1H11B9N1)]\\@

[*closo*-1-CB₉H₉-10-NH₃]

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C1H12B9N1\PIOTR\07-Oct-2009\0
 \#P MP2/6-31G(d,p) FOpt(tight) geom(noangle, nodistance) fcheck\\1-CB
 9-10-NH3, Cs, start at DFT geom\\0,1\B,0.9616913359,0.0177910467,-0.92
 76410315\B,-0.8381621794,0.462248319,0.9263393501\C,-0.5208473014,-2.1
 105144296,0.\B,-0.8381621794,0.4622483191,-0.9263393501\B,0.9616913359
 ,0.0177910467,0.9276410314\B,0.9676501485,-1.5268479081,0.\B,-0.299543
 7101,-1.213558593,-1.3049986399\B,-1.5660724624,-0.9003685032,0.\B,-0.
 29954371,-1.213558593,1.3049986399\B,0.3112107105,1.2438397328,0.\N,0.
 6754417323,2.7583315596,0.\H,1.6855781292,2.8923206286,0.\H,0.29602836
 88,3.2224220579,-0.8242558247\H,0.2960283688,3.2224220579,0.8242558247
 \H,-0.7791949486,-3.1559343519,0.\H,1.8268647416,0.2355207873,-1.71379
 54413\H,-1.4962437808,1.0664010669,1.7119036569\H,-1.4962437808,1.0664
 010669,-1.7119036568\H,1.8268647416,0.2355207873,1.7137954413\H,-0.419
 046446,-1.6955537644,-2.3784654798\H,1.8904277486,-2.2667452012,0.\H,-
 2.7273684224,-1.1246253776,0.\H,-0.4190464459,-1.6955537644,2.37846547
 98\\Version=AM64L-G03RevD.01\State=1-A'\HF=-321.5444501\MP2=-322.75874
 9\RMSD=2.727e-09\RMSF=2.491e-06\Thermal=0.\Dipole=0.7449406,3.052268,0.
 .\PG=CS [SG(C1H4B3N1),X(H8B6)]\\@

[*closo*-1-CB₉H₉-10-NH₂]⁻

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C1H11B9N1(1-)\PIOTR\07-Oct-20
 09\0\#P MP2/6-31G(d,p) FOpt(tight) geom(noangle, nodistance) fcheck\\
 1-CB9-10-NH2, Cs start at the DFT geom\\-1,1\C,-2.7569469493,-0.775284
 5688,0.\B,-0.3512627059,-0.3361539945,1.2904329135\B,-0.3512627059,-0.
 3361539945,-1.2904329135\B,-0.6043736035,0.9387904612,0.\B,-0.13306154
 17,-1.6188504781,0.\B,-1.6673492682,-1.514869078,0.9141705983\B,-2.001
 4860906,0.3019129484,-0.9142890186\B,-1.6673492682,-1.514869078,-0.914
 1705983\B,-2.0014860906,0.3019129484,0.9142890186\B,0.7396427822,-0.13
 92517408,0.\N,2.209640712,0.0931088677,0.\H,2.4720498451,0.6439583792,
 0.8102981138\H,2.4720498451,0.6439583792,-0.8102981138\H,0.0374476446,
 -0.2586337088,2.4154590374\H,0.0374476446,-0.2586337088,-2.4154590374\
 H,-0.393812254,2.1123550634,0.\H,0.4774798688,-2.6400933244,0.\H,-2.02
 39817686,-2.3514031288,1.6790010494\H,-3.8157936096,-0.9714392061,0.\H
 ,-2.6295013615,0.9574845486,-1.6811905369\H,-2.0239817686,-2.351403128
 8,-1.6790010494\H,-2.6295013615,0.9574845486,1.6811905369\\Version=AM6
 4L-G03RevD.01\State=1-A'\HF=-321.0089477\MP2=-322.2286319\RMSD=6.677e-
 09\RMSF=3.869e-06\Thermal=0.\Dipole=-0.3506395,0.4298195,0.\PG=CS [SG(
 C1H3B3N1),X(H8B6)]\\@

3[6] [*closo*-1-CB₉H₈-1-COOH-6-N₂]

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C2H9B9N2O2\PIOTR\24-Sep-2009\
 0\#P MP2/6-31G(d,p) FOpt geom(noangle, nodistance) fcheck\\1-CB9-6-N2
 -1-COOH, C1, start at DFT\\0,1\B,1.1986964018,0.9131741638,1.306975883
 1\B,1.5556200753,-0.2545468307,-0.0074120666\B,1.1503267629,0.89484118
 55,-1.3256083436\B,0.7301791617,2.1097773988,-0.0092779562\B,-0.534044
 9744,1.2359239213,0.9451927099\B,0.0813611486,-0.4746859285,0.97060816

3\B,0.0463044447,-0.4892251046,-0.9293087439\B,-0.56824334,1.224055430
 2,-0.9056431471\B,2.2167792926,1.2985636161,-0.0311747245\C,-1.1112357
 984,0.0374081161,0.0376423994\C,-2.5018321756,-0.4845450388,0.11782559
 \O,-3.0869428254,-0.7427055382,1.1527465159\O,-3.0366260186,-0.6399843
 044,-1.1173002996\N,2.5295033775,-1.386308449,-0.0163599754\N,3.299323
 0465,-2.2215637355,-0.023468903\H,1.625911061,1.0026786544,2.406206377
 \H,1.5379602803,0.9691041613,-2.4406605276\H,0.7241929498,3.2930171945
 ,-0.0180565318\H,-1.2504054468,1.7784009713,1.7097444241\H,-0.07165249
 94,-1.3774631737,1.7163371913\H,-0.1267054514,-1.4029988922,-1.6575664
 614\H,-1.3072560636,1.7615539104,-1.6518688966\H,3.3452793346,1.640532
 4253,-0.0553100141\H,-3.9378382775,-0.976038028,-0.9726638442\\Version
 =AM64L-G03RevD.01\State=1-A\HF=-561.8184564\MP2=-563.6578442\RMSD=8.02
 4e-09\RMSF=8.430e-06\Thermal=0.\Dipole=0.6991393,-1.5011116,-0.490991\
 PG=C01 [X(C2H9B9N2O2)]\\@

