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Computational Studies on Nitro-Azaboriridine—A High-Energetic Material

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Nitrogen heterocycles and their derivatives are one of the classes of compounds that have been widely used in developing high-energetic materials. The energy content of the heterocycle ring systems can be increased by inclusion of nitro, cyano, and azido groups. In the present study nitro derivatives of small three-membered B-N-C ring compounds, viz. 1-nitro-1,2-azaboriridine, 1,3-dinitro-1,2-azaboriridine, and 1,3,3-trinitro-1,2-azaboriridine, have been considered. Thermodynamic properties and energetics of the above compounds have been taken for detailed computational study using G2, G3, and CBSQB3 compound methods. Studies reveal that these compounds can be considered for use as high-energetic materials. Detonation velocity (D) and detonation pressure (P) of the title compounds have also been evaluated using the Kamlet-Jacobs method based on the theoretical densities and heats of formation calculated at G3 level. Calculation shows that 1,3,3-trinitro-1,2-azaboriridine yields a detonation velocity of 9.14 km/s and a detonation pressure of 40.2 GPa at a loading density of 1.91 g/cm^3 that is comparable to powerful commercial explosives such as HMX (9.10 km/s,

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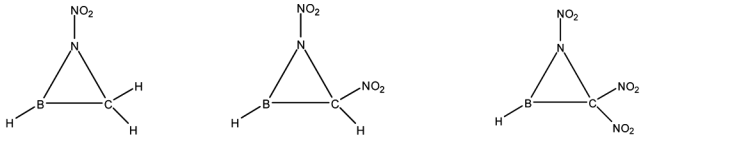
1.91 g/cm^3, 39.0 GPa) and RDX (8.75 km/s, 1.82 g/cm^3, 34.0 GPa).

Keywords: nitro-1, 2-azaboriridines, CBSQB3 calculation, detonation pressure, detonation velocity, G2, G3, high-energy-density material, kamlet-jacobs method, oxygen balance

Introduction

The search for novel high-energy-density materials (HEDMs) with a given performance is one of the major challenges of the chemical industry and it is an ongoing process [1–3]. The discovery of new energetic materials could be facilitated, accelerated, and made more cost effective with the use of computer modeling and simulations for the identification of compounds that have significant advantages over materials currently in use. A key property for the design and synthesis of new energetic materials is that the designed compound should possess a high positive heat of formation (HOF). Additionally, such compounds should be thermally stable and impact and shock resistant. Thus, synthesis of high-nitrogen-content compounds has always fascinated chemists with regards to energetics consideration. Other studies offer additional traits, such as using boron and aluminum due to the stability of their combustion products and release of high energy as a result of formation of their oxides during explosion [4]. In designing HEDMs, the criteria that are generally looked upon are that the designed compound should have high density and release a large amount of energy during its decomposition. Ringed and caged compounds substituted with nitro, amino, and azido groups have always drawn attention. Synthesis of polynitrocubanes during the recent past is a result of utilizing such an approach [5]. Recently, boron-containing compounds have drawn significant attention by Ball and his group [6–9]. They pursued computational studies on three- and four-membered B- and N-containing ring compounds to look into the possibility of using such ring compounds as potential HEDMs. With an enthalpy of formation of −1273.5 kJ/mol, diboron trioxide (B_2O_3) contributes almost 60 kJ of energy given



1-nitro-1,2-azaboriridine 1,3-dinitro-1,2-azaboriridine 1,3,3-trinitro-1,2-azaboriridine

Figure 1. Schematic representation of nitro derivatives of 1,2-azaboriridine.

off per gram of boron combusted [10]. The attachment of NO_2 groups (the so-called energetic function) to the heterocyclic ring to form an energetic molecule with good performance has always drawn the attention of scientists. Keeping in view this fact we attempted to study the effect of addition of NO_2 group on the energetics and explosive characteristics of 1,2-azboriridine, the simplest three-membered B-N-C ring compound. As such, three members of this group, 1-nitro-1,2-azaboriridine, 1,3-dinitro-1,2-azaboriridine, and 1,3,3-trinitro-1,2-azaboriridine, are taken for detailed computational study using G2, G3, and CBSQB3 methods. These compounds are shown schematically in Fig. 1.

