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THE CRYSTAL STRUCTURE DETERMINATION OF
TRIAMINOGUANIDINIUM NITRATE: A BURNING
RATE MODIFIER FOR NITRAMINE PROPELLANTS

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20. Abstract (continued)

by van der Waals' forces and hydrogen bonding. It was concluded that no definitive explanation for the burning rate behavior could be made until other data were obtained. It was recommended that the charge distribution on each ion be studied with a semi-empirical SCF-MO treatment, that thermal decomposition (gas analysis) and reaction mechanism be determined, and that a wide temperature range (liquid nitrogen temperature to melting point) differential scanning calorimetry (DSC) or differential thermal analysis (DTA) study be undertaken.

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INTRODUCTION

High-force nitramine propellants such as RDX and HMX formulations have, in general, lower flame temperatures than do energetically comparable nitrate ester propellants. This characteristic lower flame temperature constitutes a definite advantage for nitramines because there is an apparent correlation between gun barrel temperature and its rate of erosion. On the other hand, nitramine propellants display slower burning rates than nitrate ester propellants. Adding triaminoguanidinium nitrate to nitramines will produce propellants that burn faster and cooler with only slight reduction in force. Therefore, triaminoguanidinium nitrate-nitramine propellants show promise for future military application.

This investigation was conducted to determine how triaminoguanidinium nitrate accelerates the burning rates of nitramines because understanding this mechanism could lead to new and improved propellant systems. For the initial phase of this study, a crystal and molecular determination using single crystal x-ray diffraction was undertaken to ascertain if burning rate acceleration is structure related.

As part of an investigation of hydrazine derivatives of carbonic acid, Keim used x-ray diffraction powder techniques to determine some of the crystallographic parameters of triaminoguanidinium nitrate (ref. 1). The compound was classified as orthorhombic with the non-centrosymmetric space group $P2_1ca$ (non-standard setting) and unit-cell parameters $a = 6.55(3)$, $b = 8.37(5)$, and $c = 12.61(6)$ Å. Since Keim's study, the only structure study involving the triaminoguanidinium ion was carried out by Okaya and Pepinsky (ref. 2) on the chloride salt.

EXPERIMENTAL

Colorless, transparent, acicular crystals of triaminoguanidinium nitrate were prepared from aqueous solution. Optical measurements of crystal face normals indicated the crystal is bounded by the planes of the forms $\{101\}$, $\{110\}$, and $\{001\}$. Cleavage planes were observed parallel to $\{001\}$.

Oscillation and Weissenberg photographs taken with the crystal mounted on the c axis were used to determine approximate unit-cell parameters. Intensity measurements were obtained (crystal dimensions $0.5 \times 0.5 \times 0.7$ mm) with a computer-controlled diffractometer using

MoK α x-radiation. The measured intensities were corrected for Lorentz and polarization effects to obtain the structure amplitudes. Absorption corrections were applied with a maximum transmission factor of 0.952 and a minimum of 0.928. A total of 885 independent reflections were collected, of which 140 were rejected as unobserved because they violated an imposed acceptance criterion, $F \geq 2 \sigma (F_0)$.

The crystal data are:

Orthorhombic, $a = 8.389(7)$, $b = 12.684(8)$, $c = 6.543(5)$ Å; space group Pbcm (no. 57); $D_0 = 1.60$, $D_c = 1.594$ G cm $^{-3}$; $Z = 4$; $V = 692.2(9)$ Å 3 ; molecular weight = 167.13; $\mu = 1.563$ cm $^{-1}$ (MoK α 0.7107); $F(000) = 352$; systematic absences $k = 2n + 1$ for $0k\ell$, $\ell = 2n + 1$ for $h0\ell$, chemical formula C(NH) $_3$ (NH $_2$) $_3$ NO $_3$.

Systematic absences observed with Weissenberg photographs are indicative of space groups Pbcm and Pca 2_1 . On the basis of intensity distribution statistics (table 1), the centrosymmetric space group Pbcm was selected rather than the noncentrosymmetric space group Pca 2_1 reported by Keim (ref. 1). Since the unit cell contains four formula weights of triaminoguanidinium nitrate, and the general positions of this space group are eightfold, the cation and anion centers must occupy the fourfold special positions located on the mirror planes at $\pm 1/4c$. This arrangement is consistent with the molecular symmetries of both the planar nitrate and triaminoguanidinium ions (ref. 2).

