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MNDO Calculations on Borazine Derivatives. 2. Substitution of Two [HNBH] Fragments for Two [HCCH] Fragments in Benzene To Form the Diazadiborines and the Novel Open Structure of the 1,2,4,5-Isomer

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The 11 diazadiborine isomers of formula $C_2H_6B_2N_2$, 1,3,2,4-, 1,4,2,6-, 1,3,2,5-, 1,3,4,6-, 1,4,2,5-, 1,4,2,3-, 1,2,3,6-, 1,3,4,5-, 1,2,3,5-, 1,2,3,4-, and 1,2,4,5-diazadiborine (**4**–**14**), have been examined by using MNDO (*m*odified *n*eglect of *d*iatomic *o*verlap) calculations. The thermodynamically most stable diazadiborine was **4**, the 1,3,2,4-isomer (heat of formation −60.16 kcal/mol). With the exceptions of **12**–**14**, the diazadiborines optimized as planar molecules. For the 1,2,4,5-isomer, **14**, the cyclic structure was neither a local nor an absolute minimum on the MNDO potential energy surface. (No orbital overlap or bonding was calculated to exist between the two nitrogen atoms in the molecule.) Rather, **14** optimized as the novel chain structure $HN{=}CH(BH)_2CH{=}NH$, 2,3-didehydro-2,3-diborabutane-1,4-diimine (the lowest energy structure of this molecule is **14o**). The diazadiborines **4**, **9**, **10**, and **13**, which can be represented by classical, uncharged valence bond structures, optimized as molecules with localized double and single bonds. Of the remaining diazadiborines, none of which can be represented by classical, uncharged valence-bond structures and which are thus termed mesionic, **5**, **6**, and **8** optimized as molecules with approximately uniform bond delocalization among ring atoms, while **7**, **11**, and **12**, although containing some delocalized bonds, exhibited single-bond localization between certain ring atoms.

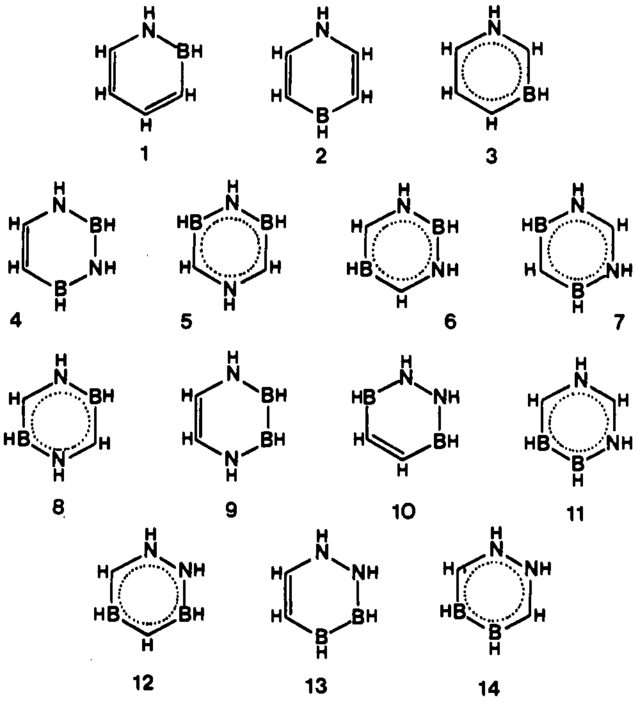
Introduction

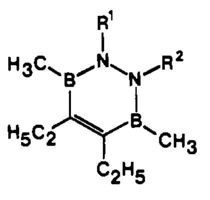
Borazine, prepared by Stock and Pohland[1] in 1923, has often been referred to as "inorganic benzene".[2] However, even though borazine has a planar structure[3] and physical properties which closely resemble benzene,[4a] the chemical properties of borazine suggest little aromatic character.[5]

The contrast between the physical and chemical properties of benzene and borazine suggest that "hybrid" structures which contain both [HNBH] and [HCCH] moieties might exhibit a mixture of the properties of both molecules. We have previously reported[6] our MNDO (*m*odified *n*eglect of *d*iatomic *o*verlap) calculations on the three possible azaborine isomers, 1,2-azaborine (**1**), 1,4-azaborine (**2**), and 1,3-azaborine (**3**), which each contain one [HNBH] and two [HCCH] moieties (see Chart I). Of these molecules, only the 1,3-isomer exhibited significant bond delocalization; the 1,2- and 1,4-isomers appeared to be best described as heterocyclic dienes.

