New Atom/Group Volume Additivity Method to Compensate for the Impact of Strong Hydrogen Bonding on Densities of Energetic Materials

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The quantitative impact of strong hydrogen bonding on the densities of energetic materials is discussed. On the basis of our new volume parameters designated for neutral high-energy density materials, the volume of each NH_2 or NH group must be corrected by -8 Å^3 to compensate for strong bonding: i.e., (1) when both carbon atoms vicinal to an NH_2 or NH group have nitro groups or one $C-NO_2$ and one N−oxide; or (2) if the molecule has *C*2 symmetry, e.g., at least two nitro and two NH_2 groups in the vicinal position, two NH_2 groups may be corrected by -8 Å^3 in total (exemplified by 1,1-diamino-2,2-dinitroethene (FOX-7), 2,4,6-triamino-3,5-dinitropyridine (Cambridge Crystallographic Data Centre (CCDC) Refcode: TIBMUM), 2,6-diamino-3,5-dinitropyrimidine (CCDC refcode: CIWMAW01, etc.); or (3) when some heterocycles (triazole, pyrazole, etc.) contain the fragment $-NHNO_2$. For 261 explosives with an average density of 1.803 $g\cdot cm^{-3}$, the mean absolute deviation (MAD) for the proposed current method is 0.026 $g\cdot cm^{-3}$, and the mean relative absolute error is 1.5 %.

Introduction

During the past three decades, considerable effort has been focused on the development of high-energy density materials (HEDM) with higher performance and/or decreased sensitivity with respect to thermal, shock, and friction stability and electrostatic discharge. [1–5] Higher performance has always been a prime requirement in the field of research and development of explosives, but more recently, a combination of properties have become desirable.[1] The development of space programs, the drilling of deep oil wells, etc., has resulted in the need for "heat-resistant" or "thermally stable" explosives, such as heat-resistant explosives for warheads of high-speed missiles, perforation of oil and gas wells, and high-performance and insensitive high explosives (IHEs) for low-vulnerability munitions.[4]

It has long been recognized that the presence of strong hydrogen bonding has a special impact on the physical and chemical properties of an explosive owing to the existence of strong intra- or interhydrogen bonding. The attractive forces confining the respective species in the crystal lattice are high. Because the solubility of a compound can legitimately be regarded as a partitioning of the compound between a crystal lattice and solvent, explosives with very strong bonding normally have poor solubility in common solvents. For the same reason, they also have very high or no observable melting points and high-impact insensitivities as well as low toxicities due to their low solubility in water and low volatilities. Perhaps more importantly, the strong hydrogen bonding also leads to much more efficient packing in the crystal lattice and thus results in higher density. Density is one of the most important factors that determines the performance of a given explosive, since the detonation pressure (*P*) is dependent on the square of the density and the detonation velocity (*D*) is proportional to the density according to an empirical equation proposed by Kamlet and Jacobs.[6] In general, a density increase outweighs the concomitant decrease in both oxygen balance and heat of formation which arise, for example, with the introduction of amino groups and results in better performance.[5] A typical example is 1,3,5-triamino-2,4,6-trinitrobenzene [TATB, CCDC Refcode TATNBZ], because due to the six bifurcated hydrogen bonds this molecule has very short C−N (amino) (1.31 Å), short C−N (nitro) (1.42 Å), and long C−C bonds (1.45 Å) in the benzene ring, and the molecule is almost planar. The net result is that TATB lacks an observable melting point and has low solubility in all solvents except concentrated H_2SO_4. The density is ~1.937 $g\cdot cm^{-3}$. In sharp comparison, in 1,3,5-trinitrobenzene (CCDC Refcode TNBENZ10), C−N (nitro) (1.48 Å) is nearly normal length, and the molecule is not planer since one nitro group has a torsion angle of about 28° off the benzene plane. Its density is 1.676 $g\cdot cm^{-3}$.

