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DENSITY FUNCTIONAL B3LYP AND B3PW91 STUDIES OF THE PROPERTIES OF FOUR CYCLIC ORGANODIBORANES WITH TETRAMETHYLENE FRAGMENTS

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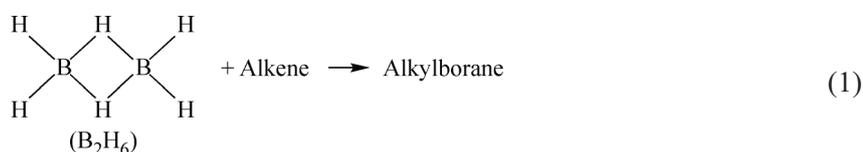
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Molecular structure and vibrational spectra of 1,2-tetramethylenediborane ($B_2C_4H_{12}$), 1,2:1,2-bis(tetramethylene)diborane ($B_2C_8H_{18}$), 1,1-tetramethylenediborane ($B_2C_4H_{12}$) and 1,1:2,2-bis(tetramethylene)diborane ($B_2C_8H_{18}$), have been studied using quantum computational density functional B3LYP and B3PW91 methods and 6-31G*, 6-31G** and 6-31++G** basis sets. Natural bond orbital analyses have been carried out to study in detail the nature of the B—C, C—C and B—H bonds in these molecules. This study showed that all these compounds are thermodynamically stable in the gas phase, but bicyclic structures are more stable than monocyclic structures.

Keywords: density functional theory, alkylborane, boranes, vibrational frequencies, natural bond orbital.

INTRODUCTION

Boranes are among the most important synthetic reagents [1] widely used in modern organic syntheses. Although the catalytic function of ethers in the hydroboration of alkenes has been comprehensively studied both experimentally [2—4] and theoretically [5—7], the mechanistic aspects of the dissociation of diborane involving ethers molecules still remain unclear. Experimentally, it is well known that diborane reacts with alkenes in hydrocarbon solvents with great difficulty or unsuccessfully (Eq.(1)).

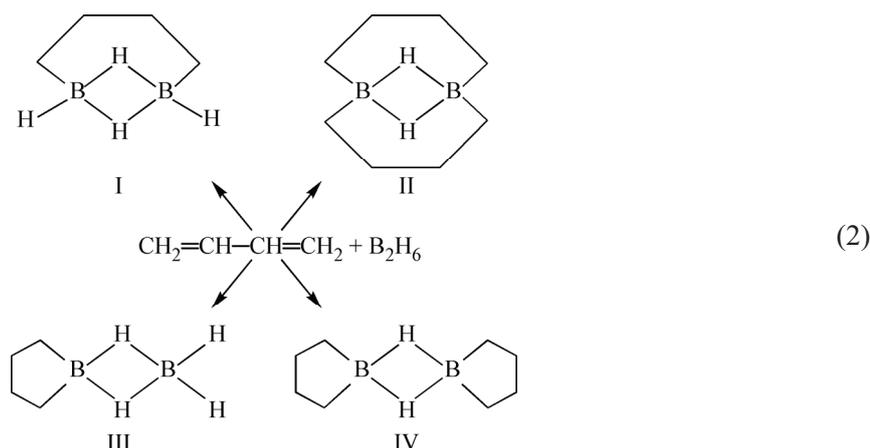


However, the reaction is considerably accelerated in the ether media, especially in tetrahydrofuran [8]. It was evident that the extension of the hydroboration reaction to dienes would probably involve many difficulties. First, the reaction of a polyfunctional olefin, such as a diene, with the polyfunctional diborane molecule, could lead to the formation of polymers which would not exhibit the normal behavior of organoboranes. Second, conjugated dienes are less reactive than related olefins

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toward simple addition reactions. Consequently, the controlled monohydroboration of such dienes was a questionable possibility [9].