Cyclic structures containing one [HCCH] and two [HNBH] moieties are commonly referred to as diazadiborines, $C_2H_6B_2N_2$.[7] There are 11 possible six-membered ring isomers with this formula: 1,3,2,4- (**4**), 1,4,2,6- (**5**), 1,3,2,5- (**6**), 1,3,4,6- (**7**), 1,4,2,5- (**8**), 1,4,2,3- (**9**), 1,2,3,6- (**10**), 1,3,4,5- (**11**), 1,2,3,5- (**12**), 1,2,3,4- (**13**), and 1,2,4,5-diazadiborine (**14**) (see Chart I). Apparently, only **4**, **7**, and **8** have been investigated (computationally) as the unsubstituted parent molecules.[8,9] The 1,2,3,6-isomer (**10**) has been synthesized in substituted form (**10a**–**c**) and as the tricarbonylchromium complex.[10]

Chart I





10a $R^1 = R^2 = H$

10b $R^1 = R^2 = CH_3$

10c $R^1 = H$, $R^2 = CH_3$

No reports of the isolation and characterization of any of the unsubstituted diazadiborines appear to have been published. A number of reports[11-20] of substituted derivatives of the azaborines

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[1] Stock, A.; Pohland, E. *Chem. Ber.* **1923**, *56*, 789.

[2] (a) Wiberg, E. *Naturwissenschaften* **1948**, *35*, 182. (b) Huheey, J. E. *Inorganic Chemistry: Principles of Structure and Reactivity*, 3rd ed.; Harper and Row: New York, 1983; pp 701–706.

[3] (a) Stock, A.; Wierl, R. *Z. Anorg. Allg. Chem.* **1932**, *203*, 228. (b) Bauer, S. H. *J. Am. Chem. Soc.* **1938**, *60*, 524. (c) Harshbarger, W.; Lee, G.; Porter, R. F.; Bauer, S. H. *Inorg. Chem.* **1969**, *8*, 1683.

[4] (a) Greenwood, N. N.; Earnshaw, A. *Chemistry of the Elements*; Pergamon Press: Oxford, England, 1985; pp 234–240. (b) *Ibid.*, pp 155–242 and 466–545.

[5] Niedenzu, K.; Dawson, J. W. In *The Chemistry of Boron and its Compounds*; Muetterties, E. W., Ed.; John Wiley and Sons: New York, 1967; pp 377–442.

[6] Massey, S. T.; Zoellner, R. W. MNDO Calculations on Borazine Derivatives. 1. *Int. J. Quantum Chem.* **1991**, in press.

[7] The nomenclature of these compounds has changed, such that a compound with the formula $C_2H_6B_2N_2$ formerly known[8] as, for example, 2,4-dibora-1,3-diazarobenzene, is now referred to as 1,3,2,4-diazadiborine. *Chemical Abstracts* terms this molecule 1,2,3,4-tetrahydro-1,3,2,4-diazadiborine, and refers to a molecule with the formula $C_2H_2B_2N_2$, which does not have hydrogen atoms bound to either nitrogen or boron, as a simple diazadiborine.

[8] Hoffmann, R. *J. Chem. Phys.* **1964**, *40*, 2474. EHT results on all 11 isomeric diazadiborines were mentioned, but only **4** and **7** were explicitly discussed.

[9] Michl, J. *Collect. Czech. Chem. Commun.* **1971**, *36*, 1248.