3[6]⁻ [*closo*-1-CB₉H₈-1-COO-6-N₂]⁻

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C2H8B9N2O2(1-)\PIOTR\19-Nov-2
 010\0\#P MP2/6-31G(d,p) FOpt(tight) geom(noangle, nodistance) fcheck\
 \1-CB9-6-N2-1-COO, Cs, co-planar, start at DFT\\-1,1\B,1.0443788001,-0
 .0104597205,-1.3105819339\B,0.8007638703,1.1855102015,0.\B,1.044378800
 1,-0.0104597205,1.3105819339\B,1.27703321,-1.2703650403,0.\B,-0.291659
 1766,-1.1586928563,-0.9094504305\B,-0.6256661876,0.6272588971,-0.93065
 30011\B,-0.6256661876,0.6272588971,0.9306530011\B,-0.2916591766,-1.158
 6928563,0.9094504305\B,2.1536860439,0.177813397,0.\C,-1.3926724105,-0.
 415958016,0.\C,-2.9572401394,-0.6506848896,0.\O,-3.2755296402,-1.86012
 55966,0.\O,-3.61178918,0.417710587,0.\N,1.0600311703,2.6334669657,0.\N
 ,1.2753085076,3.7540838626,0.\H,1.4297201432,0.1262393982,-2.424336928
 8\H,1.4297201432,0.1262393982,2.4243369288\H,1.8805010206,-2.292786801
 1,0.\H,-0.620189903,-1.9889103495,-1.6835841043\H,-1.1941804102,1.3386
 716536,-1.6847916012\H,-1.1941804102,1.3386716536,1.6847916012\H,-0.62
 0189903,-1.9889103495,1.6835841043\H,3.3049254373,0.4521008657,0.\\Ver
 sion=EM64L-G09RevA.02\State=1-A'\HF=-561.2511216\MP2=-563.1031165\RMSD
 =8.037e-09\RMSF=8.376e-07\Dipole=3.4162123,2.6670508,0.\PG=CS [SG(C2H2
 B3N2O2),X(H6B6)]\\@

3[10]⁻ [*closo*-1-CB₉H₈-1-COO-10-N₂]⁻

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C2H8B9N2O2(1-)\PIOTR\21-Nov-2
 010\0\#P MP2/6-31G(d,p) FOpt(tight) geom(noangle, nodistance) #P SCF=
 tight fcheck\\N2-CB9H8-COO anion, C2v preopt\\-1,1\B,-1.3226698336,0.,
 -1.0500612392\B,1.3226698336,0.,-1.0500612392\B,0.,1.3197983123,-1.043
 6359727\B,0.,-1.3197983123,-1.0436359727\B,-0.922194385,-0.9150568584,
 0.4535821748\B,-0.922194385,0.9150568584,0.4535821748\B,0.922194385,0.
 9150568584,0.4535821748\B,0.922194385,-0.9150568584,0.4535821748\B,0.,
 0.,-2.0855245431\N,0.,0.,-3.5180034702\N,0.,0.,-4.6648151508\C,0.,0.,1
 .3940441806\C,0.,0.,2.9739177308\O,-1.151185469,0.,3.4660964838\O,1.15
 1185469,0.,3.4660964838\H,-2.4253596716,0.,-1.4909206271\H,0.,2.424731
 3045,-1.479133056\H,2.4253596716,0.,-1.4909206271\H,0.,-2.4247313045,-
 1.479133056\H,-1.6819391921,-1.682302288,0.9329398525\H,-1.6819391921,
 1.682302288,0.9329398525\H,1.6819391921,1.682302288,0.9329398525\H,1.6
 819391921,-1.682302288,0.9329398525\\Version=EM64L-G09RevA.02\State=1-
 A1\HF=-561.246628\MP2=-563.1033534\RMSD=5.142e-09\RMSF=8.495e-07\Dipol
 e=0.,0.,-5.2306471\PG=C02V [C2(C1C1B1N1N1),SGV(H2B2O2),SGV'(H2B2),X(H4
 B4)]\\@

4[6]a [*closo*-1-CB₉H₈-1-COOH-6-C₅H₅N] (orient 5)

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C7H14B9N1O2\PIOTR\18-Nov-2010
 \0\#P MP2/6-31G(d,p) FOpt geom(noangle, nodistance) fcheck\\1-CB9-1-C
 OOH-6-Pyr, 5, started at DFT geom\\0,1\B,1.5478557772,-1.3149592769,0.

