ЖУРНАЛ СТРУКТУРНОЙ ХИМИИ

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SUPPLEMENTARY MATERIALS TO: MOLECULAR STRUCTURAL PROPERTIES OF [*n*]-ANNULENE (*n* = 8, 10, 12, 14) AND ITS BORON NITRIDE DERIVATIVES: ANALYSIS OF NMR, NBO, ELF AND PDI

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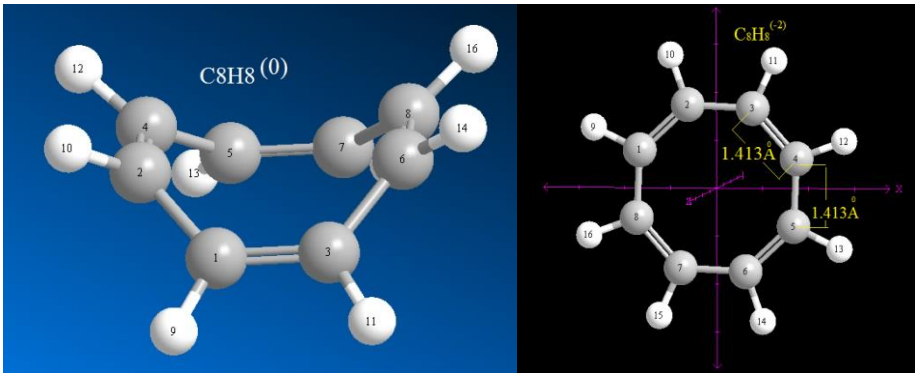
NBO ANALYSIS



Calculation method: CAM-b3lyp/cc-pvdz pop=NBO;
For **$C_8H_8^{(0)}$:** the minimum occupancy is for the (π) system; all coefficients in wave functions are 0.7; not only σ bonds but also (π) bonds are mixing of SP^n hybrids.
For **$C_8H_8^{(-2)}$:** the minimum occupancy is for the (π) system, all coefficients in wave functions are 0.7 , (π) bonds are completely pure with $\theta = 0.0$ and $\varphi = 0.0$ and $Dev = 0.0$ for all items.
For $B_2N_2C_4H_8^{(2-)}$ and $B_2N_2C_4H_8^{(0)}$ in some items, (π) bonds are not pure and also the coefficients are not symmetrical.

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Table 1

$C_8H_8^{(0)}$

NBO	Line of center		Hybride 1			Hybride 2			Wave function	OCC.
	θ	φ	θ	φ	Dev	φ	θ	Dev		
C1-C2 (σ)	58.6	125.6	59.2	126.9	1.3	120.8	304.2	1.3	$0.7SP^{1.97}$of C1 + 0.7 $SP^{1.97}$of C2	1.97
C1-C3 (σ)	90.0	350.6	101.1	358.3	13.6	101.2	162.8	13.6	$0.7SP^{1.68}$of C1 + 0.7 $SP^{1.68}$of C3	1.98
C1-C3 (π)	90.0	350.6	39.5	276.5	79.9	39.5	244.6	79.9	$0.7SP^{89.4}$ of C1 + 0.7 $SP^{89.4}$ of C3	1.92
C3-C6 (σ)	58.6	35.6	59.2	34.2	1.3	120.8	216.9	1.3	$0.7SP^{1.97}$of C3 + 0.7 $SP^{1.97}$of C6	1.97
C2-C4 (σ)	90.0	80.6	78.8	72.8	13.6	78.9	268.3	13.6	$0.7SP^{1.68}$of C2 + 0.7 $SP^{1.68}$of C4	1.98
C1-C3 (π)	90.0	80.6	140.5	154.6	79.9	140.5	186.5	79.9	$0.7SP^{89.4}$ of C1 + 0.7 $SP^{89.4}$ of C3	1.92
C4-C5 (σ)	121.4	35.6	120.8	36.9	1.3	59.2	214.2	1.3	$0.7SP^{1.97}$of C4 + 0.7 $SP^{1.97}$of C5	1.97
C5-C7 (σ)	90.0	350.6	101.1	342.8	13.6	101.1	178.3	13.6	$0.7SP^{1.68}$of C5 + 0.7 $SP^{1.68}$of C7	1.98
C5-C7 (π)	90.0	350.6	39.5	64.6	79.9	39.5	96.5	79.9	$0.7SP^{89.4}$ of C1 + 0.7 $SP^{89.4}$ of C3	1.92
					$C_8H_8^{(2-)}$					
C1-C2 (σ)	90.0	337.5	90.0	333.2	4.3	90.0	161.8	4.3	$0.7SP^{1.60}$ of C1 + 0.7 $SP^{1.60}$ of C2	1.98
C1-C2 (π)	90.	337.5	0.0	0.0	90.0	0.0	0.0	90.0	0.7 P^1 of C1 + 0.7 P^1 of C2	1.84
C1-C8 (σ)	90.0	202.5	90.0	206.8	4.3	90.0	18.2	4.3	$0.7SP^{1.60}$ of C1 + 0.7 $SP^{1.60}$ of C8	0.198
C2-C3 (σ)	90.0	292.5	90.0	288.2	4.3	90.0	116.8	4.3	$0.7SP^{1.60}$ of C2 + 0.7 $SP^{1.60}$ of C3	1.98
C3-C4 (σ)	90.0	247.5	90.0	243.2	4.3	90.0	71.8	4.3	$0.7SP^{1.60}$ of C3 + 0.7 $SP^{1.60}$ of C4	1.98
C3-C4 (π)	90.0	247.5	0.0	0.0	90.0	0.0	0.0	90.0	0.7 P^1 of C3 + 0.7 P^1 of C4	1.84
C4-C5 (σ)	90.0	202.5	90.0	198.2	4.3	90.0	26.8	4.3	$0.7SP^{1.60}$ of C4 + 0.7 $SP^{1.60}$ of C5	1.98
C5-C6 (σ)	90.0	157.5	90.0	153.2	4.3	90.0	341.8	4.3	$0.7SP^{1.60}$ of C5 + 0.7 $SP^{1.60}$ of C6	1.98
C5-C6 (π)	90.0	157.5	0.0	0.0	90.0	0.0	0.0	90.0	0.7 P^1 of C1 + 0.7 P^1 of C2	1.84
					$B_2N_2C_4H_8^{(2-)}$					
B1-N2 (σ)	90.0	314.6	90.0	312.8	1.8	90.0	140.4	5.7	$0.46SP^{2.47}$of B1 + 0.88 $SP^{1.15}$ of N2	1.98
B1-N2 (π)	90.0	314.6	0.0	0.0	90.0	0.0	0.0	90.0	0.31 P^1 of B1 + 0.94 P^1 of N2	1.83
B1-C3 (σ)	90.0	185.9	90.0	190.4	4.5	90.0	358.4	7.5	$0.56SP^{1.67}$of B1 + 0.82 $SP^{1.30}$ of C3	1.97
C3-C6 (σ)	90.0	224.6	90.0	228.5	3.9	90.0	42.2	2.4	$0.7SP^{2.07}$of C3 + 0.7 $SP^{1.37}$ of C6	1.98
C3-C6	90.0	224.6	180.0	0.0	90.0	0.0	0.0	90.0	0.77 P^1 of C3 +	1.85