To date, density has been estimated by several methods: (1) empirical atom/group volume additivity;[7–13] and (2) direct computation of molecular volume using an electronic structure method or molecular mechanics.[14–19] Computer programs, exemplified by MOLPACK,[20] that search the minimum lattice energy of different space groups based on an optimized geometry and LOTUSES,[21] etc., are also available to calculate density, heat of formation ($\Delta_f H$), and detonation properties. In 1979, Tarver[8] used 73 volume parameters and achieved a mean absolute deviation, MAD, of 0.019 $g\cdot cm^{-3}$ in density predictions compared with experimental values for a database of 188 explosives and related compounds of diverse composition. In the same year, Cady[9] also reported an independent method for density estimation. A reasonably extensive investigation by Stine[10] used data for 2051 supposedly "error-free" crystal structures to determine 34 atomic volumes for C, H, N, O, and F. Ammon published new parametrizations based on more than 11 000 crystal structures to provide 78 atoms and group volumes for C-, H-, N-, O-, and F-containing materials.[11] This method was extended to 96 atoms/groups for C-, H-, N-, O-, F-, S-, P-, Cl-, and Br-containing compounds which were determined from approximately 26 000 error-free crystal structures.[12] These

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Table 1. Volume Parameters for Atoms, Groups, and Fragments

species	V/Å^3	species	V/Å^3
Neutral			
imidazole	84	1,2,4-triazole	79
tetrazole	75	*s*-triazine	90
1,2,4,5-tetrazine	87	pyrimidine	100
cubane	135	furazan	77
benzene	110	pyridine	105
Groups			
H (bonded to N in above species)	7	H (in other cases)	5
CH_3	30	CH_2 (acyclic)	24
CH_2 (3- or 4-membered ring)	22.5	CH_2 (5- or 6-membered ring)	22
CH_2 (8-membered ring)	21	CH (in isoWurtzitane)[a]	13.5
−C=C−	26.5	-C=N-	25
C’N	30	-*N* = N-	26
NH_2	20	NO_2	36
NH	15	N_3	41
N (in tetraazapentalene)	9.5	N (in other cases)	10
C=O (not in a ring)	25	C=O (in a ring)	22
COOH	41	OH	15
O (in ether or −*O*-NO_2)	11.5	O (in other cases)	10
F	12.5	CF_2	37.5
NF_2	37	SF_5	82
Corrections			
strong hydrogen bonds for each NH_2 or NH	−8		
each sp^3 C or sp^3 N in two or more rings	−1		
each sp^2 C in two or three rings[b]	−2		

[a] Volumes of other CH moieties were derived from respective CH_2: $V(CH) = V(CH_2) -5$/Å^3; while $V(C) = V(CH_2) -10$/Å^3. [b] Except in tetrazole where sp^2 C does not need be corrected. These corrections are empirical values arising from perusing large numbers of experimental values.

parameters were also extended to 1000 ionic solids by Mathieu.[22] In addition, Hofmann derived a 100 atom code based on 182 239 crystals.[13]

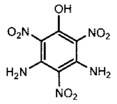
However, none of the current empirical methods can predict successfully the density of explosives with strong hydrogen bonding. Computational programs including MOLPACK also fail to identify the correct packing arrangements of crystals with strong intermolecular hydrogen bonds.[20] Although the impact of strong hydrogen bonding on density has long been recognized by military communities and utilized in the design of high explosives, the quantitative relationship had not been established until our preliminary effort in which 8 Å^3 was proposed to account for strong hydrogen bonding in energetic ionic salts.[23] For 150 energetic salts, the MAD is 0.035 g·cm^{-3}. When several more parameters and corrections are added, our empirical volume additivity can be successfully extended to neutral explosives with much more complicated structures (Table 1).