[10] (a) Siebert, W.; Full, R. *Angew. Chem., Int. Ed. Engl.* **1976**, *15*, 45; *Angew. Chem.* **1976**, *88*, 55. (b) Siebert, W. *Adv. Organomet. Chem.* **1980**, *18*, 301. (c) Siebert, W.; Full, R.; Schmidt, H.; von Seyerl, J.; Halstenberg, M.; Huttner, G. *J. Organomet. Chem.* **1980**, *191*, 15. (d) Siebert, W. *Pure Appl. Chem.* **1987**, *59*, 947.

[11] Schreyer, P.; Paetzold, P.; Boese, R. *Chem. Ber.* **1988**, *121*, 195.

[12] Tanaka, K.; Yamanaka, S.; Ueda, K.; Takeda, S.; Yamebe, T. *Synth. Met.* **1987**, *20*, 333.

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and diazadiborines have appeared, but for the unsubstituted diazadiborines, the reports have been theoretical studies at a relatively simplistic level.

We have been intrigued by these compounds and by the comparative dearth of information concerning the unsubstituted diazadiborines. The semiempirical computational program MNDO[21] has been shown to accurately calculate the structures, ionization potentials, heats of formation, and other molecular properties of both borazine[22] and benzene.[23] Our results[6] from the application of this method to the azaborines were also in accord with the literature data available. Thus, we felt MNDO would be an appropriate probe of the properties of the diazadiborines as well. Further, Maouche and Gayoso[24] report the MNDO study of a series of linear and cyclic unsaturated boron–nitrogen compounds and concluded that MNDO is a suitable semiempirical method for describing the ground state of boron- and nitrogen-containing compounds.

Herein we report our MNDO-calculated results for the ground-state properties, the structures, and the relative thermodynamic stabilities of the 11 isomers of diazadiborine.

Methods

*M*odified *n*eglect *of* *d*iatomic *o*verlap (MNDO) calculations were performed by using QCPE[25a] program number 353, (MNDO: Molecular Orbital Calculations by the MNDO Method with Geometry Optimization (IBM 370)), suitably modified to run on a Honeywell DPS-8 computer. This program uses the Davidon–Fletcher–Powell algorithm[26] to locate equilibrium geometries on the MNDO potential energy surface.

Three different sets of initial trial geometries (ITGs) were used for the MNDO calculations: (a) a heavy atom–heavy atom bond distance of 1.8 Å with a heavy atom–hydrogen bond distance of 1.2 Å; (b) bond distances of 1.2 and 0.8 Å, respectively; (c) bond distances of 1.0 and 0.8 Å, respectively. All cyclic molecules were assumed to be regular hexagons for the ITGs, while for the ITG of the open-chain molecule (**14o**), a planar chain of conjugated trans double bonds (all bond angles of 120°) with bond distances are given above was used.

The ITGs as described above were used to construct the **Z** matrices for each calculation, and *all* optimizable parameters in each molecule were allowed to optimize fully. With the exception of bond distances and relative heavy-atom positions, all of the **Z** matrices were identical. In addition to changing bond distances, each molecule was calculated by using different atom arrangements. For example, **4** was calculated from the arrangement N–B–N–B–C–C but also from the arrangements B–N–B–C–C–N, N–B–C–C–N–B, and so forth. These are equivalent arrangements of atoms for the same cyclic molecule, but each **Z** matrix begins with a different ring atom.

The ITGs were empirically determined and gave a good range of initial points from which to optimize the molecules. The calculated properties and equilibrium geometries of the diazadiborines were not extremely sensitive to the ITGs. However, in some cases additional ITGs, with values for bond distances which more closely approximated the expected equilibrium geometries, were used in order to explore more completely the MNDO potential energy surface near the final equilibrium geometry of the molecule. In every case, all parameters were optimized; no symmetry conditions were imposed.