3610005634\B,0.6513127425,-0.0088566634,-0.4991437008\B,1.5235384166,1.2939026899,0.3905878321\B,2.4481763971,-0.0124635968,1.2966279477\B,1.1156589785,-0.9540208962,2.0738931393\B,-0.1769782945,-0.9539278401,0.7636306574\B,-0.1941849089,0.8917379569,0.7845645066\B,1.0985071008,0.8862166238,2.0947574875\B,2.334683454,0.0056309951,-0.392538675\C,-0.2126984296,-0.0461492476,2.0793649624\C,-1.3159904414,-0.0677010264,3.0702744666\O,-2.5031518795,-0.0766873888,2.7941920227\O,-0.8424200043,-0.0779060327,4.3404561472\N,0.0128587794,0.0010705428,-1.9017409666\C,-0.2403879526,-1.1699080789,-2.5304948381\C,-0.7932134687,-1.1851435487,-3.8033046506\C,-1.0890716788,0.0195368767,-4.4398957722\C,-0.8156020618,1.2148014643,-3.7761249488\C,-0.2623192913,1.1810597567,-2.5038698074\H,1.8111606473,-2.4291476261,0.0466140045\H,1.7659475256,2.4196520344,0.1016082515\H,3.5134814914,-0.0084164161,1.8151753853\H,1.2875134834,-1.7265543484,2.9508765283\H,-1.063656782,-1.7036923789,0.5318442618\H,-1.0947420676,1.6299022159,0.5696572753\H,1.2561098866,1.6417434344,2.9890579923\H,3.1358680264,0.0229558513,-1.2617794561\H,-1.6309530421,-0.0922919995,4.9090907839\H,0.0195623255,-2.0625001742,-1.9796572851\H,-0.9848064817,-2.1351427639,-4.281073701\H,-1.5198760949,0.0267507716,-5.4317573203\H,-1.0249834392,2.1716373727,-4.23229828\H,-0.0189467137,2.0656427171,-1.9329058135\Version=EM64L-G09RevA.02\State=1-A\HF=-699.6650266\MP2=-702.0030268\RMSD=4.360e-09\RMSF=2.592e-05\Dipole=-1.7025193,0.0237547,-3.4795248\PG=C01 [X(C7H14B9N1O2)]\@

4[6]a⁻ [closo-1-CB₉H₈-1-COO-6-C₅H₅N]⁻ (orient 1)

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C7H13B9N1O2(1-)\PIOTR\20-Nov-2010\0\#P MP2/6-31G(d,p) FOpt(tight) geom(noangle, nodistance) fcheck\1-CB9-1-COO-6-Pyr, Cs, orientation 1, ring perpend, COO perpend\1,1\B,1.4477498908,-0.0283330366,1.3018978602\B,0.2607033718,-0.3649247197,0.\B,1.4477498908,-0.0283330366,-1.3018978602\B,2.683294164,0.3385840594,0.\B,1.8762221031,1.6879769067,0.9107715305\B,0.1320608502,1.1626878953,0.9160975208\B,0.1320608502,1.1626878953,-0.9160975208\B,1.8762221031,1.6879769067,-0.9107715305\B,1.7755937187,-1.0936499138,0.\C,0.715346326,2.3323575999,0.\N,-0.9905901642,-1.2577911882,0.\C,-1.5362380516,-1.648299775,1.1744942646\C,-2.6633323459,-2.4572895295,1.1989282843\C,-3.2420872703,-2.8717343619,0.\C,-2.6633323459,-2.4572895295,-1.1989282843\C,-1.5362380516,-1.648299775,-1.1744942646\C,0.2018324452,3.8207357175,0.\O,1.1176920908,4.6751108077,0.\O,-1.0510300779,3.9117007759,0.\H,1.5190819284,-0.4164567812,2.4263798465\H,1.5190819284,-0.4164567812,-2.4263798465\H,3.870619815,0.275636861,0.\H,2.4609755287,2.3674674232,1.6826448903\H,-0.7649991173,1.3555841601,1.6683830977\H,-0.7649991173,1.3555841601,-1.6683830977\H,2.4609755287,2.3674674232,-1.6826448903\H,2.0614139247,-2.2456176421,0.\H,-1.0337958087,-1.2833232342,2.058836376\H,-3.0776116122,-2.7504725337,2.1531514154\H,-4.1230130766,-3.4994909869,0.\H,-3.0776116122,-2.7504725337,-2.1531514154\H,-1.0337958087,-1.2833232342,-2.058836376\Version=EM64L-G09RevA.02\State=1-A\HF=-699.082793\MP2=-701.4300547\RMSD=6.692e-09\RMSF=4.849e-07\Dipole=-4.0477633,-7.2407819,0.\PG=CS [SG(C3H3B3N1O2),X(C4H10B6)]\@

4[10]a⁻ [closo-1-CB₉H₈-1-COO-10-C₅H₅N]⁻

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C7H13B9N1O2(1-)\PIOTR\20-Aug-2009\0\#P MP2/6-31G(d,p) FOpt geom(noangle, nodistance) #P SCF=tight fcheck\PyrCB9COO anion at C2 symmetry start at DFT geom\1,1\B,-0.3057177324,1.2594538756,2.0902822587\B,-1.2618084144,-0.2955126105,2.0952499181\B,0.3057177324,-1.2594538756,2.0902822587\B,1.2618084144,0.2955126105,2.0952499181\B,0.6891968108,1.1116971786,0.5888506934\B,-1.1190358245,0.6826613158,0.5826366479\B,-0.6891968108,-1.1116971786,0.5888506934\B,1.1190358245,-0.6826613158,0.5826366479\B,0.,0.,-0.4552920949\N,0.,0.,-1.972408209\C,1.1412487722,0.2780228282,-2.6458315332\C,1.16