(π)									0.63 P^1 of C6	
C4-C5	90.0	224.6	90.1	222.2	2.5	90.1	48.8	4.2	0.7 $SP^{1.37}$ of C4	1.98
(σ)									+0.7$SP^{2.07}$of C5	
C4-C5	90.0	224.6	0.1	161.7	90.0	179.7	295.1	90.1	0.63 P^1 of C4 +	1.85
(π)									0.76 P^1 of C5	
					$B_2N_2C_4H_8^{(0)}$					
C1-C3	90.0	270.0	100.4	274.8	11.4	100.4	85.2	11.4	0.7 $SP^{1.68}$ of C1 +0.7	1.98
(σ)									$SP^{1.68}$ of C3	
C1-C3	90.0	270.0	36.0	195.2	81.2	36.0	164.9	81.2	0.7 P^1 of C1 +	1.90
(π)									0.7 P^1 of C3	
B2-N4	92.5	356.6	81.9	347.7	13.7	73.2	186.9	17.6	0.46 $SP^{2.52}$ of B2	1.98
(σ)									+0.88 $SP^{1.24}$ of N4	
B2-N4	92.5	356.6	141.1	68.8	77.0	141.2	109.5	77.8	0.37 $SP^{84.8}$ of B2	1.92
(π)									+0.92 $SP^{84.8}$ of N4	
C5-C7	90.0	270.0	92.7	264.9	5.7	92.7	95.0	5.7	0.7 $SP^{1.41}$ of C5 +0.7	1.98
(σ)									$SP^{1.41}$ of C7	
C5-C7	90.0	270.0	40.4	353.5	85.8	40.4	6.5	85.8	0.7 P^1 of C5 +	1.96
(π)									0.7 P^1 of C7	

Donor and acceptor of some bonds in several molecules;

For **$C_8H_8^{(0)}$:** Among various interactions two groups are strongest, the first interaction between those double bonds together, the interaction between (π) to ($\pi*$), with 8.81 kcal/mol which appears only between carbon-carbon bonds in the rings. The second, interaction between (σ C-H) and (σ star C-C) appear around 7.5 kcal/mol, which are seen to give the strongest stabilization series among the numerous interactions.

It is notable that this interaction between (σ C-H) and (σ star C-C) causes $C_8H_8^{(0)}$ to be unplanar.

For **$C_8H_8^{(-2)}$:** the strongest one (19.30 kcal/mol) belongs to C_m-C_n (π) with C_p-C_q ($\pi*$) which are equal in all items. It is notable that due to the lack of any strong interactions of (σ C-H) with (σ star C-C), the molecule is completely planar.

For $B_2N_2C_4H_8^{(0)}$ and $B_2N_2C_4H_8^{(-2)}$ compounds the interaction of X-H (X=C, B, and N) with (X-X) bonds is very weak while the interaction between the ring bonds are strong.

Table 2

Donor NBO (i)	Acceptor NBO (j)	E(2) Kcal/mol	E(j)-E(i) a.u.	F (i,j) a.u.
		$C_8H_8^{(0)}$		
C1-C2 (π)	C2-C4 ($\pi*$)	8.81	0.48	0.058
C1-H9 (σ)	C3-C6($\sigma*$)	7.44	1.13	0.082
C2-H10(σ)	C4-C3($\sigma*$)	7.44	1.13	0.082
C3-H11(σ)	C1-C2($\sigma*$)	7.44	1.13	0.082
C4-H12(σ)	C1-C2($\sigma*$)	7.44	1.13	0.082
C5-H13(σ)	C7-C8($\sigma*$)	7.44	1.13	0.082
C6-H14(σ)	C7-C8($\sigma*$)	7.44	1.13	0.082
C2-C4 (π)	C1-C3 ($\pi*$)	8.80	0.48	0.058
C2-C4 (π)	C5-C7 ($\pi*$)	8.80	0.48	0.058
C5-C7 (π)	C2-C4 ($\pi*$)	8.80	0.48	0.058
C5-C7 (π)	C6-C8 ($\pi*$)	8.80	0.48	0.058
C6-C8 (π)	C1-C3 ($\pi*$)	8.80	0.48	0.058
C6-C8 (π)	C5-C7 ($\pi*$)	8.80	0.48	0.058
		$C_8H_8^{(-2)}$		
C1-C2 (π)	C7-C8 ($\pi*$)	19.30	0.34	0.083
C1-C2 (π)	C3-C4 ($\pi*$)	19.29	0.34	0.083
C3-C4 (π)	C1-C2 ($\pi*$)	19.30	0.34	0.083
C3-C4 (π)	C5-C6 ($\pi*$)	19.29	0.34	0.083
C5-C6 (π)	C7-C8 ($\pi*$)	19.29	0.34	0.083
C5-C6 (π)	C3-C4 ($\pi*$)	19.30	0.34	0.083
C7-C8 (π)	C1-C2($\pi*$)	19.30	0.34	0.083
C7-C8 (π)	C5-C6($\pi*$)	19.30	0.34	0.083
		$B_2N_2C_4H_8^{(0)}$		
C1-C3 (π)	B2-N4 ($\pi*$)	11.36	0.45	0.064
C1-C3 (π)	B6-N8 ($\pi*$)	11.36	0.45	0.064
B2-N4 (π)	C5-C7($\pi*$)	15.81	0.47	0.078
B6-N8 (π)	C5-C7($\pi*$)	15.80	0.47	0.078
		$B_2N_2C_4H_8^{(2-)}$		
B1-N2 (π)	C4-C5($\pi*$)	39.60	0.41	0.114
C3-C6 (π)	B1-N2 ($\pi*$)	37.71	0.40	0.110
C4-C5 (π)	B7-N8 ($\pi*$)	36.76	0.41	0.109
B7-N8 (π)	C3-C6 ($\pi*$)	40.05	0.40	0.114
C3-C6 (π)	B1-N2 ($\pi*$)	42.75	0.04	0.094
C4-C5 (π)	B7-N8 ($\pi*$)	39.04	0.04	0.094