Table I. MNDO-Optimized Results[a] for the Isomers of Diazadiborine, $C_2H_6B_2N_2$

compd	heat of formn, kcal/mol	ionizn pot., eV	dipole moment, D
1,3,2,4-diazadiborine (**4**)	−60.16	9.282	1.932
1,4,2,6-diazadiborine (**5**)	−30.71	8.216	2.210
1,3,2,5-diazadiborine (**6**)	−30.67	8.375	2.625
1,3,4,6-diazadiborine (**7**)	−25.72	8.339	6.146
1,4,2,5-diazadiborine (**8**)	−25.47	8.004	0.00301
1,4,2,3-diazadiborine (**9**)	−22.04	8.920	3.162
1,2,3,6-diazadiborine (**10**)	−12.70	10.01	2.380
1,3,4,5-diazadiborine (**11**)	+12.34	8.106	6.542
1,2,3,5-diazadiborine (**12**)	+19.66	8.867	5.561
1,2,3,4-diazadiborine (**13**)	+26.57	9.681	3.585
1,2,4,5-diazadiborine (**14c**)	+39.37	10.72	2.109
2,3-didehydro-2,3-dibora-butane-1,4-diimine (**14o**)	+37.26	10.88	2.521

[a] All values have been arbitrarily reported to four significant figures.[25b]

Results and Discussion

General Ground-State Properties. Table I contains the results for the heats of formation, ionization potentials, and dipole moments, as calculated by MNDO, for the isomers of diazadiborine. The heats of formation of these molecules vary from −60.16 kcal/mol for **4** to +39.37 kcal/mol for **14c**. Since MNDO-calculated stabilities are referenced to standard heats of formation for the atoms involved, the comparison of molecules whose atomic composition is different (i.e., benzene versus borazine versus the diazadiborines) is not without hazard. However, contrary to the EHT (extended Hückel theory) results of Hoffmann,[8] each of the diazadiborines was calculated to have a heat of formation more positive than that calculated for borazine (−131.1 kcal/mol[6]) and more negative (with the exception of **13** and **14**) than the heat of formation of benzene (+21.20 kcal/mol[6]). Of course, such data do not necessarily imply that the diazadiborines are more stable than benzene and less stable than borazine: benzene is indefinitely stable under ambient conditions in the absence of ignition sources, while borazine slowly decomposes on standing.[3c]

The thermodynamically most stable of the diazadiborines, as calculated by MNDO, is **4**, 1,3,2,4-diazadiborine. This result is in accord with the EHT calculations of Hoffmann,[8] although he quotes no data. Hoffmann further states, however, that the next most stable isomer is **7**, 1,3,4,6-diazadiborine, while the current MNDO calculations demonstrate that **5**, 1,4,2,6-diazadiborine, and **6**, 1,3,2,5-diazadiborine, are more stable than **7**. The heats of formation of **5** and **6** differ by less than 0.04 kcal/mol, while **7** and **8**, 1,4,2,5-diazadiborine, differ by less than 0.3 kcal/mol. These individual differences are not statistically significant, but the pairs differ in heats of formation by greater than 5 kcal/mol, which is significant. In each pair, the molecules are similar, with only the interchange of nitrogen and boron atoms to distinguish them.

The ionization potentials (calculated from the energy of the highest occupied molecular orbital of the molecule) for all of the diazadiborines were lower than the calculated value[6] for borazine (10.96 eV), and with the exception of **10**, **13**, and **14**, were also lower than the calculated ionization potential of benzene (9.392 eV).

Michl[18] has used the semiempirical SCF–PPP[28] method to investigate the diazadiborines **4**, **7**, and **8**. The ionization potentials

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Table II. MNDO-Optimized Bond Lengths[a] for the Isomers of Diazadiborine

compd	d(C–C)	d(N–B)	d(N–C)	d(B–C)	d(N–N)	d(B–B)
			Classical Structures			
4	1.3698	1.4259[b] 1.4298[c] 1.4177[d]	1.4019	1.5110		
9	1.3677	1.4034_2	1.4094_3			1.6514
10	1.3636	1.4099[e] 1.4084[f]		1.5213_2	1.3684	
13	1.3687	1.4073	1.4265	1.4988	1.3795	1.6504
			Mesionic Structures			
5		1.4189_1	1.3666_2	1.4891_3		
6		1.4255_1	1.3890_4	1.4537_1		
7		1.4645_7	1.3584_3	1.4526_3		
8		1.4216_5	1.3736_1	1.4726_5		
11		1.4381	1.3508[g] 1.4031[h] 1.3791[i]	1.4436		1.6124
12		1.4385	1.3731	1.4928[j] 1.4360[k] 1.4884[l]	1.3576	
14c			1.2887[h] 1.2912[n]	1.5417[m] 1.5339[l]	4.7027	1.5938
14o			1.2872_1	1.5309_3	4.7236	1.5955