As listed in Table 1, the current method only involves 38 atom/group parameters and three corrections. The volume of each NH_2 or NH group should be corrected by −8 Å^3 for strong bonding in three scenarios: (1) both carbons vicinal to the NH_2 or NH group have nitro groups or one C−NO_2 and one N−oxide (N−O). Typical examples are given in Table 2. When the NH_2 group was substituted by an alkyl, phenyl, or other electron-donating group, for example, *N*-methyl-2,4,6-trinitrobenzenamine (JUPROB) or *N*-methyl-2,6-dinitro-4-(trifluoromethyl) benzenamine (FMANIL), this NH group did not require correction because hydrogen bonding in this case was not strong enough owing to electronic and/or steric effects. (2) If only one vicinal carbon bears a nitro group, the volume of the amino group remains at 20 Å^3. However, if the molecule has a symmetrical structure, e.g., at least two nitro and two NH_2 groups in the molecule and in the vicinal position, two NH_2 could possibly be corrected by −8 Å^3 in total, as exemplified by FOX-7, TIBMUM, CIWMAW01, etc. (3) If some heterocycles contain an −$NHNO_2$ group and the heterocycle also has an acidic N−H on the ring, the volume of the molecule also needs a correction of −8 Å;, for example, 5-nitramino-1,2,4-triazole (NRTZ), 3-nitramino-4,5-dinitro-pyrazole, etc.

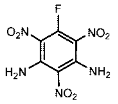
For 15 typical high explosives with strong hydrogen bonding with an average density of 1.879 g·cm^{-3}, shown in Table 2, Hoffmann’s method gives a MAD of 0.153 g·cm^{-3}, while the MAD for Ammon’s parameters is 0.079 g·cm^{-3}. Using our current method, the MAD is remarkably reduced to 0.013 g·cm^{-3}. Our 8 Å^3 rule may also apply to Hofmann’s and Ammon’s methods. For the same 15 series in Table 2, after correction for corresponding hydrogen bonding, the MAD for Hofmann’s method reduced from 0.153 g·cm^{-3} to 0.032 g·cm^{-3} according to the same rule for hydrogen bonding corrections. The MAD for results from Ammon’s method also can be reduced to 0.024 g·cm^{-3}, but different rules for hydrogen bonding corrections would apply. In general, when using Ammon’s method, hydrogen bond corrections require a reduction of −8 Å^3, whereas our method needs corrections of −16 Å^3. In some cases where Ammon’s method gives a correct result, our method needs to be corrected by −8 Å^3.

Previous density calculations[7−10] were mainly focused on picryl derivatives. With time, more and more explosives with more novel structures have been prepared. In this work, we have compiled a list of 261 of the most sophisticated explosives which contains the most promising explosive candidates including NF_2, SF_5, and fused and caged rings, with an average density of about 1.803 g·cm^{-3} (Table 3). Compounds with densities lower than 1.5 g·cm^{-3} are excluded from consideration with the only exception being mononitro cubane. Most of the values are taken from CCDC files, where the majority of crystals have an *R* factor of < 0.07. When two polymorphs both have *R* factors < 0.07, the crystal with the higher density was retained. For example, in the case of 1,3,5,7-tetranitro-1,3,5,7-tetrazocane (HMX), *β*-HMX (CCDC refcode OCHTET04 $R = 0.065$, $d = 1.903$ g·cm^{-3}) was retained over the α-HMX (CCDC refcode OCHTET, $R = 0.035$, $d = 1.84$ g·cm^{-3}) entry, although all of the empirical additivity predictions are closer to the density of α-HMX.

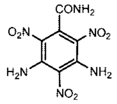
Table 2. Experimental and Predicted Densities of 15 Typical Explosives with Hydrogen Bonding[a]