Cyclic organodiboranes with a unique stable intramolecular doubly hydrogen—bridged structure, such as 1,2-tetramethylenediborane (I) and 1,2:1,2-bis(tetramethylene)diborane (II) (Eq.(2)), have been the subject of a debate [9—13]. These compounds were prepared by hydroboration reaction of butadiene with diborane (Eq.(2)) under specific conditions. The early suggestion of an intermolecular hydrogen—bridged structure was replaced with the concept of an intramolecular doubly hydrogen—bridged structure as a result of structure analysis by Young and Shore [12] and then the high ring opening reactivity of borane with borane was shown by Brown *et al.* [13].



In the present work , we have studied the structure and bonding of a family of cyclic organodiboranes including 1,2-tetramethylene diborane (I), 1,2:1,2-bis(tetramethylene)diborane (II), 1,1-tetramethylene diborane (III) and 1,1:2,2-bis(tetramethylene)diborane (IV) to elucidate their thermodynamic stabilities and the nature of bonding. In this study, density functional theory (DFT) B3LYP and B3PW91 methods have been used with a variety of basis sets using G98 program [14].

COMPUTATIONAL METHOD

All the structures were fully optimized without any symmetry limitation using B3LYP and B3PW91 methods with 6-31G, 6-31G* and 6-31++G** basis sets. Also, comparative study on the effect of basis set on the optimized structures was carried out. In addition, the characterization of alkyldiboranes we were interested in was calculated throughout with the 6-31++G** basis set. Population analysis has been studied based on the cross population between indirectly bonded atoms in the mentioned alkyldiboranes. Hybridizations of atomic orbitals have also been calculated via natural bond orbital (NBO) analysis. Vibrational analysis was performed on the DFT optimized structures using the same levels of theory and the same basis set. Harmonic frequencies and IR intensities were obtained by DFT methods. All the molecules studied in this work are shown in Fig. 1.

RESULTS AND DISCUSSION

Structural analysis. All of the optimized structural characteristics at B3LYP and B3PW91 levels of theory with different basis sets for the studied alkyldiboranes are reported in Table 1. The results show that all structures are non-planar. The values of bond lengths and angles are similar in all the methods. Application of polarized basis set has significant effects on the structural parameters of alkyldiboranes. However, diffused basis set have negligible effects on the optimized structural parameters (about 0.002 Å in bond lengths and 0.3° in angles). The B—H_(b) bond lengths for two boron atoms in the alkyldiboranes I, II and IV are completely equal. But, in the alkyldiborane III, the B_(t)—H_(b) bond is shorter than B_(c)—H_(b) bond. Furthermore, in the alkyldiboranes I and III, the B—H_(t) bond is shorter than B—H_(b) bond because of the reduction bond order in B—H_(b). In all of compounds the

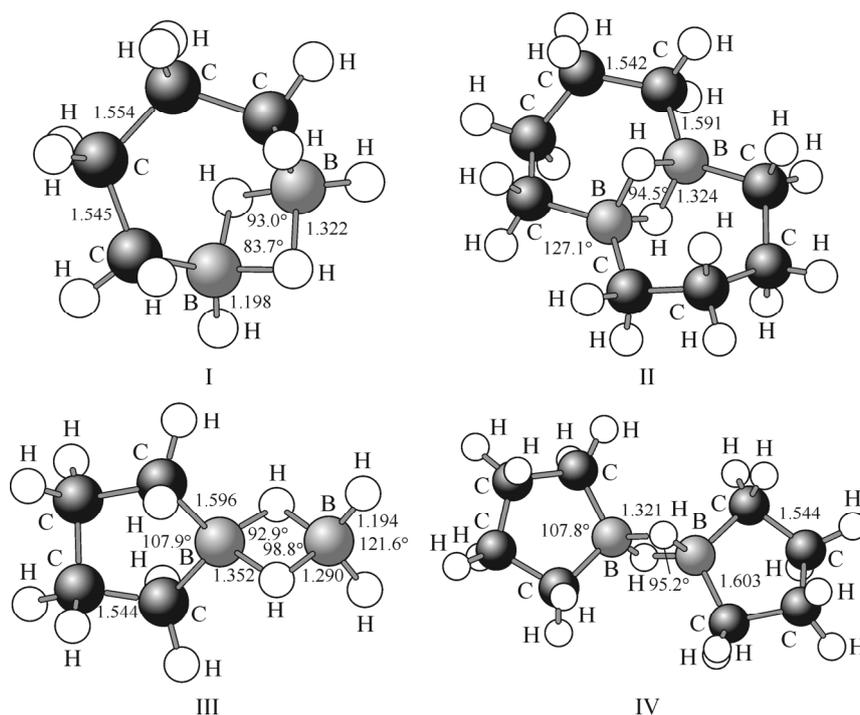


Fig. 1. Structural properties the alkyldiboranes of I, II, III and IV computed with the B3PW91 method by using 6-31++G** basis set