In addition to the energetics, parameters characterizing the explosive performance of high-energy-materials such as oxygen balance (OB_{100}), density (ρ), detonation velocity (D), and detonation parameter (P) are also calculated using Kamlet-Jacobs equations based on the predicted theoretical density (ρ) and heat of formation (HOF) Alternatively, detonation velocity (D) is also calculated using an empirical equation [11] recently formulated for explosives compositions having aluminum and a comparison is made with the values calculated by the well-accepted Kamlet-Jacobs method [12].

Computational Details

All calculations were performed with *Gaussian 03* software package [13] and the methods implemented there in. In the present study G2 [14], G3 [15], and complete basis set (CBS-QB3) [16] methods were used for the geometry optimization and thermodynamic calculations. The enthalpies of formation of

title compounds were calculated using atomization method [17]. In brief, the calculated total energies of the given molecule and its constituent atoms were used to evaluate the atomization energy. This value was then used along with thermal corrections and the known experimental enthalpies of formation for the atomic species to calculate the HOF of the title compounds at 298 K. The experimental enthalpies of formation of the atoms were taken from the *NIST Chemistry Webbook* [10].

Combustion enthalpies (ΔH_{comb}) were calculated using the following stoichiometric combustion reactions (reactions (1)–(3)) for the three nitroderivatives of 1,2-azaboriridines.

$$CH_3BN_2O_2\ (g) + 1.5\ O_2\ (g) \longrightarrow CO_2\ (g) + 1.5\ H_2O\ (1) + N_2\ (g) + 0.5\ B_2O_3\ (s) \quad (1)$$

$$CH_2BN_3O_4\,(g) + 0.25\,O_2\,(g) \longrightarrow CO_2\,(g) + H_2O\,(1) + 1.5\,N_2\,(g) + 0.5\,B_2O_3\,(s) \quad (2)$$

$$CHBN_4O_6\ (g) \longrightarrow CO_2\ (g) + 0.5H_2O\ (1) + 2N_2\ (g) + 0.5\ B_2O_3\ + O_2(g) \quad (3)$$

The enthalpies of formation of water, carbon dioxide, and diboron trioxide (B_2O_3), used in reactions (1)–(3), were taken from the *NIST Chemistry Webbook* [10]. Specific enthalpies of combustion ($\Delta H_{comb,sp}$) of compounds were determined by dividing the heat of combustion with the molar mass of the compound.

Detonation velocity (D) and detonation pressure (P) were calculated using the Kamlet-Jacobs equation [12] as given by Eqs. (4) and (5).

$$D = 1.01\ (N\ M^{1/2}\ Q^{1/2})^{1/2}\ (1 + 1.30\ \rho) \quad (4)$$

$$P = 1.588\ \rho^2\ N\ M^{1/2}\ Q^{1/2} \quad (5)$$

Each term in the above equations is defined as follows: D, the detonation velocity (km/s); P, the detonation pressure (GPa); N, moles of gaseous products per gram of explosive; M, average molecular weight of gaseous products; Q, chemical energy of detonation (kJ/mol), and ρ, the density of explosive (g/cm^3). N, M, and Q are calculated from the chemical composition of the molecules [18,19]. The heat of formation used during the calculation of Q was determined at G3 level. The density (ρ) is calculated from the molecular volume divided by the molecular weight and the molecular volume of different molecules are estimated using Monte Carlo method, based on 0.001 electron/bohr^3 density space as implemented in the *Gaussian 03* program. This approach for calculating molecular volume and subsequently the density has been successfully tested on various CHNO molecules and reasonably accurate values of the explosive properties have been predicted [20–23]. In the present study, single-point molecular volume calculations were performed at B3LYP/6-311G(d,p) level with the geometry optimized at the same level.

The oxygen balance is calculated from the molecular formula of the compound and is represented in terms of percentage of oxygen required for complete conversion of carbon to carbon dioxide, hydrogen to water, nitrogen to N_2, and boron to B_2O_3. In the present case it is determined by using Eq. (6) [24–26]:

$$OB_{100} = \frac{-1600}{\textit{Mol. wt. of compound}}\left(2X + \frac{1}{2}Y + \frac{3}{2}M - Z\right) \quad (6)$$

where X, Y, Z, and M are the number of C, H, O, and B (boron) atoms present in the molecular formula of the compound. In the formulation of the above equation it is assumed that boron is completely converted into B_2O_3 during explosive decomposition.