[a] Bond lengths in angstroms; the standard deviation of the least significant figure is subscripted. [b] Bond d(N^1–B^2). [c] Bond d(B^2–N^3). [d] Bond d(N^3–B^4). [e] Bond d(N^1–B^6). [f] Bond d(N^2–B^3). [g] Bond d(N^1–C^2). [h] Bond d(N^1–C^6). [i] Bond d(C^2–N^3). [j] Bond d(B^3–C^4). [k] Bond d(C^4–B^5). [l] Bond d(B^5–C^6). [m] Bond d(C^3–B^4). [n] Bond d(N^2–C^3).

Table III. Ring Atom Bond Indices[a] for the Isomers of Diazadiborine

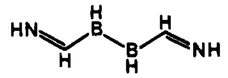
compd	bi(1–2)	bi(2–3)	bi(3–4)	bi(4–5)	bi(5–6)	bi(1–6)
			Classical Structures			
4	1.2114	1.1886	1.2502	1.0862	1.7217	1.0795
9	1.3432	0.9391	1.3427	1.0490	1.7520	1.0488
10	0.9647	1.3357	1.0470	1.7786	1.0474	1.3336
13	0.9638	1.3484	0.9310	1.1066	1.7044	1.0696
			Mesionic Structures			
5	1.2589	1.1809	1.3110	1.3102	1.1816	1.2583
6	1.2244	1.2239	1.1716	1.3665	1.3670	1.1710
7	1.3409	1.3411	1.0431	1.3576	1.3572	1.0420
8	1.2608	1.2766	1.2660	1.2606	1.2766	1.2658
11	1.3943	1.1894	1.1656	1.0060	1.4040	1.0866
12	0.9899	1.1882	1.1515	1.4535	1.1649	1.3086
14c	0.0002	1.9466	0.9576	0.9842	0.9572	1.9631
14o	1.9684	0.9589	0.9821	0.9592	1.9685	0.0005

[a] Heading numbers refer to the numbering of the atoms in the ring, with atom number 1 always being nitrogen. Note that in **14c** the atom numbering follows systematic rules for a cyclic molecule, i.e., N^1, N^2, C^3, B^4, B^5, and C^6, while for **14o**, the numbering is N^1, C^2, B^3, B^4, C^5, and N^6, which is correct for a chain molecule.

calculated by the SCF–PPP method were 8.49, 7.93, and 7.58 eV, respectively. Although not matching the absolute values calculated by the MNDO method, 9.282, 8.339, and 8.004 eV, respectively, the SCF–PPP values do mirror the order of ionization potentials calculated by MNDO and roughly reproduce the relative magnitudes of the ionization potentials. The SCF–PPP calculations were used primarily to aid in the interpretation of the electronic spectra of synthetically available molecules; the calculated results for these three diazadiborines could not be compared to known compounds.

General Structural Properties. Compounds **4–11** optimized to planar or nearly planar structures. For these eight molecules, torsion angles for the ring atoms varied from +0.09 to −0.08°, while torsion angles for the hydrogen atoms varied from 179.86 to 180.01°. In contrast to these obviously planar molecules, both **12** and **13**, 1,2,3,5- and 1,2,3,4-diazadiborine, optimized as nonplanar six-membered rings reminiscent of the cyclohexane boat conformation with atoms 1 and 4 at the "prow" and "stern" positions. The average torsion angles between either end of the molecules and the four central atoms varied from 168 to 172°.