NMR

$B_4N_4H_8^{(2-)}$

Calculating GIAO nuclear magnetic shielding tensors.
SCF GIAO Magnetic shielding tensor (ppm):
1 B Isotropic = 104.3255 Anisotropy = 32.7883
XX= 92.4781 YX= -23.0012 ZX= -0.0034
XY= -23.0032 YY= 94.3141 ZY= -0.0039
XZ= 0.0151 YZ= 0.0134 ZZ= 126.1844
Eigenvalues: 70.3755 116.4166 126.1844
2 N Isotropic = 141.0785 Anisotropy = 124.2238
XX= -9.2775 YX= 4.3352 ZX= -0.0122
XY= 4.3312 YY= 208.6186 ZY= 0.0009
XZ= 0.0077 YZ= 0.0240 ZZ= 223.8943
Eigenvalues: -9.3636 208.7047 223.8943
3 N Isotropic = 141.0801 Anisotropy = 124.2286
XX= 208.6166 YX= -4.3316 ZX= 0.0008
XY= -4.3353 YY= -9.2755 ZY= 0.0052
XZ= 0.0218 YZ= -0.0098 ZZ= 223.8992
Eigenvalues: -9.3617 208.7027 223.8992
4 B Isotropic = 104.3252 Anisotropy = 32.7887
XX= 94.3144 YX= 23.0064 ZX= 0.0050
XY= 22.9979 YY= 92.4768 ZY= -0.0046
XZ= -0.0001 YZ= -0.0010 ZZ= 126.1843
Eigenvalues: 70.3751 116.4161 126.1843
5 N Isotropic = 141.0805 Anisotropy = 124.2246
XX= 208.6185 YX= -4.3318 ZX= -0.0019
XY= -4.3352 YY= -9.2740 ZY= -0.0170
XZ= -0.0219 YZ= -0.0114 ZZ= 223.8969
Eigenvalues: -9.3601 208.7047 223.8969
6 B Isotropic = 104.3254 Anisotropy = 32.7883
XX= 94.3150 YX= 23.0062 ZX= -0.0040
XY= 22.9985 YY= 92.4770 ZY= 0.0036
XZ= 0.0009 YZ= -0.0013 ZZ= 126.1843
Eigenvalues: 70.3753 116.4167 126.1843
7 B Isotropic = 104.3253 Anisotropy = 32.7888
XX= 92.4775 YX= -23.0016 ZX= 0.0016
XY= -23.0029 YY= 94.3138 ZY= 0.0020
XZ= -0.0054 YZ= -0.0070 ZZ= 126.1845
Eigenvalues: 70.3751 116.4162 126.1845
8 N Isotropic = 141.0788 Anisotropy = 124.2237
XX= -9.2772 YX= 4.3367 ZX= 0.0044
XY= 4.3318 YY= 208.6189 ZY= -0.0017
XZ= -0.0189 YZ= -0.0192 ZZ= 223.8945
Eigenvalues: -9.3633 208.7051 223.8945
9 H Isotropic = 25.6394 Anisotropy = 7.1882
XX= 27.5056 YX= -2.8125 ZX= 0.0000
XY= -2.8124 YY= 27.7282 ZY= -0.0001
XZ= 0.0022 YZ= 0.0008 ZZ= 21.6845
Eigenvalues: 21.6845 24.8022 30.4316
10 H Isotropic = 25.4562 Anisotropy = 6.8074
XX= 29.4781 YX= 0.0104 ZX= 0.0007

XY= 0.0101 YY= 29.9943 ZY= 0.0008
XZ= 0.0010 YZ= -0.0010 ZZ= 16.8963
Eigenvalues: 16.8963 29.4779 29.9945
11 H Isotropic = 25.4561 Anisotropy = 6.8087
XX= 29.9950 YX= -0.0102 ZX= 0.0007
XY= -0.0104 YY= 29.4782 ZY= -0.0001
XZ= -0.0010 YZ= -0.0011 ZZ= 16.8951
Eigenvalues: 16.8951 29.4780 29.9952
12 H Isotropic = 25.6395 Anisotropy = 7.1882
XX= 27.7285 YX= 2.8126 ZX= 0.0004
XY= 2.8122 YY= 27.5056 ZY= 0.0000
XZ= 0.0008 YZ= 0.0009 ZZ= 21.6844
Eigenvalues: 21.6844 24.8025 30.4316
13 H Isotropic = 25.4562 Anisotropy = 6.8086
XX= 29.9951 YX= -0.0102 ZX= -0.0003
XY= -0.0104 YY= 29.4783 ZY= 0.0004
XZ= 0.0002 YZ= 0.0014 ZZ= 16.8953
Eigenvalues: 16.8953 29.4781 29.9953
14 H Isotropic = 25.6394 Anisotropy = 7.1883
XX= 27.7284 YX= 2.8126 ZX= -0.0002
XY= 2.8123 YY= 27.5055 ZY= 0.0001
XZ= -0.0002 YZ= -0.0005 ZZ= 21.6844
Eigenvalues: 21.6844 24.8023 30.4316
15 H Isotropic = 25.6395 Anisotropy = 7.1882
XX= 27.5057 YX= -2.8124 ZX= -0.0001
XY= -2.8123 YY= 27.7283 ZY= 0.0002
XZ= -0.0006 YZ= 0.0005 ZZ= 21.6844
Eigenvalues: 21.6844 24.8025 30.4316
16 H Isotropic = 25.4563 Anisotropy = 6.8074
XX= 29.4782 YX= 0.0105 ZX= -0.0005
XY= 0.0102 YY= 29.9944 ZY= -0.0002
XZ= -0.0009 YZ= 0.0001 ZZ= 16.8963
Eigenvalues: 16.8963 29.4780 29.9946
17 Bq Isotropic = 9.1725 Anisotropy = 21.6013
XX= 1.9710 YX= 0.0002 ZX= 0.0000
XY= -0.0001 YY= 1.9732 ZY= -0.0002
XZ= 0.0001 YZ= 0.0000 ZZ= 23.5734
Eigenvalues: 1.9710 1.9732 23.5734