Results and Discussion

Optimized geometrical parameters of all the three nitrocompounds of azaboriridine studied at different levels of theory are listed in Tables 1–3 and their optimized structures obtained

Table 1
Optimized geometrical parameters of 1-nitro-1,2-azaboriridine obtained by CBSQB3, G2, and G3 calculations

Parameters	CBSQB3	G2	G3
Bond length (Å)			
C1-B2	1.579	1.596	1.596
C1-N3	1.464	1.452	1.452
C1-H4	1.090	1.089	1.089
C1-H5	1.086	1.089	1.089
B2-3N	1.370	1.358	1.358
B2-H6	1.173	1.179	1.179
N3-N7	1.420	1.410	1.410
N7-O8	1.212	1.229	1.229
N7-O9	1.211	1.229	1.229
Bond angle (°)			
C1-B2-N3	59.0	58.2	58.2
B2-C1-N3	53.4	52.7	52.7
B2-N3-C1	67.6	69.1	69.1
B2-C1-H4	117.5	121.2	121.2
B2-C1-H5	124.9	121.2	121.2
N3-C1-H4	117.0	116.3	116.3
N3-C1-H5	115.1	116.3	116.3
H4-C1-H5	114.3	114.2	114.2
C1-B2-H6	154.8	155.4	155.4
N3-B2-H6	145.3	146.4	146.4
C1-N3-N7	132.5	135.8	135.9
B2-N3-N7	143.1	155.0	155.0
N3-N7-O8	115.7	115.5	115.5
N3-N7-O9	115.7	115.5	115.5
O8-N7-O9	128.6	128.9	128.9
B2-N3-N7	143.1	155.0	155.0
C1-N3-N7	132.5	135.8	135.9

Table 2
Optimized geometrical parameters of 1,3-dinitro-1,2-azaboriridine obtained by CBSQB3, G2, and G3 calculations

Parameters	CBSQB3	G2	G3
Bond length (Å)			
N1-C2	1.414	1.416	1.416
N1-B3	1.352	1.355	1.355
N1-N6	1.453	1.439	1.439
C2-B3	1.608	1.602	1.601
C2-H4	1.084	1.087	1.087
C2-N9	1.505	1.486	1.486
B3-H5	1.169	1.176	1.176
N6-O7	1.205	1.224	1.224
N6-O8	1.203	1.222	1.223
N9-O10	1.221	1.240	1.240
N9-O11	1.217	1.238	1.238
Bond angle (°)			
C2-B3-N1	56.3	56.5	56.5
B3-C2-N1	52.7	52.9	52.9
B3-N1-C2	71.0	70.6	70.6
C2-N1-N6	134.9	132.9	132.9
B3-N1-N6	153.8	155.3	155.3
N1-C2-H4	121.6	121.1	121.1
N1-C2-N9	116.3	114.9	114.9
B3-C2-H4	128.3	129.1	129.1
B3-C2-N9	116.9	116.5	116.5
H4-C2-N9	109.9	110.4	110.4
N1-B3-H5	149.9	149.4	149.4
C2-B3-H5	153.7	154.1	154.1
N1-N6-O7	114.9	114.5	114.5
N1-N6-O8	114.7	114.9	144.9
O7-N6-O8	130.4	130.6	130.6
C2-N9-O10	117.4	117.2	117.2
C2-N9-O11	115.9	116.2	116.2

(*Continued*)