B—C bond lengths are longer than the C—C bond lengths. The optimized values of the B—C—C and C—C—C bond angles in the six-membered rings (*i.e.* the alkyldiboranes I and II) are greater than in the five-membered rings (*i.e.* the alkyldiboranes III and IV), which will decrease steric pressure.

NBO population analysis. Electron population analysis was carried out at all three levels of theory in order to characterize the nature and connectivity of the chemical bonds in the studied alkyldiboranes. The results of this analysis on the cross population between indirectly bonded pair of the B—B and the $H_{(b)}-H_{(b)}$ atoms are reported in Table 2. The results obtained with the two DFT methods for the alkyldiborane with six-member ring (I) show that there are significant cross populations for the two indirectly bonded B atoms of the ring. The obtained negative values of B—B cross population for some compounds imply an anti-bonding interaction between the two mediated atoms. Also, there is a close agreement between the obtained results at the two DFT methods.

An NBO analysis was carried out (on two DFT levels) to complete picture of the ring bonding system in these compounds. The results of this analysis were used to derive local atomic orbital hybridizations and they are reported in Table 3. These results show that strain is present in the alkyldiborane rings and it is attributable largely to the $\sim sp^2$ hybridization of the boron atom. This subject indicates that it is primarily responsible for the greater reactivity. Also, NBO analysis shows that $C_{(B)}$ atoms have $\sim sp^2$ hybridization but other carbon atoms in the rings have $\sim sp^3$ hybridization.

Vibrational analysis. The vibrational harmonic frequencies of alkyldiboranes have been calculated using the same level of theory and basis set in the geometry optimization (*see* Table 5). A scaling factor of 0.8929 has been used throughout the calculations. The absence of any imaginary frequency indicates that all of the optimized structures correspond to the minimum point on the intramolecular potential energy surface. The calculated vibrational frequencies near 2500 cm^{-1} (ν_5, ν_6) in the spectra of both I and III are in agreement with available experimental data [11] and verify the presence of terminal B—H stretching region; *i.e.*, R—B—H rather than BH_2 groups as in diborane [15, 16]. It is well known that "In diboranes having two terminal hydrogens bound to boron, one observes a doublet due to in-phase asymmetrical and out-of-phase symmetrical stretches" [17]. Thus, for the reported Köster and Iwasaki structure (III) [10, 18], the terminal boron-hydrogen stretching region would most

Table 1

Optimized structural parameters for B₂C₄H₁₂ (I), B₂C₈H₁₈ (II), B₂C₄H₁₂ (III) and B₂C₈H₁₈ (IV) alkyldiboranes obtained with B3LYP and B3PW91 method and different basis sets *