47648533,0.2840647274,-4.0333238509\C,0.,0.,-4.7453221815\C,-1.1647648
533,-0.2840647274,-4.0333238509\C,-1.1412487722,-0.2780228282,-2.64583
15332\C,0.,0.,3.0363956889\C,0.,0.,4.6120162564\O,-0.9725071547,0.6123
164152,5.114429353\O,0.9725071547,-0.6123164152,5.114429353\H,-0.55060
95968,2.31363227,2.5681288862\H,-2.3119832005,-0.5523000535,2.57613360
86\H,0.5506095968,-2.31363227,2.5681288862\H,2.3119832005,0.5523000535
,2.5761336086\H,1.2696143379,2.061311433,0.1580224103\H,-2.0633238902,
1.2667547133,0.1454762908\H,-1.2696143379,-2.061311433,0.1580224103\H,
2.0633238902,-1.2667547133,0.1454762908\H,1.9987467168,0.4865383277,-2
.023191763\H,2.091763132,0.5100765095,-4.5410230874\H,0.,0.,-5.8270681
194\H,-2.091763132,-0.5100765095,-4.5410230874\H,-1.9987467168,-0.4865
383277,-2.023191763\\Version=AM64L-G03RevD.01\State=1-A\HF=-699.080790
4\MP2=-701.4237937\RMSD=5.344e-09\RMSF=8.649e-06\Thermal=0.\Dipole=0.,
0.,-10.529062\PG=C02 [C2(C1C1B1N1C1H1),X(C4H12B8O2)]\\@

5[6]⁻ [closo-1-CB₉H₈-1-COO-6-yl]

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C2H8B9O2(1-)\PIOTR\19-Nov-201
0\0\\#P MP2/6-31G(d,p) FOpt(tight) geom(noangle, nodistance) fcheck\\1
-CB9-6-ylide-1-COO, Cs, co-planar start at DFT\\-1,1\B,1.0525856852,-0
.0222250431,-1.3331551134\B,0.7710894094,1.0553833802,0.\B,1.052585685
2,-0.0222250431,1.3331551134\B,1.2794917406,-1.223750722,0.\B,-0.31070
06476,-1.1427224474,-0.9224978061\B,-0.6451911421,0.6637807679,-0.9170
007047\B,-0.6451911421,0.6637807679,0.9170007047\B,-0.3107006476,-1.14
27224474,0.9224978061\B,2.1657738215,0.2598038032,0.\C,-1.4055741924,-
0.4071550375,0.\C,-2.964429332,-0.6869952883,0.\O,-3.2509763199,-1.904
0141136,0.\O,-3.6423755855,0.3660523372,0.\H,1.4255485962,0.04361243,-
2.4532924952\H,1.4255485962,0.04361243,2.4532924952\H,1.9441875739,-2.
2076522418,0.\H,-0.6602768749,-1.965051766,-1.6948524462\H,-1.19267287
86,1.3697025738,-1.6886643077\H,-1.1926728786,1.3697025738,1.688664307
7\H,-0.6602768749,-1.965051766,1.6948524462\H,3.3295533893,0.452082856
5,0.\\Version=EM64L-G09RevA.02\State=1-A'\HF=-452.3081089\MP2=-453.806
5798\RMSD=7.696e-09\RMSF=6.094e-07\Dipole=2.7171275,1.0215923,0.\PG=CS
[SG(C2H2B3O2),X(H6B6)]\\@

5[10]⁻ [closo-1-CB₉H₈-1-COO-10-yl]

1\1\GINC-MONSTER\FOpt\RMP2-FC\6-31G(d,p)\C2H8B9O2(1-)\PIOTR\14-Aug-200
9\0\\#P MP2/6-31G(D,P) FOPT GEOM(NOANGLE, NODISTANCE) #P MAXDISK=245MW
POP=NBO\\CB9H8-COO ylide, C2v starting at the DFT geom\\-1,1\B,-1.356
8601647,0.,-1.776723699\B,1.3568601647,0.,-1.776723699\B,0.,1.35510065
48,-1.765003544\B,0.,-1.3551006548,-1.765003544\B,-0.9246850258,-0.919
7293321,-0.260689121\B,-0.9246850258,0.9197293321,-0.260689121\B,0.924
6850258,0.9197293321,-0.260689121\B,0.9246850258,-0.9197293321,-0.2606
89121\B,0.,0.,-2.6701266252\C,0.,0.,0.6522685205\C,0.,0.,2.2914900611\
O,-1.1514035384,0.,2.7607763548\O,1.1514035384,0.,2.7607763548\H,-2.46
83058228,0.,-2.1897929101\H,0.,2.4665379568,-2.1787000736\H,2.46830582
28,0.,-2.1897929101\H,0.,-2.4665379568,-2.1787000736\H,-1.6848228749,-
1.6855033334,0.220925194\H,-1.6848228749,1.6855033334,0.220925194\H,1.
6848228749,1.6855033334,0.220925194\H,1.6848228749,-1.6855033334,0.220
925194\\Version=x86-Linux-G98RevA.9\State=1-A1\HF=-452.2868002\MP2=-45
3.7851924\RMSD=6.293e-09\RMSF=9.758e-05\Dipole=0.,0.,-3.1658296\PG=C02
V [C2(B1C1C1),SGV(H2B2O2),SGV'(H2B2),X(H4B4)]\\@

6[1] [closo-1-CB₉H₉-1-N₂]

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C1H9B9N2\PIOTR\07-Dec-2010\0\
\\#P MP2/6-31G(d,p) FOpt(tight) geom(noangle, nodistance) fcheck\\1-CB9
-1-N2, C4v preopt\\0,1\B,-1.3326962377,0.,-0.0807169883\B,0.,1.3326962
377,-0.0807169883\B,1.3326962377,0.,-0.0807169883\B,0.,-1.3326962377,-
0.0807169883\B,-0.9238740934,-0.9238740934,1.3905086588\B,-0.923874093