Table 2
Continued

Parameters	CBSQB3	G2	G3
O10-N9-O11	126.7	126.6	126.6
B3-N1-N6	153.8	155.3	155.3
C2-N1-N6	134.9	132.9	132.9

at G3 level are shown in Fig. 2. The numbering of the atoms shown in Fig. 2 is given by default during computation. Results show that optimized parameters listed as bond lengths and bond angles between different atoms calculated with different computational methods are consistent. We relied upon the fact that the compound model G3 has been found to give reliable thermodynamic data for a wide variety of compounds and gives a lower mean error when compared with experimentally determined values [27]. Therefore, the results obtained with the G3 method have been considered in detail during the present study. Results show that substitution of nitro groups at N and C atoms of B-N-C ring significantly changes the C-N bond distance of the ring. The first addition of nitro group at the N atom decreases its value from 1.481 Å calculated in 1,2-azaboriridine [6] to 1.452 Å in 1-nitro-1,2-azaboriridine. This bond distance further decreases as nitro groups are attached at the C atom of the ring. The lowest value of 1.398 Å is obtained in the case of 1,3,3-trinitro-1,2-azaboriridine. Detailed analysis of the optimized structures using *Gaussview* [28] reveal that nitration of 1,2-azaboriridine first at N and subsequently at the C atom of the ring resulted in a slight increase in the bond angle B-C-N, whereas C-B-N and C-N-N angles decrease. Further analysis of the structure reveals that with a nitro group placed at the N atom of the ring, the molecule remains in plane with C_1 symmetry, whereas subsequent addition of nitro group at the C atom of the ring makes the molecule nonplanar, retaining its C_1 symmetry.

Thermochemical data for nitroazaboriridines calculated using compound methods are listed in Tables 4–6. The enthalpies of

Table 3
Optimized geometrical parameters of 1,3,3-trinitro-1,2-azaboriridine obtained by CBSQB3, G2, and G3 calculations

Parameters	CBSQB3	G2	G3
Bond length (Å)			
C1-N2	1.396	1.398	1.398
C1-B3	1.595	1.588	1.588
C1-N8	1.519	1.496	1.496
C1-N11	1.507	1.484	1.484
N2-B3	1.360	1.364	1.364
N2-N5	1.482	1.464	1.464
B3-H4	1.168	1.175	1.175
N5-O6	1.199	1.220	1.220
N5-O7	1.198	1.219	1.219
N8-O9	1.223	1.240	1.240
N8-O10	1.207	1.235	1.235
N11-O12	1.217	1.240	1.240
N11-O13	1.214	1.237	1.237
Bond angle (°)			
C1-B3-N2	55.7	55.9	55.9
B3-C1-N2	53.6	53.9	53.9
B3-N2-C1	70.7	70.2	70.2
N2-C1-N8	116.9	116.5	116.5
N2-C1-N11	118.1	117.2	117.2
B3-C1-N8	116.9	118.3	118.3
B3-C1-N11	125.8	126.5	126.5
N8-C1-N11	112.7	111.7	111.7
C1-N2-N5	133.9	131.5	131.5
B3-N2-N5	151.8	155.8	155.8
C1-B3-H4	153.3	154.1	154.1
N2-B3-H4	151.0	150.0	150.0
N2-N5-O6	114.3	113.7	113.7
N2-N5-O7	114.0	114.5	114.5
O6-N5-O7	131.7	131.8	131.8

(*Continued*)

Table 3
Continued

Parameters	CBSQB3	G2	G3
C1-N8-O9	113.3	118.7	113.7
C1-N8-O10	119.2	118.8	118.8
O9-N8-O10	127.5	127.4	127.4
C1-N11-O12	116.5	116.4	116.4
C1-N11-O13	115.7	115.8	115.8
O12-N11-O13	127.7	127.8	127.8
B3-N2-N5	151.8	155.8	155.8
C1-N2-N5	133.9	131.5	131.5

formation of different nitroazaboriridines calculated using G2, G3, and CBS-QB3 methods are listed in Table 4. The data show that G2 and CBS-QB3 methods yield almost the same result. However, the G3 method predicts a slightly higher value. Enthalpies of formation of all the compounds studied possess high positive values that fulfill one of the criteria for considering it as a potential high-energetic material.

Enthalpies of combustion of title compounds calculated using stoichiometric combustion reactions (reactions (1)–(3)) are listed in Table 5. During this calculation heats of formation of carbon dioxide, water (l), and B_2O_3 (s) are taken from NIST and these are −393.51, −285.83, and −1273.5 kJ/mol respectively [10]. The data reveal that 1-nitro-1,2-azaboriridine possesses the most negative value of heat of combustion among the three nitro compounds of azaboriridine considered.