Molecule	Parameter	B3LYP			B3PW91		
		6-31G*	6-31G**	6-31++G**	6-31G*	6-31G**	6-31++G**
B ₂ C ₄ H ₁₂ (I)	B—H _(t)	1.196	1.194	1.195	1.198	1.197	1.198
	B—H _(b)	1.322	1.321	1.320	1.323	1.322	1.322
	B—C	1.593	1.592	1.592	1.591	1.590	1.590
	C—C ₍₁₎	1.550	1.550	1.552	1.544	1.544	1.545
	C ₍₁₎ —C ₍₂₎	1.560	1.560	1.561	1.553	1.553	1.554
	∠H _(b) —B—H _(b)	92.5	92.5	92.7	92.9	92.9	93.0
	∠B—H _(b) —B	84.4	84.5	84.4	83.8	83.8	83.7
B ₂ C ₈ H ₁₈ (II)	B—H _(b)	1.323	1.323	1.322	1.324	1.324	1.324
	B—C	1.594	1.593	1.594	1.592	1.591	1.591
	C—C ₍₁₎	1.547	1.547	1.548	1.541	1.541	1.542
	∠H _(b) —B—H _(b)	93.7	93.8	93.9	94.3	94.4	94.5
	∠C—B—C	127.2	127.2	127.1	127.2	127.1	127.1
B ₂ C ₄ H ₁₂ (III)	B—H _(t)	1.193	1.191	1.192	1.195	1.194	1.194
	B ₍₁₎ —H _(b)	1.291	1.290	1.289	1.292	1.290	1.290
	B ₍₂₎ —H _(b)	1.350	1.350	1.350	1.352	1.352	1.352
	B—C	1.599	1.598	1.599	1.596	1.596	1.596
	C—C ₍₁₎	1.550	1.550	1.551	1.544	1.543	1.544
	∠H _(t) —B ₍₁₎ —H _(t)	121.8	121.7	121.6	121.7	121.7	121.6
	∠H _(b) —B ₍₁₎ —H _(b)	97.9	98.0	98.1	98.6	98.7	98.8
	∠H _(b) —B ₍₂₎ —H _(b)	92.3	92.3	92.3	92.8	92.8	92.9
	∠C—B—C	108.0	108.0	108.0	107.9	107.9	107.9
B ₂ C ₈ H ₁₈ (IV)	B—H _(b)	1.320	1.320	1.319	1.321	1.321	1.321
	B—C	1.605	1.605	1.605	1.603	1.602	1.603
	C—C ₍₁₎	1.550	1.550	1.551	1.544	1.543	1.544
	∠H _(b) —B—H _(b)	94.5	94.5	94.6	95.1	95.1	95.2
	∠C—B—C	107.9	107.9	107.9	107.8	107.8	107.8

* All bond lengths and angles are given in Angstroms and degrees, respectively.

Table 2

Cross population between two indirectly bonded boron atoms and two hydrogen atoms of the cycle of alkyldiboranes obtained with B3LYP and B3PW91 methods and 6-31++G** basis set

Method	I		II		III		IV	
	B, B	H _(b) , H _(b)	B, B	H _(b) , H _(b)	B, B	H _(b) , H _(b)	B, B	H _(b) , H _(b)
B3LYP	0.683	0.064	-1.461	0.161	-0.425	1.394	-29.924	1.454
B3PW91	0.590	0.034	-0.488	0.096	-2.614	-0.008	-25.525	0.689

likely be a doublet. The existence of the observed sharp singlet for the terminal B—H stretching frequency suggests the presence of only one terminal hydrogen per boron similar to structure I. Very strong absorptions near 1600 cm⁻¹ (ν₈) for I to IV substantiate the presence of double-hydrogen bridges, *i.e.*, the same kind of bridging as in diborane itself [11]. It is interesting to note that the infra-

Table 3

NBO analysis of carbon and boron atomic orbital hybridizations involved in the C—C and C—B bond of the alkyldiboranes of I to IV using B3LYP and B3PW91 methods with 6-31++G** basis set