4,0.9238740934,1.3905086588\B,0.9238740934,0.9238740934,1.3905086588\B,0.9238740934,-0.9238740934,1.3905086588\B,0.,0.,2.4950550326\C,0.,0.,-1.0093163392\N,0.,0.,-2.3460061255\N,0.,0.,-3.4953929713\H,0.,0.,3.6732975939\H,-2.3758396804,0.,-0.6359567975\H,0.,2.3758396804,-0.6359567975\H,2.3758396804,0.,-0.6359567975\H,0.,-2.3758396804,-0.6359567975\H,-1.7126215374,-1.7126215374,1.7862781839\H,-1.7126215374,1.7126215374,1.7862781839\H,1.7126215374,1.7126215374,1.7862781839\H,1.7126215374,-1.7126215374,1.7862781839\Version=EM64L-G09RevA.02\State=1-A1\HF=-374.1093425\MP2=-375.4839784\RMSD=9.591e-09\RMSF=7.043e-06\Dipole=0.,0.,-2.3040582\PG=C04V [C4(H1B1C1N1N1),2SGV(H2B2),2SGD(H2B2)]\@

6[2] [*closo*-1-CB₉H₉-2-N₂]

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C1H9B9N2\PIOTR\11-Dec-2010\0\ \#P MP2/6-31G(d,p) FOpt(tight) geom(noangle, nodistance) fcheck\1-CB9-2-N2, Cs, start at the DFT geom\0,1\B,0.707822863,-0.011136117,-1.315577524\B,0.3015750337,1.156025167,0.\B,0.707822863,-0.011136117,1.315577524\B,1.0647824612,-1.2416079893,0.\B,-0.4869300193,-1.2869224503,-0.920710017\B,-1.030520111,0.4634809794,-0.9256799619\B,-1.030520111,0.4634809794,0.9256799619\B,-0.4869300193,-1.2869224503,0.920710017\C,1.6116150377,0.2701479012,0.\B,-1.8131377987,-0.7314156796,0.\N,0.4783241855,2.6450430343,0.\N,0.5470298349,3.777744907,0.\H,-2.9437005006,-1.0663708144,0.\H,1.1695495951,0.1867892345,-2.3844260724\H,1.1695495951,0.1867892345,2.3844260724\H,1.8566103495,-2.1178527739,0.\H,-0.6389988352,-2.1474538314,-1.7199866291\H,-1.5906093644,1.1529152698,-1.7111380776\H,-1.5906093644,1.1529152698,1.7111380776\H,-0.6389988352,-2.1474538314,1.7199866291\H,2.6370319708,0.6032305019,0.\Version=EM64L-G09RevA.02\State=1-A'\HF=-374.1845043\MP2=-375.5464906\RMSD=6.032e-09\RMSF=1.812e-06\Dipole=1.4268589,2.2747951,0.\PG=CS [SG(C1H3B3N2),X(H6B6)]\@

6[6] [*closo*-1-CB₉H₉-6-N₂]

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C1H9B9N2\PIOTR\19-Nov-2010\0\ \#P MP2/6-31G(d,p) FOpt(tight) geom(noangle, nodistance) fcheck\1-CB9-6-N2, Cs, start at the DFT geom\0,1\B,0.6933770488,-0.0027655042,-1.3140816534\B,0.3122405365,1.1560249852,0.\B,0.6933770488,-0.0027655042,1.3140816534\B,1.0616751717,-1.2330974348,0.\B,-0.4966681144,-1.2959541094,-0.9198330941\B,-1.0278386206,0.4478480928,-0.9425392123\B,-1.0278386206,0.4478480928,0.9425392123\B,-0.4966681144,-1.2959541094,0.9198330941\B,1.7687571769,0.3041991885,0.\C,-1.6572643542,-0.6737122251,0.\N,0.4228492019,2.6426553417,0.\N,0.5461388468,3.7723048541,0.\H,-2.690959505,-0.97692239,0.\H,1.0648430552,0.1736143606,-2.4234290984\H,1.0648430552,0.1736143606,2.4234290984\H,1.765934559,-2.1843861897,0.\H,-0.7471795477,-2.1607220496,-1.6841831768\H,-1.6903970251,1.0820003831,-1.6885242548\H,-1.6903970251,1.0820003831,1.6885242548\H,-0.7471795477,-2.1607220496,1.6841831768\H,2.8783790286,0.7049266439,0.\Version=EM64L-G09RevA.02\State=1-A'\HF=-374.2059016\MP2=-375.5663475\RMSD=4.584e-09\RMSF=6.420e-07\Dipole=-0.6234105,1.5268494,0.\PG=CS [SG(C1H3B3N2),X(H6B6)]\@

6[10] [*closo*-1-CB₉H₉-10-N₂]

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C1H9B9N2\PIOTR\06-Dec-2010\0\ \#P MP2/6-31G(d,p) FOpt(tight) geom(noangle, nodistance) fcheck\1-CB9-10-N2, C4v\0,1\B,-1.3235084794,0.,-0.0839230371\B,0.,1.3235084794,-0.0839230371\B,1.3235084794,0.,-0.0839230371\B,0.,-1.3235084794,-0.0839230371\B,-0.9249459751,-0.9249459751,1.4096235453\B,-0.9249459751,0.9249459751,1.4096235453\B,0.9249459751,0.9249459751,1.4096235453\B,0.9249459751,-0.9249459751,1.4096235453\C,0.,0.,2.329578153\B,0.,0.,-1.1095537562\N,0.,0.,-2.5681262989\N,0.,0.,-3.7063990232\H,0.,0.,3.407027658