$C_8H_8^{2-}$

Calculating GIAO nuclear magnetic shielding tensors.
SCF GIAO Magnetic shielding tensor (ppm):
1 C Isotropic = 88.2139 Anisotropy = 103.5315
XX= 129.1694 YX= 0.0000 ZX= 0.0001
XY= 0.0000 YY= -21.7626 ZY= -0.0014
XZ= 0.0006 YZ= 0.0009 ZZ= 157.2349
Eigenvalues: -21.7626 129.1694 157.2349
2 C Isotropic = 88.7551 Anisotropy = 105.5001
XX= 53.5884 YX= -75.4775 ZX= -0.0010
XY= -75.4775 YY= 53.5883 ZY= -0.0009
XZ= 0.0002 YZ= 0.0011 ZZ= 159.0885
Eigenvalues: -21.8891 129.0659 159.0885

3 C Isotropic = 88.2139 Anisotropy = 103.5315
XX= -21.7626 YX= 0.0000 ZX= 0.0014
XY= 0.0000 YY= 129.1694 ZY= 0.0001
XZ= -0.0009 YZ= 0.0006 ZZ= 157.2349
Eigenvalues: -21.7626 129.1694 157.2349
4 C Isotropic = 88.7551 Anisotropy = 105.5001
XX= 53.5883 YX= 75.4775 ZX= 0.0009
XY= 75.4775 YY= 53.5884 ZY= -0.0010
XZ= -0.0011 YZ= 0.0002 ZZ= 159.0885
Eigenvalues: -21.8891 129.0659 159.0885
5 C Isotropic = 88.2139 Anisotropy = 103.5315
XX= 129.1694 YX= 0.0000 ZX= -0.0001
XY= 0.0000 YY= -21.7626 ZY= 0.0014
XZ= -0.0006 YZ= -0.0009 ZZ= 157.2349
Eigenvalues: -21.7626 129.1694 157.2349
6 C Isotropic = 88.7551 Anisotropy = 105.5001
XX= 53.5884 YX= -75.4775 ZX= 0.0010
XY= -75.4775 YY= 53.5883 ZY= 0.0009
XZ= -0.0002 YZ= -0.0011 ZZ= 159.0885
Eigenvalues: -21.8891 129.0659 159.0885
7 C Isotropic = 88.2139 Anisotropy = 103.5315
XX= -21.7626 YX= 0.0000 ZX= -0.0014
XY= 0.0000 YY= 129.1694 ZY= -0.0001
XZ= 0.0009 YZ= -0.0006 ZZ= 157.2349
Eigenvalues: -21.7626 129.1694 157.2349
8 C Isotropic = 88.7551 Anisotropy = 105.5001
XX= 53.5883 YX= 75.4775 ZX= -0.0009
XY= 75.4775 YY= 53.5884 ZY= 0.0010
XZ= 0.0011 YZ= -0.0002 ZZ= 159.0885
Eigenvalues: -21.8891 129.0659 159.0885
9 H Isotropic = 26.0182 Anisotropy = 9.0697
XX= 32.0646 YX= 0.0000 ZX= 0.0000
XY= 0.0000 YY= 28.1220 ZY= 0.0000
XZ= 0.0001 YZ= 0.0002 ZZ= 17.8679
Eigenvalues: 17.8679 28.1220 32.0646
10 H Isotropic = 26.0968 Anisotropy = 8.9201
XX= 30.0891 YX= -1.9544 ZX= 0.0000
XY= -1.9544 YY= 30.0891 ZY= 0.0000
XZ= 0.0000 YZ= 0.0002 ZZ= 18.1121
Eigenvalues: 18.1121 28.1347 32.0435
11 H Isotropic = 26.0182 Anisotropy = 9.0697
XX= 28.1220 YX= 0.0000 ZX= 0.0000
XY= 0.0000 YY= 32.0646 ZY= 0.0000
XZ= -0.0002 YZ= 0.0001 ZZ= 17.8679
Eigenvalues: 17.8679 28.1220 32.0646
12 H Isotropic = 26.0968 Anisotropy = 8.9201
XX= 30.0891 YX= 1.9544 ZX= 0.0000
XY= 1.9544 YY= 30.0891 ZY= 0.0000
XZ= -0.0002 YZ= 0.0000 ZZ= 18.1121
Eigenvalues: 18.1121 28.1347 32.0435
13 H Isotropic = 26.0182 Anisotropy = 9.0697
XX= 32.0646 YX= 0.0000 ZX= 0.0000

XY= 0.0000 YY= 28.1220 ZY= 0.0000
XZ= -0.0001 YZ= -0.0002 ZZ= 17.8679
Eigenvalues: 17.8679 28.1220 32.0646
14 H Isotropic = 26.0968 Anisotropy = 8.9201
XX= 30.0891 YX= -1.9544 ZX= 0.0000
XY= -1.9544 YY= 30.0891 ZY= 0.0000
XZ= 0.0000 YZ= -0.0002 ZZ= 18.1121
Eigenvalues: 18.1121 28.1347 32.0435
15 H Isotropic = 26.0182 Anisotropy = 9.0697
XX= 28.1220 YX= 0.0000 ZX= 0.0000
XY= 0.0000 YY= 32.0646 ZY= 0.0000
XZ= 0.0002 YZ= -0.0001 ZZ= 17.8679
Eigenvalues: 17.8679 28.1220 32.0646
16 H Isotropic = 26.0968 Anisotropy = 8.9201
XX= 30.0891 YX= 1.9544 ZX= 0.0000
XY= 1.9544 YY= 30.0891 ZY= 0.0000
XZ= 0.0002 YZ= 0.0000 ZZ= 18.1121
Eigenvalues: 18.1121 28.1347 32.0435
17 Bq Isotropic = 15.9019 Anisotropy = 37.6409
XX= 3.3550 YX= 0.0000 ZX= 0.0000
XY= 0.0000 YY= 3.3550 ZY= 0.0000
XZ= 0.0000 YZ= 0.0000 ZZ= 40.9958
Eigenvalues: 3.3550 3.3550 40.9958