Bond	Atom	B3LYP				B3PW91			
		I	II	III	IV	I	II	III	IV
(C _(B) —H) ₁	C _(B)	S ¹ P ^{3.78}	S ¹ P ^{3.79}	S ¹ P ^{3.79}	S ¹ P ^{3.74}	S ¹ P ^{3.78}	S ¹ P ^{3.76}	S ¹ P ^{3.80}	S ¹ P ^{3.74}
(C _(B) —H) ₂ *	C _(B)	S ¹ P ^{3.53}	S ¹ P ^{3.66}	S ¹ P ^{3.29}	S ¹ P ^{3.30}	S ¹ P ^{3.50}	S ¹ P ^{3.63}	S ¹ P ^{3.28}	S ¹ P ^{3.28}
(C—H) ₁	C	S ¹ P ^{3.39}	S ¹ P ^{3.40}	S ¹ P ^{3.34}	S ¹ P ^{3.35}	S ¹ P ^{3.40}	S ¹ P ^{3.38}	S ¹ P ^{3.33}	S ¹ P ^{3.35}
(C—H) ₂ *	C	S ¹ P ^{3.28}	S ¹ P ^{3.27}	S ¹ P ^{3.06}	S ¹ P ^{3.07}	S ¹ P ^{3.29}	S ¹ P ^{3.25}	S ¹ P ^{3.06}	S ¹ P ^{3.07}
C _(B) —C	C _(B)	S ¹ P ^{2.96}	S ¹ P ^{2.93}	S ¹ P ^{3.09}	S ¹ P ^{3.08}	S ¹ P ^{2.95}	S ¹ P ^{2.95}	S ¹ P ^{3.08}	S ¹ P ^{3.08}
	C	S ¹ P ^{2.70}	S ¹ P ^{2.70}	S ¹ P ^{2.83}	S ¹ P ^{2.81}	S ¹ P ^{2.70}	S ¹ P ^{2.72}	S ¹ P ^{2.83}	S ¹ P ^{2.81}
C—C	C	S ¹ P ^{2.71}	S ¹ P ^{2.72}	S ¹ P ^{2.82}	S ¹ P ^{2.81}	S ¹ P ^{2.71}	S ¹ P ^{2.73}	S ¹ P ^{2.83}	S ¹ P ^{2.82}
C _(B) —B	C _(B)	S ¹ P ^{2.16}	S ¹ P ^{2.12}	S ¹ P ^{2.20}	S ¹ P ^{2.22}	S ¹ P ^{2.18}	S ¹ P ^{2.13}	S ¹ P ^{2.21}	S ¹ P ^{2.24}
	B	S ¹ P ^{2.17}	S ¹ P ^{2.09}	S ¹ P ^{2.32}	S ¹ P ^{2.45}	S ¹ P ^{2.19}	S ¹ P ^{2.09}	S ¹ P ^{2.33}	S ¹ P ^{2.47}
B—H _(t)	B	S ¹ P ^{2.08}		S ¹ P ^{2.22}		S ¹ P ^{2.09}		S ¹ P ^{2.24}	

Note that all of the S-containing NBO hybridizations are normalized to make the power of S-orbital to be equal to 1.

All hydrogens have S¹ hybridization. C_(B) is carbon that connected to boron. H_(t) is terminal hydrogen.

* For this compound, hybridization of two different C—H bonds have been listed.

Table 4

The NBO charges calculated for the B3LYP and B3PW91 optimized structures of alkyldiboranes using 6-31++G** basis set

Method	Bond	Atom	I	II	III	IV
B3LYP	C _(B) —H	C _(B)	-0.75	-0.74	-0.76	-0.73
		H	+0.24 (+0.25)*	+0.24 (+0.25)	+0.25	+0.24 (+0.25)
	C—H	C	-0.44	-0.44	-0.44	-0.44
		H	+0.22 (+0.23)	+0.22 (+0.23)	+0.22 (+0.23)	+0.22 (+0.23)
	B _(C) —H _(b)	B _(C)	+0.10	+0.37	+0.40	+0.34
		H _(b)	+0.12	+0.11	+0.12	+0.12
B—H _(t)	B	+0.10		-0.20		
	H _(t)	+0.02		+0.02		
B3PW91	C _(B) —H	C _(B)	-0.76	-0.76	-0.77	-0.75
		H	+0.25 (+0.26)	+0.25 (+0.26)	+0.26	+0.25 (+0.26)
	C—H	C	-0.46	-0.46	-0.46	-0.46
		H	+0.23 (+0.24)	+0.23 (+0.24)	+0.23 (+0.24)	+0.23 (+0.24)
	B _(C) —H _(b)	B _(C)	+0.07	+0.34	+0.38	+0.32
		H _(b)	+0.14	+0.13	+0.14	+0.14
B—H _(t)	B	+0.07		-0.24		
	H _(t)	+0.03		+0.03		

* This compound has two types of hydrogen atoms.

red spectrum of II is identical with the spectrum assigned to IV by Köster [10, 18]. The calculated vibrational frequencies for I to IV qualitatively agree with available experimental data [10b—12, 17, 18] with the percent differences ranging from 1% to as high as 8%.