2\H,-2.4273811302,0.,-0.5133907835\H,0.,2.4273811302,-0.5133907835\H,2
.4273811302,0.,-0.5133907835\H,0.,-2.4273811302,-0.5133907835\H,-1.682
8112471,-1.6828112471,1.9061256072\H,-1.6828112471,1.6828112471,1.9061
256072\H,1.6828112471,1.6828112471,1.9061256072\H,1.6828112471,-1.6828
112471,1.9061256072\\Version=EM64L-G09RevA.02\State=1-A1\HF=-374.20901
13\MP2=-375.5702712\RMSD=3.846e-09\RMSF=6.166e-06\Dipole=0.,0.,-1.0735
501\PG=C04V [C4(H1C1B1N1N1),2SGV(H2B2),2SGD(H2B2)]\\@

7[1] [*closo*-1-CB₉H₉-1-yl]

1\1\GINC-MONSTER\FOpt\RMP2-FC\6-31G(d,p)\C1H9B9\PIOTR\10-Jun-2005\0\#\#
P MP2/6-31G(D,P) FOPT(TIGHT) GEOM(CHECK, NOANGLE, NODISTANCE) #P FCHEC
K GUESS=CHECK\\1-CB9 reactive intermediate (no H at C1), C4v starting
at DFT geom\\0,1\B,-1.3635748252,0.,-0.7942863345\B,0.,-1.3635748252,-
0.7942863345\B,1.3635748252,0.,-0.7942863345\B,0.,1.3635748252,-0.7942
863345\B,-0.9469818259,-0.9469818259,0.7134369246\B,0.9469818259,-0.94
69818259,0.7134369246\B,0.9469818259,0.9469818259,0.7134369246\B,-0.94
69818259,0.9469818259,0.7134369246\B,0.,0.,1.7243262315\C,0.,0.,-1.491
9583454\H,-2.4142700176,0.,-1.3306568582\H,0.,-2.4142700176,-1.3306568
582\H,2.4142700176,0.,-1.3306568582\H,0.,2.4142700176,-1.3306568582\H,
-1.7391428365,-1.7391428365,1.0904601504\H,1.7391428365,-1.7391428365,
1.0904601504\H,1.7391428365,1.7391428365,1.0904601504\H,-1.7391428365,
1.7391428365,1.0904601504\H,0.,0.,2.9078939429\\Version=x86-Linux-G98R
evA.9\State=1-A1\HF=-265.1445543\MP2=-266.1683397\RMSD=9.464e-09\RMSF=
5.855e-06\Dipole=0.,0.,-0.9915298\PG=C04V [C4(H1B1C1),2SGV(H2B2),2SGD(
H2B2)]\\@

7[2] [*closo*-1-CB₉H₉-2-yl]

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C1H9B9\PIOTR\11-Dec-2010\0\#\#
P MP2/6-31G(d,p) FOPT(tight) geom(noangle, nodistance) fcheck\\1-CB9-2
-ylide, Cs start at the DFT geom\\0,1\B,0.7370115215,-0.0317470949,-1.
3275482192\B,0.2934058146,1.014928362,0.\B,0.7370115215,-0.0317470949,
1.3275482192\B,1.0870207402,-1.2382819763,0.\B,-0.4966819901,-1.279540
3575,-0.9254262338\B,-1.0305164229,0.4988675595,-0.9393820755\B,-1.030
5164229,0.4988675595,0.9393820755\B,-0.4966819901,-1.2795403575,0.9254
262338\C,1.644136034,0.2839817198,0.\B,-1.8118401238,-0.6879327225,0.\
H,-2.9382894164,-1.0352457098,0.\H,1.1806381088,0.1289079427,-2.406687
0222\H,1.1806381088,0.1289079427,2.4066870222\H,1.8818039311,-2.112050
2997,0.\H,-0.6701327148,-2.1284468844,-1.7314852183\H,-1.5507684017,1.
1758798143,-1.7573629097\H,-1.5507684017,1.1758798143,1.7573629097\H,-
0.6701327148,-2.1284468844,1.7314852183\H,2.6641228111,0.6297826672,0.
\\Version=EM64L-G09RevA.02\State=1-A'\HF=-265.2295132\MP2=-266.2406049
\RMSD=7.067e-09\RMSF=2.046e-06\Dipole=1.2995554,1.0392016,0.\PG=CS [SG
(C1H3B3),X(H6B6)]\\@

7[6] [*closo*-1-CB₉H₉-6-yl]

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C1H9B9\PIOTR\19-Nov-2010\0\#\#
P MP2/6-31G(d,p) FOPT(tight) geom(noangle, nodistance) fcheck\\1-CB9-6
-ylide, Cs, start at DFT\\0,1\B,0.7116372645,-0.0177198901,-1.33992589
96\B,0.3254569787,1.0150656473,0.\B,0.7116372645,-0.0177198901,1.33992
58996\B,1.0570032027,-1.1952257295,0.\B,-0.5122245338,-1.2869592198,-0.
933289252\B,-1.0353551383,0.4744307275,-0.9323707935\B,-1.0353551383,
0.4744307275,0.9323707935\B,-0.5122245338,-1.2869592198,0.933289252\B,
1.7924453459,0.3697891579,0.\C,-1.6637025436,-0.6650550078,0.\H,-2.694
0593477,-0.9785109713,0.\H,1.0869630698,0.0847315093,-2.4531871494\H,1.
0869630698,0.0847315093,2.4531871494\H,1.8230179282,-2.0974650323,0.\
H,-0.7834033946,-2.1462453534,-1.6959321568\H,-1.6722491104,1.12247508
48,-1.684658349\H,-1.6722491104,1.1224750848,1.684658349\H,-0.78340339
46,-2.1462453534,1.6959321568\H,2.9285621171,0.6730002207,0.\\Version=

EM64L-G09RevA.02\State=1-A'\HF=-265.2546059\MP2=-266.2647456\RMSD=9.55
7e-09\RMSF=2.598e-06\Dipole=-0.7271018,0.408799,0.\PG=CS [SG(C1H3B3),X
(H6B6)]\@