The specific enthalpies of combustion of different nitroazaboriridines calculated using G2, G3, and CBS-QB3 methods are listed in Table 6. The specific enthalpy of combustion per unit mass varies. The specific combustion energies for title compounds are much higher than the combustion or decomposition energies of some known HEDMs. For example, the specific decomposition energy of ammonium nitrate, NH_4NO_3, is

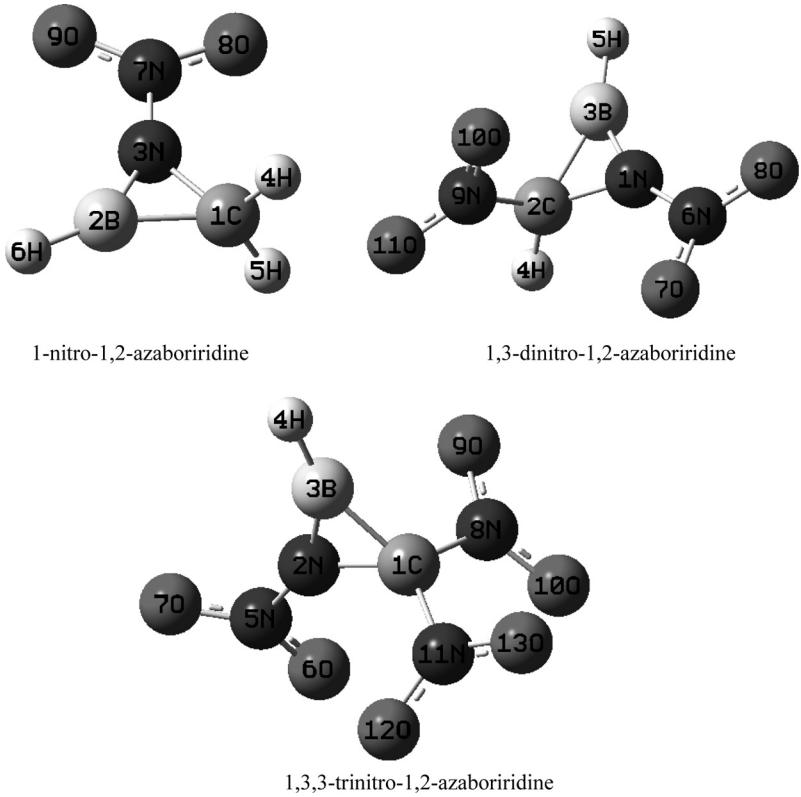


Figure 2. Optimized geometries of nitro-azaboriridines obtained using the G3 method.

Table 4
Enthalpies of formation (kJ mol^{-1}) of nitro derivatives of 1,2-azaboriridine as determined by various compound methods

Compounds	CBS-QB3	G2	G3
1-Nitro-1,2-azaboriridine	186.7	186.2	196.0
1,3-Dinitro-1,2-azaboriridine	150.8	152.8	170.5
1,3,3-Trinitro-1,2-azaboriridine	167.8	168.5	194.8

Table 5
Enthalpies of combustion (kJ mol^{-1}) of nitro derivatives of azaboriridine as determined by various compound methods

Compounds	CBS-QB3	G2	G3
1-Nitro-1,2-azaboriridine	−1645.7	−1645.2	−1655.0
1,3-Dinitro-1,2-azaboriridine	−1466.9	−1468.9	−1486.6
1,3,3-Trinitro-1,2-azaboriridine	−1340.9	−1341.7	−1367.9

2.58 kJ/g, whereas that of trinitrotoluene, TNT, is 2.18 kJ/g [29]. The explosive HMX, which is octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine, has a specific combustion energy of 8.9 kJ/g [10]. The results show that nitro-azaboriridine considered during the present study has a high potential to be used as high-density energetic materials.