$B_4N_4H_8^{(0)}$

Calculating GIAO nuclear magnetic shielding tensors.
SCF GIAO Magnetic shielding tensor (ppm):
1 N Isotropic = 152.2263 Anisotropy = 121.5054
XX= 22.3016 YX= 4.3458 ZX= 0.2234
XY= 4.3405 YY= 201.1476 ZY= -0.0052
XZ= 0.2313 YZ= -0.0048 ZZ= 233.2296
Eigenvalues: 22.1959 201.2530 233.2299
2 B Isotropic = 83.2314 Anisotropy = 46.8512
XX= 68.1694 YX= 11.6306 ZX= 0.0273
XY= 11.6231 YY= 67.0595 ZY= 0.0559
XZ= 0.0247 YZ= 0.1030 ZZ= 114.4654
Eigenvalues: 55.9743 79.2544 114.4655
3 B Isotropic = 83.2322 Anisotropy = 46.8504
XX= 67.0462 YX= -11.6269 ZX= 0.0270
XY= -11.6206 YY= 68.1846 ZY= -0.0501
XZ= 0.0217 YZ= -0.0922 ZZ= 114.4656
Eigenvalues: 55.9777 79.2530 114.4658
4 N Isotropic = 152.2466 Anisotropy = 121.4938
XX= 201.1550 YX= -4.3539 ZX= 0.0090
XY= -4.3379 YY= 22.3424 ZY= 0.1373
XZ= -0.0352 YZ= 0.1180 ZZ= 233.2424
Eigenvalues: 22.2367 201.2606 233.2425
5 B Isotropic = 83.2335 Anisotropy = 46.8503
XX= 67.0506 YX= -11.6261 ZX= -0.0819
XY= -11.6246 YY= 68.1831 ZY= -0.0415
XZ= -0.0626 YZ= -0.0329 ZZ= 114.4669

Eigenvalues: 55.9776 79.2560 114.4671
6 N Isotropic = 152.2523 Anisotropy = 121.5025
XX= 201.1472 YX= -4.3456 ZX= 0.0030
XY= -4.3388 YY= 22.3558 ZY= -0.1692
XZ= -0.0322 YZ= -0.1005 ZZ= 233.2538
Eigenvalues: 22.2503 201.2526 233.2539
7 N Isotropic = 152.2298 Anisotropy = 121.5036
XX= 22.3110 YX= 4.3433 ZX= -0.2762
XY= 4.3529 YY= 201.1463 ZY= 0.0056
XZ= -0.1308 YZ= -0.0040 ZZ= 233.2320
Eigenvalues: 22.2052 201.2520 233.2322
8 B Isotropic = 83.2339 Anisotropy = 46.8475
XX= 68.1718 YX= 11.6314 ZX= -0.0645
XY= 11.6225 YY= 67.0645 ZY= 0.0343
XZ= -0.0387 YZ= 0.0229 ZZ= 114.4655
Eigenvalues: 55.9779 79.2582 114.4656
9 H Isotropic = 27.0626 Anisotropy = 6.2074
XX= 31.1987 YX= -0.0869 ZX= -0.0100
XY= -0.0882 YY= 27.5869 ZY= 0.0000
XZ= -0.0017 YZ= -0.0002 ZZ= 22.4022
Eigenvalues: 22.4022 27.5847 31.2009
10 H Isotropic = 27.3424 Anisotropy = 2.6263
XX= 28.7368 YX= -0.3403 ZX= -0.0013
XY= -0.3403 YY= 28.7684 ZY= -0.0031
XZ= -0.0017 YZ= 0.0003 ZZ= 24.5221
Eigenvalues: 24.5221 28.4119 29.0933
11 H Isotropic = 27.3423 Anisotropy = 2.6263
XX= 28.7678 YX= 0.3405 ZX= -0.0016
XY= 0.3408 YY= 28.7365 ZY= 0.0031
XZ= -0.0014 YZ= -0.0005 ZZ= 24.5227
Eigenvalues: 24.5227 28.4111 29.0932
12 H Isotropic = 27.0628 Anisotropy = 6.2125
XX= 27.5904 YX= 0.0864 ZX= 0.0020
XY= 0.0866 YY= 31.2024 ZY= -0.0079
XZ= 0.0013 YZ= -0.0004 ZZ= 22.3957
Eigenvalues: 22.3956 27.5884 31.2045
13 H Isotropic = 27.3426 Anisotropy = 2.6264
XX= 28.7686 YX= 0.3406 ZX= 0.0061
XY= 0.3405 YY= 28.7366 ZY= 0.0007
XZ= 0.0046 YZ= 0.0019 ZZ= 24.5227
Eigenvalues: 24.5226 28.4117 29.0936
14 H Isotropic = 27.0630 Anisotropy = 6.2136
XX= 27.5909 YX= 0.0872 ZX= 0.0017
XY= 0.0867 YY= 31.2033 ZY= 0.0084
XZ= 0.0015 YZ= 0.0065 ZZ= 22.3949
Eigenvalues: 22.3949 27.5888 31.2054
15 H Isotropic = 27.0627 Anisotropy = 6.2081
XX= 31.1994 YX= -0.0867 ZX= 0.0090
XY= -0.0868 YY= 27.5873 ZY= 0.0002
XZ= 0.0139 YZ= -0.0005 ZZ= 22.4015
Eigenvalues: 22.4015 27.5852 31.2015
16 H Isotropic = 27.3426 Anisotropy = 2.6264

XX= 28.7363 YX= -0.3404 ZX= 0.0054
XY= -0.3407 YY= 28.7688 ZY= 0.0000
XZ= 0.0039 YZ= -0.0019 ZZ= 24.5226
Eigenvalues: 24.5226 28.4116 29.0935
17 Bq Isotropic = -4.2046 Anisotropy = 13.7854
XX= 4.9686 YX= 0.0003 ZX= 0.0009
XY= 0.0003 YY= 4.9857 ZY= -0.0002
XZ= -0.0079 YZ= 0.0001 ZZ= -22.5680
Eigenvalues: -22.5680 4.9686 4.9857