The 1,2,4,5-diazadiborine isomer, **14**, presented a unique problem: the cyclic structure was neither a local nor an absolute minimum on the MNDO potential energy surface. (No orbital overlap or bonding was calculated to exist between N^1 and N^2.) When any of the cyclic ITGs was minimized, the lowest energy structure which resulted was **14c**, a noncyclic chain molecule, which was a *local* minimum on the potential energy surface. The apparent absolute minimum was found by using open-chain ITG structures to begin the minimization. These latter ITGs resulted in the lowest energy structure **14o**. In both **14c** and **14o**, the result



14o

is not the cyclic 1,2,4,5-diazadiborine; rather, the product is best described as 2,3-didehydro-2,3-diborabutane-1,4-diimine. (Both structures **14c** and **14o** are slightly different conformers of the same diimine; **14o** is the lower energy conformer.)

Classical Diazadiborines. Compounds **4**, **9**, **10**, and **13** are the only diazadiborines for which classical, uncharged valence-bond structures may be constructed. Bond lengths (Table II) and bond indices[29] (Table III) reflect such structures, particularly in their short C–C bond lengths (1.36–1.37 Å) and high bond orders (1.72–1.78) for the C–C bonds.

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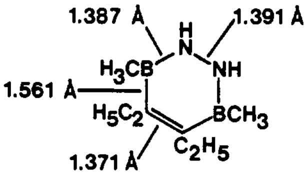
(29) Armstrong, D. R.; Perkins, P. G.; Stewart, J. J. P. *J. Chem. Soc., Dalton Trans.* **1973**, 838. This article allows the concept of bond "delocalization" to be addressed through comparisons of bond indices in adjacent bonds.

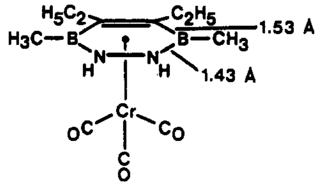
The single-bond covalent radii[4b] for boron, carbon, and nitrogen are 0.88, 0.77, and 0.70 Å, respectively, allowing the prediction of upper bounds for the covalent single-bond distances for C—C bonds (1.54 Å), N—B bonds (1.58 Å), N—C bonds (1.47 Å), B—C bonds (1.65 Å), N—N bonds (1.40 Å), and B—B bonds (1.76 Å). Double-bond covalent radii[4b] for carbon and nitrogen are generally taken as 0.67 and 0.60 Å, allowing the prediction of C=C, N=C, and N=N bond distances of 1.34, 1.27, and 1.20 Å but making the prediction of the hypothetical C=B and N=B bonds difficult.

Given the above values, all of the ring atom to ring atom bond lengths are longer than the predicted double-bond lengths but shorter than predicted single-bond lengths. Examination of bond indices, however, indicates that, especially in the cases of **9**, **10**, and **13**, significant bond index alternation occurs in these molecules, as would be expected for a cyclic, nondelocalized alkene. In the case of **4**, the molecule appears to adopt some bond delocalization between N^1, B^2, N^3, and B^4 (average bond index of 1.217; compare the average bond index of borazine[6] of 1.187).

X-ray crystallographic data have been reported[10] for **10a** and the **10a**–tricarbonylchromium complex, **10d**. The MNDO-calculated values for *d*(C–C), *d*(N–N), and *d*(B–C) are shorter than the values for the diethyl-*B,B'*-dimethyl-substituted derivative **10a**, while *d*(B–C) is longer than that found experimentally. Surprisingly, values for *d*(B–N) and *d*(B–C) in the tricarbonylchromium complex are nearly identical with the MNDO-calculated values.



10a



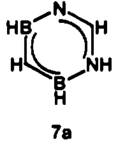
10d

Michl's calculated bond orders[18] for N–B bonds were 0.556, 0.586, and 0.547 for **4**, indicating significant π-bonding between these atoms. The present results do not support the magnitude of the π-bonding reported by Michl but do indicate that a degree of π-bonding does occur between the nitrogen and boron atoms in **4**.

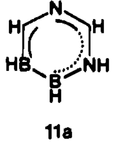
Mesionic[18] Diazadiborines. Compounds **5–8**, **11**, **12**, and **14** are defined as mesionic molecules because they cannot be described by using classical uncharged valence-bond depictions. Bond lengths (Table II), with the exception of **14** (vide infra), are shorter than predicted single-bond lengths but are longer than those predicted for "pure" double bonds.