Detonation performances evaluated using Kamlet-Jacobs method based on predicted densities are recorded in Table 7. Other significant parameters such as oxygen balance (OB_{100}) and heat of detonation (Q) are also provided in Table 7. The data show that the calculated theoretical densities of 1-nitro and 1,3-dinitro-1,2-azaboriridines as 1.637 and 1.639 g/cm^3 are comparable to a conventional explosive TNT (1.64) [30]. On the other hand, the calculated density of 1,3,3-trinitro-1,2-azaboriridine is 1.91 g/cm^3, which is even higher than the RDX (1.82 g/cm^3), and therefore it may be considered to be

Table 6
Specific enthalpies of combustion (kJ g^{-1}) of nitro derivatives of azaboriridine as determined by various compound methods

Compounds	CBS-QB3	G2	G3
1-Nitro-1,2-azaboriridine	−19.2	−19.2	−19.3
1,3-Dinitro-1,2-azaboriridine	−11.2	−11.2	−11.4
1,3,3-Trinitro-1,2-azaboriridine	−7.63	−7.63	−7.78

Table 7
Predicted densities and detonation properties of the title compounds

Compounds	OB_{100}	Q	V	ρ	D^a	P
1-Nitro-1, 2-azaboriridine	−55.94	1286.67	52.415	1.637	7.49 (7.18)	28.73
1,3-Dinitro-1, 2-azaboriridine	−06.12	1521.18	79.793	1.639	8.18 (7.43)	34.19
1,3,3-Trinitro-1, 2-azaboriridine	+18.20	1635.92	92.303	1.905	9.14 (9.04)	40.20
RDX[b]				1.82	8.75	34.00
HMX[b]				1.91	9.10	39.00

Notes. Units: Q in $kJ.g^{-1}$, V in $cm^3.mol^{-1}$, ρ in $g.cm^{-3}$, D in $km.s^{-1}$, and P in GPa.

[a]Velocity of detonation using Kamlet-Jacobs method [12]. Values in parentheses are calculated using the empirical formula given in Keshavarz [11].

[b]Values taken from Talawar et al. [32].

better option if such a compound is synthesized in future. The calculated density and detonation velocity of 1,3,3-trinitro-1,2-azaboriridine as $1.91\,g/cm^3$ and $9.14\,km/s$ put this compound into the category of HEDMs ($\rho \approx 1.9\,g/cm^3$, $D \approx 9.0\,km/s$, $P \approx 40.0\,GPa$) [31]. With increasing number of NO_2 groups substituted on 1,2-azaboriridine, ρ, D, and P all increase, so do V, OB_{100}, and Q. Detonation velocities are also calculated using an empirical equation recently formulated for aluminized explosives [11]. During the formulation it was assumed that Al was completely oxidized into its oxide. During the calculation we also assumed that B was completely oxidized to B_2O_3 during explosive decomposition. Comparable values of detonation velocities were obtained and these are also listed in Table 7.

The explosive power or energy release of high-energy compounds that contain oxygen may be qualitatively assessed and predicted from their oxygen balance. It can have positive,

negative, or zero values. Deficiency of oxygen in the compound gives a negative balance. On the other hand, a zero oxygen balance indicates maximum energy release. For the three nitroazaboriridines considered during the present investigation, OB_{100} for 1-nitro-1,2-azaboriridine is −55.9, whereas for 1,3-dinitro-1,2-azaboriridine and 1,3,3-trinitro-1,2-azaboriridine it is −6.1 and +18.2, respectively, as recorded in Table 7. Data show that 1,3-dinitro-1,2-azaboriridine and 1,3,3-trinitro-1,2-azaboriridine have the potential to be used as explosive materials. The high oxygen balance associated with the latter gives it an additional advantage to be used as commercial explosives because there will little chance of producing toxic CO gas during explosive decomposition.

Conclusion

Optimized geometries, enthalpies of formation, enthalpies of combustion, and specific enthalpies of combustion for 1-nitro-1,2-azaboriridine, 1,3-dinitro-1,2-azaboriridine, and 1,3,3-trinitro-1,2-azaboriridine are determined using G2, G3, and CBS-QB3 compound methods. Based on the quantum chemical calculation of molecular volumes, theoretical densities and detonation velocities of the title compounds are also determined. The study reveals that nitro derivatives of azaboriridine possess potential properties to be used as high-energy materials. In addition to its high density and detonation velocity (1.91 g/cm^3; 9.1 km/s), the positive high oxygen balance (+18.2) of 1,3,3-trinitro-1,2-azaboriridine would further increase its potential to be used as a commercial explosive because of absence of any CO as toxic gas produced during explosive decomposition in industrial applications.

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