$B_4N_4H_8^{(2-)}$

Calculating GIAO nuclear magnetic shielding tensors.
SCF GIAO Magnetic shielding tensor (ppm):
1 B Isotropic = 104.3255 Anisotropy = 32.7883
XX= 92.4781 YX= -23.0012 ZX= -0.0034
XY= -23.0032 YY= 94.3141 ZY= -0.0039
XZ= 0.0151 YZ= 0.0134 ZZ= 126.1844
Eigenvalues: 70.3755 116.4166 126.1844
2 N Isotropic = 141.0785 Anisotropy = 124.2238
XX= -9.2775 YX= 4.3352 ZX= -0.0122
XY= 4.3312 YY= 208.6186 ZY= 0.0009
XZ= 0.0077 YZ= 0.0240 ZZ= 223.8943
Eigenvalues: -9.3636 208.7047 223.8943
3 N Isotropic = 141.0801 Anisotropy = 124.2286
XX= 208.6166 YX= -4.3316 ZX= 0.0008
XY= -4.3353 YY= -9.2755 ZY= 0.0052
XZ= 0.0218 YZ= -0.0098 ZZ= 223.8992
Eigenvalues: -9.3617 208.7027 223.8992
4 B Isotropic = 104.3252 Anisotropy = 32.7887
XX= 94.3144 YX= 23.0064 ZX= 0.0050
XY= 22.9979 YY= 92.4768 ZY= -0.0046
XZ= -0.0001 YZ= -0.0010 ZZ= 126.1843
Eigenvalues: 70.3751 116.4161 126.1843
5 N Isotropic = 141.0805 Anisotropy = 124.2246
XX= 208.6185 YX= -4.3318 ZX= -0.0019
XY= -4.3352 YY= -9.2740 ZY= -0.0170
XZ= -0.0219 YZ= -0.0114 ZZ= 223.8969
Eigenvalues: -9.3601 208.7047 223.8969
6 B Isotropic = 104.3254 Anisotropy = 32.7883
XX= 94.3150 YX= 23.0062 ZX= -0.0040
XY= 22.9985 YY= 92.4770 ZY= 0.0036
XZ= 0.0009 YZ= -0.0013 ZZ= 126.1843
Eigenvalues: 70.3753 116.4167 126.1843
7 B Isotropic = 104.3253 Anisotropy = 32.7888
XX= 92.4775 YX= -23.0016 ZX= 0.0016
XY= -23.0029 YY= 94.3138 ZY= 0.0020
XZ= -0.0054 YZ= -0.0070 ZZ= 126.1845
Eigenvalues: 70.3751 116.4162 126.1845
8 N Isotropic = 141.0788 Anisotropy = 124.2237
XX= -9.2772 YX= 4.3367 ZX= 0.0044
XY= 4.3318 YY= 208.6189 ZY= -0.0017
XZ= -0.0189 YZ= -0.0192 ZZ= 223.8945
Eigenvalues: -9.3633 208.7051 223.8945

9 H Isotropic = 25.6394 Anisotropy = 7.1882
XX= 27.5056 YX= -2.8125 ZX= 0.0000
XY= -2.8124 YY= 27.7282 ZY= -0.0001
XZ= 0.0022 YZ= 0.0008 ZZ= 21.6845
Eigenvalues: 21.6845 24.8022 30.4316
10 H Isotropic = 25.4562 Anisotropy = 6.8074
XX= 29.4781 YX= 0.0104 ZX= 0.0007
XY= 0.0101 YY= 29.9943 ZY= 0.0008
XZ= 0.0010 YZ= -0.0010 ZZ= 16.8963
Eigenvalues: 16.8963 29.4779 29.9945
11 H Isotropic = 25.4561 Anisotropy = 6.8087
XX= 29.9950 YX= -0.0102 ZX= 0.0007
XY= -0.0104 YY= 29.4782 ZY= -0.0001
XZ= -0.0010 YZ= -0.0011 ZZ= 16.8951
Eigenvalues: 16.8951 29.4780 29.9952
12 H Isotropic = 25.6395 Anisotropy = 7.1882
XX= 27.7285 YX= 2.8126 ZX= 0.0004
XY= 2.8122 YY= 27.5056 ZY= 0.0000
XZ= 0.0008 YZ= 0.0009 ZZ= 21.6844
Eigenvalues: 21.6844 24.8025 30.4316
13 H Isotropic = 25.4562 Anisotropy = 6.8086
XX= 29.9951 YX= -0.0102 ZX= -0.0003
XY= -0.0104 YY= 29.4783 ZY= 0.0004
XZ= 0.0002 YZ= 0.0014 ZZ= 16.8953
Eigenvalues: 16.8953 29.4781 29.9953
14 H Isotropic = 25.6394 Anisotropy = 7.1883
XX= 27.7284 YX= 2.8126 ZX= -0.0002
XY= 2.8123 YY= 27.5055 ZY= 0.0001
XZ= -0.0002 YZ= -0.0005 ZZ= 21.6844
Eigenvalues: 21.6844 24.8023 30.4316
15 H Isotropic = 25.6395 Anisotropy = 7.1882
XX= 27.5057 YX= -2.8124 ZX= -0.0001
XY= -2.8123 YY= 27.7283 ZY= 0.0002
XZ= -0.0006 YZ= 0.0005 ZZ= 21.6844
Eigenvalues: 21.6844 24.8025 30.4316
16 H Isotropic = 25.4563 Anisotropy = 6.8074
XX= 29.4782 YX= 0.0105 ZX= -0.0005
XY= 0.0102 YY= 29.9944 ZY= -0.0002
XZ= -0.0009 YZ= 0.0001 ZZ= 16.8963
Eigenvalues: 16.8963 29.4780 29.9946
17 Bq Isotropic = 9.1725 Anisotropy = 21.6013
XX= 1.9710 YX= 0.0002 ZX= 0.0000
XY= -0.0001 YY= 1.9732 ZY= -0.0002
XZ= 0.0001 YZ= 0.0000 ZZ= 23.5734
Eigenvalues: 1.9710 1.9732 23.5734