7[10] [*closo*-1-CB₉H₉-10-yl]

1\1\GINC-MONSTER\FOpt\RMP2-FC\6-31G(d,p)\C1H9B9\PIOTR\13-Aug-2009\0\#\n
P MP2/6-31G(D,P) FOPT GEOM(NOANGLE, NODISTANCE) #P SCF=TIGHT MAXDISK=2
45MW\1-CB9-10-ylide, C4v start at the DFT geom\0,1\B,-1.3633511058,0
.,-0.8257505343\B,0.,1.3633511058,-0.8257505343\B,1.3633511058,0.,-0.8
257505343\B,0.,-1.3633511058,-0.8257505343\B,-0.9306548105,-0.93065481
05,0.6676508718\B,-0.9306548105,0.9306548105,0.6676508718\B,0.93065481
05,0.9306548105,0.6676508718\B,0.9306548105,-0.9306548105,0.6676508718
\C,0.,0.,1.5672026636\B,0.,0.,-1.715493464\H,0.,0.,2.6446775953\H,-2.4
667150311,0.,-1.2507367135\H,0.,2.4667150311,-1.2507367135\H,2.4667150
311,0.,-1.2507367135\H,0.,-2.4667150311,-1.2507367135\H,-1.6850133513,
-1.6850133513,1.1736284618\H,-1.6850133513,1.6850133513,1.1736284618\H
,1.6850133513,1.6850133513,1.1736284618\H,1.6850133513,-1.6850133513,1
.1736284618\Version=x86-Linux-G98RevA.9\State=1-A1\HF=-265.2398138\MP
2=-266.245421\RMSD=6.098e-09\RMSF=3.873e-05\Dipole=0.,0.,-0.2112804\PG
=C04V [C4(B1C1H1),2SGV(H2B2),2SGD(H2B2)]\@

8[1] [*closo*-1-CB₉H₉-1-C₅H₅N]

1\1\GINC-MONSTER\FOpt\RMP2-FC\6-31G(d,p)\C6H14B9N1\PIOTR\15-May-2007\0
\#P MP2/6-31G(D,P) FOPT GEOM(NOANGLE, NODISTANCE) FCHECK\1-CB9 1-Pyr
idine, C2v\0,1\B,-2.5753719608,0.,1.303868\B,-2.5753719608,0.,-1.3038
68\B,-2.5747199608,1.302464,0.\B,-2.5747199608,-1.302464,0.\B,-1.08676
49608,-0.925448,0.928776\B,-1.0867649608,0.925448,0.928776\B,-1.086764
9608,0.925448,-0.928776\B,-1.0867649608,-0.925448,-0.928776\B,-3.67258
39608,0.,0.\C,-0.1651499608,0.,0.\N,1.2702280392,0.,0.\C,3.3185450392,
0.,1.200105\C,3.3185450392,0.,-1.200105\C,1.9323770392,0.,1.183268\C,1
.9323770392,0.,-1.183268\C,4.0282320392,0.,0.\H,-2.9658519608,0.,2.423
69\H,-2.9658519608,0.,-2.42369\H,-2.9570829608,2.424776,0.\H,-2.957082
9608,-2.424776,0.\H,-0.5407629608,-1.674707,1.669258\H,-0.5407629608,1
.674707,1.669258\H,-0.5407629608,1.674707,-1.669258\H,-0.5407629608,-1
.674707,-1.669258\H,-4.8528829608,0.,0.\H,3.8258400392,0.,2.153967\H,3
.8258400392,0.,-2.153967\H,1.3093470392,0.,2.064418\H,1.3093470392,0.,
-2.064418\H,5.1094150392,0.,0.\Version=x86-Linux-G98RevA.9\State=1-A1
\HF=-511.9848497\MP2=-513.8464645\RMSD=4.320e-09\RMSF=2.151e-06\Dipole
=0.,5.9005816,0.\PG=C02V [C2(H1B1C1N1C1H1),SGV(C4H6B2),SGV'(H2B2),X(H4
B4)]\@

8[2] [*closo*-1-CB₉H₉-2-C₅H₅N]

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C6H14B9N1\PIOTR\12-Dec-2010\0
\#P MP2/6-31G(d,p) FOPT(tight) geom(noangle, nodistance) fcheck\1-CB
9-2-Pyr, Cs, (perpendicular) start at DFT geom\0,1\B,1.4353490751,0.0
004437987,1.3066609857\B,0.1829224165,-0.0280910496,0.\B,1.4353490751,
0.0004437987,-1.3066609857\B,2.7236539455,0.0621906729,0.\B,2.25998267
,1.5485306437,0.9211969004\B,0.4318552201,1.4644216847,0.9206370856\B,
0.4318552201,1.4644216847,-0.9206370856\B,2.25998267,1.5485306437,-0.9
211969004\C,1.4772330014,-0.944866053,0.\B,1.290732697,2.607436902,0.\
N,-1.1907368365,-0.71831139,0.\C,-1.788578005,-1.0141844015,1.17739449
77\C,-3.0272433101,-1.6399708285,1.2010406571\C,-3.6596256564,-1.95898
89108,0.\C,-3.0272433101,-1.6399708285,-1.2010406571\C,-1.788578005,-1
.0141844015,-1.1773944977\H,1.2274850346,3.7866942957,0.\H,1.421114927
7,-0.5046038808,2.3790668458\H,1.4211149277,-0.5046038808,-2.379066845
8\H,3.8176226937,-0.3869854445,0.\H,3.0268709853,1.9789348814,1.716394
7733\H,-0.4070396956,1.7778365899,1.7038999308\H,-0.4070396956,1.77783
65899,-1.7038999308\H,3.0268709853,1.9789348814,-1.7163947733\H,1.5091