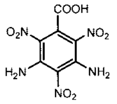
BAKLII



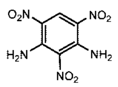
BEWYOR



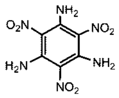
BICWEP



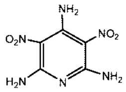
DACYEL



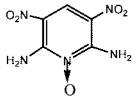
DATB



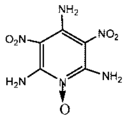
TATB



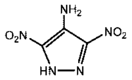
TIBMUM



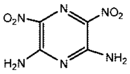
TIBMIA



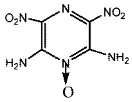
TIBMOG



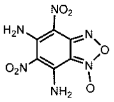
LLM-116



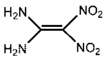
CIWMAW01



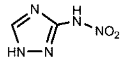
YEKQAG01



CI-14



FOX-7



NATA

compd	d_{obsd}/g·cm^{-3}	Hofmann V/Å^3	 d/g·cm^{-3}	Ammon V/Å^3	 d/g·cm^{-3}	this work V/Å^3	 d/g·cm^{-3}
BAKLII	1.890	247.35	1.740	236.439	1.820	227	1.895
		(231.35)	(1.860)	(228.439)	(1.884)		
BEWYOR	1.946	242.05	1.791	234.84	1.846	224.5	1.931
		(226.05)	(1.918)	(226.84)	(1.912)		
BICWEP	1.887	278.10	1.709	269.958	1.760	256	1.856
		(262.10)	(1.813)	(253.958)	(1.871)		
DACYEL	1.863	272.61	1.749	262.368	1.817	253	1.885
		(256.61)	(1.858)	(254.368)	(1.875)		
DATB	1.839	235.96	1.711	228.871	1.764	217	1.861
		(219.96)	(1.836)	(220.871)	(1.828)		
TATB	1.937	252.84	1.695	242.265	1.769	224	1.914
		(228.84)	(1.873)	(218.265)	(1.964)		
TIBMUM	1.819	216.19	1.645	198.260	1.794	196	1.814
		(200.19)	(1.776)				
TIBMIA	1.878	210.70	1.695	200.281	1.784	191	1.870
		(194.70)	(1.837)	(192.281)	(1.858)		
TIBMOG	1.876	227.58	1.679	213.675	1.789	206	1.855
		(211.58)	(1.806)	(205.675)	(1.858)		
LLM-116	1.900	161.41	1.781	156.960	1.831	153	1.879
		(153.41)	(1.874)				
CIWMAW01	1.812	192.16	1.729	184.828	1.798	184	1.806
		(184.16)	(1.804)				
YEKQAG01	1.922	203.55	1.763	192.216	1.867	186	1.929
		(187.55)	(1.913)	(184.216)	(1.948)		
Cl-14[b]	1.910	242.68	1.753	228.924	1.858	222	1.916
		(226.68)	(1.877)	(220.924)	(1.925)		
FOX-7	1.883	140.82	1.742	139.214	1.766	130.5	1.884
		(132.32)	(1.851)	(131.214)	(1.874)		
NATA[c]	1.83	124.76	1.718	122.618	1.748	117	1.831
		(116.76)	(1.836)				
average density/g·cm^{-3}	1.879		1.727		1.801		1.875
			(1.849)		(1.865)		
MAD/g·cm^{-3}			0.153		0.079		0.013
			(0.032)		(0.025)		

[a] Number in parentheses is molecular volume or density after correction for hydrogen bonding. [b] Ref 24. [c] Ref 25.

Table 3. MAD of Different Methods for 261 High-Density Explosives

type of explosive	no. of candidates	MAD/g·cm^{-3} Hofmann	 Ammon	 this work
acyclic	31	0.042	0.040	0.034
four-membered ring	6	0.020	0.023	0.029
five-membered ring	34	0.063	0.042	0.026
six-membered nonaromatic ring	13	0.053	0.028	0.020
eight-membered ring	7	0.085	0.033	0.045
aromatic heterocycles	15	0.118	0.046	0.015
nitrobenzene	33	0.060	0.037	0.018
furazan	19	0.085	0.087	0.026
nonfused rings	39	0.061	0.043	0.031
fused ring	39	0.087	0.036	0.027
caged ring	25	0.115	0.030	0.025
overall	261	0.072	0.042	0.026
average density/g·cm^{-3}	1.801	1.764	1.809	1.803