Table 5

Vibrational harmonic frequencies in cm^{-1} and their IR intensities in km/mol (given in parentheses) for the optimized structures of alkyldiboranes obtained with B3LYP and B3PW91 methods using 6-31++G** basis set

Vib No	Method		B3LYP				B3PW91			
	Fundamental group	Vibrational mode	I	II	III	IV	I	II	III	IV
ν_1	CH ₂	antisymmetric stretch	2747 (76)	2725 (183)	2755 (60)	2751 (135)	2764 (61)	2742 (142)	2774 (49)	2771 (107)
ν_2	CH ₂ h	antisymmetric stretch	2738 (72)	2712 (92)	2747 (58)	2740 (114)	2758 (59)	2731 (82)	2764 (52)	2756 (102)
ν_3	CH ₂	symmetric stretch	2712 (69)	2684 (78)	2710 (54)	2699 (96)	2723 (68)	2697 (75)	2714 (50)	2712 (90)
ν_4	CH ₂	symmetric stretch	2686 (36)	2678 (35)	2697 (36)	2696 (65)	2702 (30)	2692 (48)	2711 (42)	2709 (51)
ν_5	B—H _(t)	antisymmetric stretch	2352 (177)		2402 (103)		2349 (170)		2402 (99)	
ν_6	B—H _(t)	symmetric stretch	2339 (84)		2327 (107)		2335 (84)		2325 (109)	
ν_7	B—H _(b)	stretch	1755 (15)	1722 (18)	1984 (38)	1779 (15)	1784 (11)	1749 (15)	1990 (32)	1804 (12)
ν_8	B—H _(b) —B	rock	1466 (435)	1523 (594)	1497 (657)	1514 (1148)	1471 (399)	1532 (549)	1497 (599)	1519 (1062)
ν_9	C _(B) H ₂	scissor	1323 (12)	1305 (38)	1300 (18)	1307 (14)	1316 (13)	1297 (40)	1293 (20)	1300 (23)
ν_{10}	CH ₂	twist	1046 (39)	1063 (60)	1039 (30)	1030 (44)	1042 (38)	1203 (40)	1044 (38)	1033 (49)
ν_{11}	H _(t) —B—H _(t)	scissor			1063 (47)				1054 (34)	
ν_{12}	CH ₂	wag	1003 (86)	971 (11)	917 (16)	917 (17)	1002 (72)		969 (17)	928 (12)
ν_{13}	CH ₂	wag		846 (15)	864 (36)	738 (67)		857 (17)	874 (40)	745 (60)
ν_{14}	B—H _(b) —B	wag	1046 (39)	884 (16)	965 (18)	939 (32)	1042 (38)	1064 (59)		865 (14)
ν_{15}	C _(B) H ₂	rock		743 (35)		659 (18)		743 (36)		657 (20)

CONCLUSION

Density functional B3LYP and B3PW91 calculations were carried out on some alkyldiboranes. Results of the structural investigation showed that all these alkyldiboranes have non-planar structures. In I and III alkyldiboranes the B—H_(t) bonds are shorter than the B—H_(b) bonds, which is indicative of a reduced bond order in B—H_(b) bonds. The vibrational analysis was carried out on the optimized structures in the B3LYP and B3PW91 method by using 6-31++G** basis set. The results indicate that all the optimized structures have minima on the potential energy surface without any negative mode. The obtained results show that B—H_(t) stretching band is higher in frequency than the B—H_(b) adsorption band and verify the bond B—H_(t) is shorter than B—H_(b). The population analysis showed that there are significant cross populations between indirectly bonded B—B atoms of the ring at the two DFT methods for the alkyldiborane with six-membered ring (I). The NBO analysis demonstrated that the strain present in the alkyldiborane rings is attributable largely to the $\sim\text{sp}^2$ hybridization of the bo-

ron atom. However, the possibility must also be considered that the excess stability of the double hydrogen bridge of compounds I and III, as evidenced by its relatively low reactivity toward terminal olefins, may also be playing an important role in the ease of the ring opening reaction with diboranes.

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