$C_4B_2N_2H_8^{(0)}$

Calculating GIAO nuclear magnetic shielding tensors.
SCF GIAO Magnetic shielding tensor (ppm):
1 C Isotropic = 49.9107 Anisotropy = 189.0273
XX= 23.2470 YX= 12.8030 ZX= -100.1844
XY= 19.1861 YY= 31.5366 ZY= 3.1357

```
 XZ=  -122.1494   YZ=    15.3598   ZZ=    94.9485
 Eigenvalues:   -61.3423    35.1455   175.9289
 2  B    Isotropic =    74.1028   Anisotropy =    71.8387
 XX=    54.1958   YX=     6.9463   ZX=     4.7341
 XY=     3.2985   YY=    81.2593   ZY=   -34.7600
 XZ=     6.1057   YZ=   -40.9045   ZZ=    86.8533
 Eigenvalues:    41.6911    58.6220   121.9953
 3  C    Isotropic =    49.9010   Anisotropy =   189.0458
 XX=    23.2433   YX=   -12.7903   ZX=  -100.1937
 XY=   -19.1734   YY=    31.5227   ZY=    -3.1502
 XZ=  -122.1653   YZ=   -15.3763   ZZ=    94.9370
 Eigenvalues:   -61.3601    35.1316   175.9316
 4  N    Isotropic =   140.6532   Anisotropy =   103.8972
 XX=   161.8783   YX=   -15.6573   ZX=     5.2741
 XY=   -26.7500   YY=    89.2003   ZY=   -74.6564
 XZ=    10.4779   YZ=   -48.0572   ZZ=   170.8810
 Eigenvalues:    54.2146   157.8270   209.9180
 5  C    Isotropic =    69.7520   Anisotropy =   110.7057
 XX=    42.5119   YX=   -11.2570   ZX=    84.3077
 XY=   -15.3038   YY=    93.4500   ZY=    12.1384
 XZ=    83.7132   YZ=     1.0029   ZZ=    73.2940
 Eigenvalues:   -29.1993    94.8995   143.5558
 6  B    Isotropic =    74.1055   Anisotropy =    71.8403
 XX=    54.2031   YX=    -6.9403   ZX=     4.7306
 XY=    -3.2977   YY=    81.2739   ZY=    34.7638
 XZ=     6.1042   YZ=    40.9094   ZZ=    86.8394
 Eigenvalues:    41.6944    58.6230   121.9990
 7  C    Isotropic =    69.7573   Anisotropy =   110.6956
 XX=    42.5254   YX=    11.2593   ZX=    84.3035
 XY=    15.3015   YY=    93.4581   ZY=   -12.1383
 XZ=    83.7101   YZ=    -1.0085   ZZ=    73.2886
 Eigenvalues:   -29.1904    94.9081   143.5544
 8  N    Isotropic =   140.6618   Anisotropy =   103.8875
 XX=   161.8860   YX=    15.6466   ZX=     5.2731
 XY=    26.7471   YY=    89.2438   ZY=    74.6689
 XZ=    10.4820   YZ=    48.0695   ZZ=   170.8556
 Eigenvalues:    54.2351   157.8301   209.9201
 9  H    Isotropic =    24.9361   Anisotropy =     2.9519
 XX=    24.4061   YX=     0.4892   ZX=    -1.5331
 XY=     0.2013   YY=    26.7200   ZY=     0.3647
 XZ=    -2.2165   YZ=     1.1482   ZZ=    23.6822
 Eigenvalues:    21.9978    25.9065    26.9040
 10  H    Isotropic =    26.4342   Anisotropy =     1.8808
 XX=    27.1938   YX=    -0.1089   ZX=     0.1842
 XY=    -1.1222   YY=    26.8792   ZY=    -0.0888
 XZ=    -0.2329   YZ=    -0.6157   ZZ=    25.2295
 Eigenvalues:    25.1458    26.4688    27.6881
 11  H    Isotropic =    24.9357   Anisotropy =     2.9523
 XX=    24.4055   YX=    -0.4888   ZX=    -1.5334
 XY=    -0.2015   YY=    26.7201   ZY=    -0.3643
 XZ=    -2.2175   YZ=    -1.1479   ZZ=    23.6815
 Eigenvalues:    21.9966    25.9065    26.9039
```

12 H Isotropic = 26.9339 Anisotropy = 8.4905
XX= 28.4381 YX= 2.6615 ZX= 0.4252
XY= 1.8179 YY= 27.9016 ZY= 4.1513
XZ= 1.9637 YZ= 4.9824 ZZ= 24.4620
Eigenvalues: 21.2887 26.9188 32.5942
13 H Isotropic = 25.7082 Anisotropy = 3.4724
XX= 25.3769 YX= -0.3017 ZX= -1.6485
XY= -0.4035 YY= 27.8520 ZY= 0.8991
XZ= -1.0772 YZ= 0.0422 ZZ= 23.8957
Eigenvalues: 23.0745 26.0270 28.0231
14 H Isotropic = 26.4345 Anisotropy = 1.8802
XX= 27.1935 YX= 0.1091 ZX= 0.1844
XY= 1.1215 YY= 26.8802 ZY= 0.0889
XZ= -0.2328 YZ= 0.6154 ZZ= 25.2299
Eigenvalues: 25.1462 26.4694 27.6880
15 H Isotropic = 25.7083 Anisotropy = 3.4724
XX= 25.3772 YX= 0.3014 ZX= -1.6487
XY= 0.4039 YY= 27.8520 ZY= -0.8990
XZ= -1.0770 YZ= -0.0425 ZZ= 23.8957
Eigenvalues: 23.0746 26.0271 28.0232
16 H Isotropic = 26.9345 Anisotropy = 8.4915
XX= 28.4385 YX= -2.6614 ZX= 0.4271
XY= -1.8175 YY= 27.8994 ZY= -4.1518
XZ= 1.9652 YZ= -4.9843 ZZ= 24.4655
Eigenvalues: 21.2893 26.9186 32.5955
17 Bq Isotropic = -1.9739 Anisotropy = 10.5827
XX= 4.2090 YX= -0.0003 ZX= 1.1854
XY= 0.0001 YY= 5.0813 ZY= -0.0006
XZ= 2.5989 YZ= -0.0008 ZZ= -15.2120
Eigenvalues: -15.3946 4.3917 5.0813