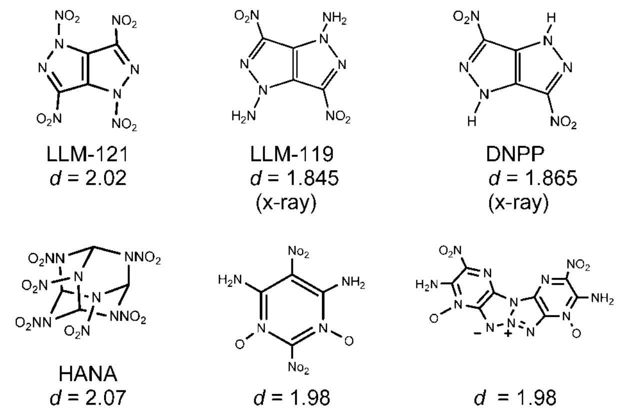


Figure 1. Predicted densities of some proposed explosives (*d* in g·cm^{-3}).

In general, Hofmann's method overestimates densities of explosives containing azide (N_3), nitrile (CN), and high nitrogen explosives and underestimates densities of fused, bridged, and caged rings; however, these errors are systematic and could be canceled by corresponding corrections. Notably, Hofmann's method gives very accurate density prediction for some acyclic and cyclic explosives with small rings. From the data listed in Table 3, our method compares favorably with Ammon's parameters, especially for five-membered rings and furazan explosives. Moreover, our method is much simpler for users since fewer parameters are involved and the majority of parameters are in whole numbers, which does not lead to inaccuracy in density predictions as is clearly shown in Table 3.

Some Proposed High Explosives

1,3,4,6-Tetranitro-1,4-dihydropyrazolo[4,3-c]pyrazole (LLM-121)[26] has been synthesized, but the high-density polymorph is still being sought. Its density is predicted to be 2.2 g·cm^{-3} using MOLPACK and 2.08 g·cm^{-3}using Ammon's parameters,[3] both of which give values which are higher than that of 2,4,6,8,10,12-hexanitro-2,4,6,8,10,12-hexaazaisowurtzitane (Cl-20). However, based on our method, the best prediction is only 2.02 g·cm^{-3}, which is lower than that of Cl-20. Our method also offers more accurate density predictions for analogues of LLM-121), e.g., 1,4-diamino-3,6-dinitropyrazolo[4,3-c]pyrazole (LLM-119) (our method 1.848 g·cm^{-3}, X-ray 1.845 g·cm^{-3}) and 3,6-dinitro-1,4-dihydropyrazolo[4,3-c]pyrazole (DNPP) (our method: 1.859 g·cm^{-3}; X-ray 1.865 g·cm^{-3}) (Figure 1).

Hexaazohexanitroadamantine (HANA) is a long-sought explosive, with a very high estimated density of 2.1 g·cm^{-3} when using Ammon's method or 2.07 g·cm^{-3} by our method. This is predicted to be the densest explosive at 2.1 g·cm^{-3} which seems to be a threshold for C, H, N, and O nonpolymeric explosives. Synthesis of the nitropyrimidine derivatives as proposed has been attempted without success.[27] The density of this compound should approach 1.98 g·cm^{-3}. Tetraazapentalene (TAP)[28,29] derivatives are of special interest due to their thermal stability and novel chemical structure, which suggest that they be used as insensitive explosives for down hole high-energy materials.[30] One of the suggested TAP candidates here should also be insensitive and promising owing to the presence of strong intramolecular hydrogen bonding and an impressive estimated density of 1.98 g·cm^{-3}.

Conclusion

A new atom/group additivity method for crystal density prediction of high-density explosives has been created. There are 38 atoms and groups and three corrections, which cover explosives containing C, H, O, N, and F. The quantitative impact of strong hydrogen bonding on the densities of energetic materials is addressed. For 261 explosives with an average density of 1.803 g·cm^{-3}, our current method gives a mean absolute deviation (MAD) of 0.026 g·cm^{-3} and a mean relative absolute error of 1.5 %.

Supporting Information Available:

Four instructional examples and a compilation of 261 high-density explosives. This material is available free of charge via the Internet at http://pubs.acs.org.

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