STRUCTURE DETERMINATION

The trial structure was obtained with a multisolution direct method (program Multan, ref. 3). The program calculated an overall temperature factor of 3.28 Å 2 and the quasi-normalized structure factors (E values). It also automatically generated and ranked 293 reflections with $E \geq 1.0$, selected three origin defining reflections, and produced eight sets of phased reflections. The set with the highest combined figure of merit (3.0) produced a computed E-map that revealed the molecular shape of the triaminoguanidinium ion and the positions of its six nitrogen atoms and one carbon atom. Locations of the nitrogen and oxygen atoms of the nitrate ion were also evident, but the molecular shape was distorted and the weights of the oxygen peaks were small, suggesting the possibility of disorder in the nitrate ion. This trial structure yielded an R value of 0.320 ($R = \sum |F_0 - F_c| / \sum |F_0|$).

Table 1. Intensity distribution statistics.

	Experimental	Theoretical	
		(Centrosymmetric)	(Non-centrosymmetric)
$\langle E^2 \rangle$	1.0000	1.0000	1.0000
$\langle (E^2 - 1) \rangle$	0.9335	0.9680	0.7360
$\langle E \rangle$	0.8082	0.7980	0.8860
$ E > 0.5$	0.643	0.617	0.779
$ E > 1.0$	0.383	0.368	0.445
$ E > 1.5$	0.137	0.134	0.105
$ E > 2.0$	0.043	0.046	0.018
$ E > 2.5$	0.006	0.012	0.002
$ E > 3.0$	0.002	0.003	0.000

Isotropic, full matrix least squares refinement with Flinus, a modified ORFLS program (ref. 4), with observed reflections weighted by $w = 1/\sigma^2(F)$ reduced the R value to 0.228. Continued least squares refinement with anisotropic temperature factors and an isotropic extinction correction led to an R value of 0.107. At this point, the hydrogen atoms' positions, located by means of an ($F_o - F_c$) synthesis, were refined by least squares analysis. The anisotropic temperature factors of each hydrogen atom were constrained to equal the temperature factors of the nitrogen atom to which each hydrogen atom is bonded.

After three cycles of refinement, the R value reduced to 0.083. The final shifts of both the positional and thermal parameters were equal to or less than two percent of the standard deviation. The extinction was made with the formula $F_{cor} = F_o (1 + gBF^2)^{1/4}$ in which F is the calculated structure factor on the absolute scale B is a function of both the diffraction angle (θ) and the average path length in the crystal for a given reflection, and g is the isotropic extinction parameter (ref. 5), which refined to 0.31×10^{-4} cm. The largest extinction correction was 0.77 for the 002 reflection.

The atomic and thermal parameters (tables 2 and 3) demonstrate the planarity of the triaminoguanidinium ion, and its anisotropy with the greatest thermal vibrations occurring perpendicular to the plane of the ion. The nitrate ion is very nearly planar (table 4) and anisotropic. The large thermal parameters of the oxygen atoms, b_{33} of O(1) in particular, are harbingers of disorder in the nitrate ion.

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

The molecular configuration of the triaminoguanidinium ion (fig. 1) is similar to that reported by Okaya and Pepinsky (ref. 2) in the structure determination of triaminoguanidinium chloride. In both cases, the ion is planar with the exception of the three pairs of amino hydrogen atoms. In the hexagonal chloride salt, the ion has the molecular symmetry C_{3h} yielding exact bond angles of 120.0° , and values of 1.318(9) Å for each C-N bond and 1.450(14) Å for each N-N bond. Since the variation observed in the C-N bond lengths and bond angles (table 5) is about one standard deviation, the three C-N bonds are considered equivalent with an average bond length of 1.322 Å, and average bond angle of 120.0° . This is consistent with the bond lengths observed in triaminoguanidinium chloride, guanidinium chloride (ref. 6), and guanidinium oxylate dihydrate monoperhydrate

Table 2. Atomic coordinates and their standard deviations.