$BNC_6H_8^{(0)}$

Calculating GIAO nuclear magnetic shielding tensors.
SCF GIAO Magnetic shielding tensor (ppm):
1 N Isotropic = 130.1031 Anisotropy = 110.4519
XX= 103.1514 YX= 32.1509 ZX= 45.1882
XY= 50.7166 YY= 130.0183 ZY= -62.4213
XZ= 39.5768 YZ= -53.1966 ZZ= 157.1396
Eigenvalues: 33.9810 152.5906 203.7377
2 B Isotropic = 73.3146 Anisotropy = 72.0479
XX= 70.2213 YX= -14.9028 ZX= 19.0876
XY= -12.9638 YY= 64.4975 ZY= -28.5093
XZ= 24.2035 YZ= -35.3264 ZZ= 85.2250
Eigenvalues: 41.1930 57.4043 121.3465
3 C Isotropic = 59.9807 Anisotropy = 165.5945
XX= 57.8118 YX= -12.2032 ZX= 69.7388
XY= -12.3075 YY= 31.3075 ZY= 70.6977
XZ= 81.2053 YZ= 72.0332 ZZ= 90.8227
Eigenvalues: -47.0613 56.6263 170.3770
4 C Isotropic = 55.5185 Anisotropy = 157.0852
XX= 30.9072 YX= -13.7674 ZX= 67.3853
XY= -16.7186 YY= 56.6995 ZY= 62.2722
XZ= 94.0634 YZ= 68.9138 ZZ= 78.9489

```
 Eigenvalues:   -55.1871    61.5007   160.2420
 5  C    Isotropic =    58.4328   Anisotropy =   146.7568
  XX=    47.1493   YX=    18.4492   ZX=   -62.1089
  XY=    19.2740   YY=    54.1519   ZY=    69.9796
  XZ=   -71.3054   YZ=    81.1763   ZZ=    73.9971
 Eigenvalues:   -49.9201    68.9478   156.2706
 6  C    Isotropic =    68.2769   Anisotropy =   135.7825
  XX=    75.0380   YX=    17.5943   ZX=   -54.9887
  XY=    16.1915   YY=    39.3761   ZY=    72.4185
  XZ=   -61.1053   YZ=    65.3003   ZZ=    90.4166
 Eigenvalues:   -31.1723    77.2044   158.7986
 7  C    Isotropic =    73.4834   Anisotropy =   124.9723
  XX=    77.7020   YX=   -26.5615   ZX=   -60.1690
  XY=   -26.4956   YY=    54.4366   ZY=   -69.3622
  XZ=   -67.3497   YZ=   -53.3406   ZZ=    88.3115
 Eigenvalues:   -28.4004    92.0522   156.7982
 8  C    Isotropic =    60.8938   Anisotropy =   124.7903
  XX=    46.1121   YX=   -21.8406   ZX=   -63.3614
  XY=   -25.5194   YY=    68.4747   ZY=   -55.2693
  XZ=   -79.8558   YZ=   -60.6657   ZZ=    68.0944
 Eigenvalues:   -44.1207    82.7147   144.0873
 9  H    Isotropic =    26.7356   Anisotropy =     7.3428
  XX=    30.0945   YX=    -0.7362   ZX=    -2.6280
  XY=     0.2805   YY=    25.7091   ZY=     2.4486
  XZ=    -3.3873   YZ=     2.2757   ZZ=    24.4033
 Eigenvalues:    21.9230    26.6531    31.6308
10  H    Isotropic =    26.5241   Anisotropy =     1.6518
  XX=    26.5903   YX=    -0.2025   ZX=    -0.1921
  XY=     0.5158   YY=    27.5964   ZY=     0.0144
  XZ=     0.7790   YZ=    -0.3157   ZZ=    25.3857
 Eigenvalues:    25.3035    26.6436    27.6254
11  H    Isotropic =    25.6309   Anisotropy =     2.6978
  XX=    25.9609   YX=    -1.2001   ZX=     1.1972
  XY=    -1.2986   YY=    26.3119   ZY=     1.2117
  XZ=     1.1126   YZ=     1.3981   ZZ=    24.6199
 Eigenvalues:    23.0086    26.4547    27.4295
12  H    Isotropic =    25.2900   Anisotropy =     3.5475
  XX=    26.1404   YX=    -0.2940   ZX=    -0.0226
  XY=    -2.2426   YY=    26.3765   ZY=    -0.1697
  XZ=     1.7794   YZ=    -0.1716   ZZ=    23.3532
 Eigenvalues:    23.0868    25.1282    27.6551
13  H    Isotropic =    25.4182   Anisotropy =     3.6748
  XX=    26.8355   YX=     1.0470   ZX=    -0.1866
  XY=     1.6894   YY=    25.9192   ZY=     0.1316
  XZ=    -1.5935   YZ=     0.8271   ZZ=    23.4999
 Eigenvalues:    23.0261    25.3604    27.8681
14  H    Isotropic =    25.9328   Anisotropy =     2.9937
  XX=    26.9860   YX=     1.7237   ZX=     0.6947
  XY=     0.5268   YY=    26.5232   ZY=    -0.2889
  XZ=     0.2883   YZ=     0.0321   ZZ=    24.2892
 Eigenvalues:    24.1497    25.7200    27.9286
15  H    Isotropic =    26.0828   Anisotropy =     3.0629
```

XX= 26.4697 YX= -1.3707 ZX= 0.5177
XY= -1.1047 YY= 27.1729 ZY= -0.2431
XZ= 0.0412 YZ= 0.0567 ZZ= 24.6059
Eigenvalues: 24.5608 25.5630 28.1248
16 H Isotropic = 25.3720 Anisotropy = 3.7136
XX= 26.1365 YX= -0.6369 ZX= 1.0059
XY= -1.7762 YY= 26.9015 ZY= 1.2851
XZ= -0.7180 YZ= 0.2668 ZZ= 23.0781
Eigenvalues: 22.8794 25.3889 27.8478
17 Bq Isotropic = -3.0052 Anisotropy = 13.3455
XX= 5.7644 YX= -1.1863 ZX= -0.6114
XY= 0.3138 YY= 3.2885 ZY= -0.7076
XZ= -1.8685 YZ= -0.5095 ZZ= -18.0683
Eigenvalues: -18.1512 3.2439 5.8919