An examination of ring atom bond indices (Table III) allows the classification of these mesionic structures into two groups. The first group contains diazadiborines **5**, **6**, and **8**, wherein the bond indices indicate moderate bond delocalization throughout the ring atoms. These three molecules are adequately represented by the depictions in Chart I, wherein a dotted circle in the ring is used to obviate the necessity of drawing a charged valence-bond structure. Michl's calculated bond orders[18] for N–B bonds were 0.473 for **7** and 0.575 for **8**. As was discussed for **4** earlier, these values are greater than would be predicted from the present calculations but are indicative of the π-bonding that the present calculations demonstrate.

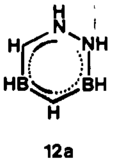
In the second group of diazadiborines, bond delocalization is not uniform about the ring. The diazadiborine **7**, for example, is better represented as **7a**, wherein the molecule appears to resemble two fused allyl systems. The picture is considerably more complicated for **11** and **12**, wherein no simple symmetrical bond delocalization occurs. Representations such as **11a** and **12a** are attempts to depict the bond delocalization which does arise in these molecules.



7a



11a



12a

As has been mentioned earlier, **14** does not optimize to a cyclic structure but rather to the open-chain molecule 2,3-didehydro-2,3-diborabutane-1,4-diimine. This molecule is formally the ring-opened version of 1,2,3,6-diazadiborine wherein the N–N bond has been cleaved. It is interesting to note that in **12** and **13**, the only other molecules with N–N bonds, the N–N bonds are definitely single and that these two molecules are the only two molecules which did not optimize as planar molecules. The orientation of two adjacent nitrogen atoms in these molecules may not be favorable, leading to ring distortion and, in the case of **14**, to actual ring opening.

Conclusions

Scant synthetic experimental data exist with which to compare our MNDO-calculated data for the diazadiborines. In the sole case where structural data are extant,[10] the case of 4,5-diethyl-3,6-dimethyl-1,2,3,6-diazadiborine, calculated values overestimate the extent of C–C (1.3636 Å calculated versus 1.371 Å found experimentally), N–N (1.3684 Å versus 1.391 Å), and B–C (1.5213 Å versus 1.561 Å) bonding and underestimate the extent of N–B (1.409 Å versus 1.387 Å) bonding. The MNDO-calculated bond lengths for the parent molecule **10**, however, match the values much more closely for the analogous bonds in the tricarbonylchromium complex, **10d**.

Although none of the diazadiborines had heats of formation more negative than borazine, all except the 1,2,3,4- and 1,2,4,5-isomers had heats of formation more negative than benzene. Further, many of the diazadiborines exhibited significant bond delocalization and, with **10d** as a guide, might afford stable complexes with transition-metal-containing moieties such as tricarbonylchromium. However, it is interesting to note that the only example of a transition-metal complex of a diazadiborine contains a diazadiborine isomer which is calculated to exhibit generalized bond localization and little or no delocalization.

In the single case of **14**, a novel open-chain molecule, 2,3-didehydro-2,3-diborabutane-1,4-diimine, was shown to be a minimum on the MNDO potential energy surface. Such a molecule, if appropriately substituted, might also be a target for synthetic studies.

There is a continuing interest in the study of novel monomeric and polymeric precursors to ceramic materials.[30] The demonstration of the potential stability of the diazadiborines may lend impetus to new synthetic studies of these interesting molecules. Further, some of these compounds might see use as precursors to "boron-nitride-carbide" materials in the same way that borazine is used as a precursor to boron nitride. We are continuing our computational investigations of these and other interesting borazine derivatives.

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Supplementary Material Available: Tables of final atomic coordinates, molecular orbital energies, and ring atom bond angles for all molecules (13 pages). Ordering information is given on any current masthead page.

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(30) Lynch, A. T.; Sneddon, L. G. *J. Am. Chem. Soc.* **1989**, *111*, 6201 and references therein.