Triaminoguan- idinium cation	x/a	y/b	z/c
C	0.7188(5)	0.7600(3)	0.75
N(1)	0.6671(5)	0.8586(3)	0.75
N(2)	0.8740(4)	0.7405(3)	0.75
N(3)	0.6159(4)	0.6814(3)	0.75
N(4)	0.7800(5)	0.9407(3)	0.75
N(5)	0.9238(4)	0.6340(4)	0.75
N(6)	0.4530(5)	0.7035(3)	0.75
H(1)	0.562(6)	0.873(4)	0.75
H(2)	0.922(6)	0.776(5)	0.75
H(3)	0.645(6)	0.624(4)	0.75
H(4)	0.754(4)	0.978(3)	0.654(6)
H(5)	0.996(4)	0.631(3)	0.652(6)
H(6)	0.405(4)	0.680(3)	0.646(6)
Nitrate anion			
N	0.2405(4)	0.9024(3)	0.75
O(1)	0.3602(4)	0.9549(3)	0.75
O(2)	0.1808(5)	0.8765(3)	0.9092(5)

Table 3. Thermal parameters and their standard deviations ($\chi 10^4$).

$$T = \exp \left[-(b_{11}h^2 + b_{22}k^2 + b_{33}l^2 + 2b_{12}hk + 2b_{13}hl + 2b_{23}kl) \right]$$

Triaminoguan- idinium cation	b_{11}	b_{22}	b_{33}	b_{12}	b_{13}	b_{23}
C	105(6)	44(2)	110(8)	9(3)	0	0
N(1)	82(5)	40(2)	275(11)	-8(3)	0	0
N(2)	93(6)	47(3)	288(12)	-3(3)	0	0
N(3)	94(5)	35(2)	226(10)	2(3)	0	0
N(4)	128(7)	43(2)	290(14)	-21(3)	0	0
N(5)	108(6)	61(3)	299(13)	25(4)	0	0
N(6)	84(5)	50(3)	266(12)	-8(3)	0	0

Nitrate anion

N	76(5)	32(2)	270(12)	3(3)	0	0
O(1)	80(6)	40(2)	1711(51)	-3(3)	0	0
O(2)	309(8)	126(3)	240(9)	76(4)	69(6)	0

Table 4. Least-squares plane for nitrate ion and deviations of atoms from it.

Plane defined by N, O(1), O(2)*, O(2)* $4.6274A - 10.5800B - 0.00006C = -8.4355$.

Atom	Deviation(A)
N	0.0017
O(1)	-0.0006
O(2)	-0.0010
O(2)	-0.0001

Symmetry related pair of oxygen atoms at (x,y,z) and (x,y, 1/2+z).