031636,-2.0226325852,0.\H,-1.2435226441,-0.7241846223,2.0640370079\H,-
3.4843430519,-1.864485975,2.153924401\H,-4.6272837971,-2.4419242201,0.
\H,-3.4843430519,-1.864485975,-2.153924401\H,-1.2435226441,-0.72418462
23,-2.0640370079\\Version=EM64L-G09RevA.02\State=1-A'\HF=-512.0380671\
MP2=-513.8972191\RMSD=9.671e-09\RMSF=1.928e-06\Dipole=-4.0905561,-3.36
0757,0.\PG=CS [SG(C2H4B3N1),X(C4H10B6)]\\@

8[6] [*closo*-1-CB₉H₉-6-C₅H₅N]

1\1\GINC-OCTOPUS\FOpt\RMP2-FC\6-31G(d,p)\C6H14B9N1\PIOTR\20-Nov-2010\0
\\#P MP2/6-31G(d,p) FOpt(tight) geom(noangle, nodistance) fcheck\\1-CB
9-6-Pyr, Cs, orientation 1 (perpendicular), start at DFT\\0,1\B,1.4519
591604,-0.0090863835,1.3043330956\B,0.2125156783,-0.0752461,0.\B,1.451
9591604,-0.0090863835,-1.3043330956\B,2.7415636812,0.0829065976,0.\B,2
.2520015135,1.5613243278,0.9212515648\B,0.4278179118,1.4356728271,0.92
57005244\B,0.4278179118,1.4356728271,-0.9257005244\B,2.2520015135,1.56
13243278,-0.9212515648\B,1.5424671613,-1.1122364894,0.\C,1.2648414902,
2.4297438569,0.\N,-1.1916780422,-0.7107800374,0.\C,-1.7942823741,-1.00
43549952,1.1754052325\C,-3.0444061544,-1.606424951,1.1999548641\C,-3.6
851309329,-1.9125802183,0.\C,-3.0444061544,-1.606424951,-1.1999548641\
C,-1.7942823741,-1.0043549952,-1.1754052325\H,1.1858754326,3.503971685
4,0.\H,1.440582399,-0.4049432551,2.4240918156\H,1.440582399,-0.4049432
551,-2.4240918156\H,3.8852403338,-0.2281538079,0.\H,2.9701077803,2.110
3906076,1.6837558818\H,-0.3984968992,1.8436781604,1.6720527532\H,-0.39
84968992,1.8436781604,-1.6720527532\H,2.9701077803,2.1103906076,-1.683
7558818\H,1.565116396,-2.2947779812,0.\H,-1.2354911527,-0.7461428691,2
.0635562909\H,-3.5007847451,-1.8299957683,2.1535156683\H,-4.6588270611
, -2.383084893,0.\H,-3.5007847451,-1.8299957683,-2.1535156683\H,-1.2354
911527,-0.7461428691,-2.0635562909\\Version=EM64L-G09RevA.02\State=1-A
'\HF=-512.0496439\MP2=-513.9087967\RMSD=3.760e-09\RMSF=6.859e-07\Dipol
e=-4.0297917,-1.105514,0.\PG=CS [SG(C2H4B3N1),X(C4H10B6)]\\@

8[10] [*closo*-1-CB₉H₉-10-C₅H₅N]

1\1\GINC-MONSTER\FOpt\RMP2-FC\6-31G(d,p)\C6H14B9N1\PIOTR\14-Aug-2009\0
\\#P MP2/6-31G(D,P) FOPT GEOM(CHECK, NOANGLE, NODISTANCE) FCHECK #P GU
ESS=CHECK\\10-CB9-1-Pyridine, C2v\\0,1\B,0.,1.3048148339,-2.6466167742
\B,0.,-1.3048148339,-2.6466167742\B,1.3045597656,0.,-2.6454178537\B,-1
.3045597656,0.,-2.6454178537\B,-0.9250600456,0.9275973077,-1.148294408
8\B,0.9250600456,0.9275973077,-1.1482944088\B,0.9250600456,-0.92759730
77,-1.1482944088\B,-0.9250600456,-0.9275973077,-1.1482944088\C,0.,0.,-
3.5711464956\B,0.,0.,-0.1042488508\N,0.,0.,1.4162310325\C,0.,1.2001451
556,3.4749754533\C,0.,-1.2001451556,3.4749754533\C,0.,1.1758833233,2.0
875545357\C,0.,-1.1758833233,2.0875545357\C,0.,0.,4.1846679753\H,0.,2.
3787479176,-3.1429467602\H,0.,-2.3787479176,-3.1429467602\H,2.37900800
26,0.,-3.1403560305\H,-2.3790080026,0.,-3.1403560305\H,-1.7115036387,1
.7121251986,-0.7243414676\H,1.7115036387,1.7121251986,-0.7243414676\H,
1.7115036387,-1.7121251986,-0.7243414676\H,-1.7115036387,-1.7121251986
, -0.7243414676\H,0.,0.,-4.6480643004\H,0.,2.1534429136,3.9835569602\H,
0.,-2.1534429136,3.9835569602\H,0.,2.0621440071,1.4705762578\H,0.,-2.0
621440071,1.4705762578\H,0.,0.,5.2661420501\\Version=x86-Linux-G98RevA
.9\State=1-A1\HF=-512.0556231\MP2=-513.9104998\RMSD=1.166e-09\RMSF=2.1
41e-06\Dipole=0.,0.,3.9873565\PG=C02V [C2(H1C1B1N1C1H1),SGV(C4H6B2),SG
V'(H2B2),X(H4B4)]\\@