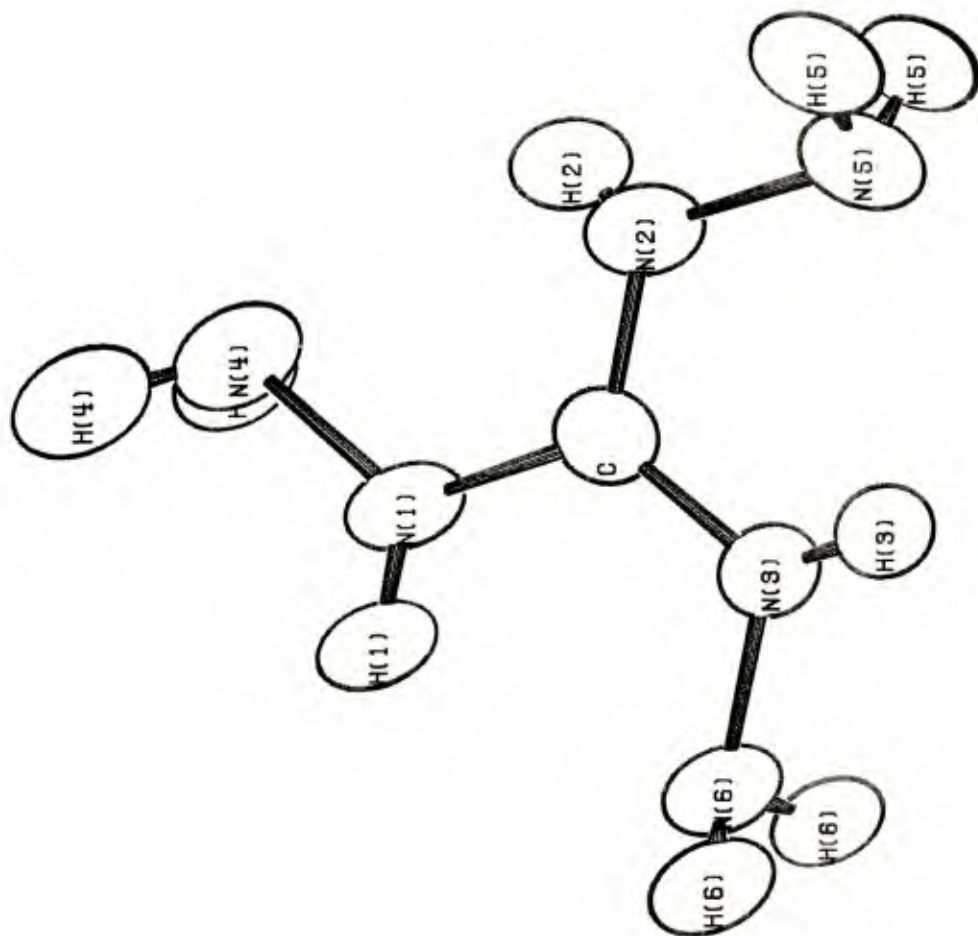


Figure 1. Molecular configuration and numbering scheme of triaminoguanidinium ion.

(ref. 7). The N-N bond lengths, on the other hand, exhibit a variation exceeding one standard deviation and are much shorter than the N-N bond length observed in triaminoguanidinium chloride. The N-H bond lengths corrected for thermal motion are in agreement with N-H bond lengths observed in guanidinium oxylate dihydrate monoperhydrate (ref. 7).

Table 5 shows that the average bond angle for the nitrate ion is 120° , and the observed bond lengths for N-O(1) and N-O(2) are 1.206 and 1.203A, respectively. These data indicate the oxygen atoms are equivalent and the D_{3h} symmetry usually observed with the nitrate ion is maintained. However, these bond lengths are short compared to the average N-O bond lengths listed in the International Tables for X-ray Crystallography (ref. 8).

This shortened bond suggests a model for the nitrate ion consisting of rigid-body thermal motion as well as atomic thermal variations. The directions for the greatest thermal vibrations of each atom are parallel to the plane of the nitrate ion and perpendicular to the N-O bond, while the smallest vibrations occur perpendicularly to the plane of the nitrate ion and parallel to the N-O bond. This suggests a rotation or rotary-oscillation of the nitrate ion, probably hindered by the forces of hydrogen bonding, around an axis parallel to the ion's three-fold axis. No attempt was made to analyze the rigid-body motion. The bond lengths, corrected for thermal vibrations only (oxygen atom riding on the nitrogen atom), are 1.341 and 1.262A for N-O(1) and N-O(2), respectively. With these bond lengths, the oxygen atoms are no longer equivalent and the classic D_{3h} symmetry is not maintained. These values, however, do agree with the N-O bond lengths observed in the structure determination of $NH_4NO_3 \cdot 2HNO_3$ by Einstein and Tuck (ref. 9). The N-O(1) bond which is coplanar with the triaminoguanidinium ion is probably stretched because of the influence of two hydrogen bonds (table 6). The N-O(2) bond is stretched to a lesser extent because it is involved with only one hydrogen bond.

The crystal structure presented in figure 2 consists of layers of triaminoguanidinium ions and nitrate ions located on mirror planes perpendicular to the c axis at $\pm 1/4$. The triaminoguanidinium ions are coplanar with mirror planes (except for the amino hydrogen atoms). Each nitrate ion is bisected by a mirror plane with only the center nitrogen atom and one oxygen atom located on the mirror. This results in a dihedral angle of 90° between the planes of the two ions. The inter-layer packing of the ions consists of stacking the cations along the c axis

Table 5. Bond lengths and angles with their e. s. d. 's.

Triaminoguanidinium cation

C-N(1)	1.324(4)A		N(1)-C-N(2)	119.8(4)
C-N(2)	1.324(6)		N(2)-C-N(3)	120.1(4)
C-N(3)	1.318(5)		N(3)-C-N(1)	120.0(4)
N(1)-N(4)	1.407(5)		C-N(1)-N(4)	118.6(4)
N(2)-N(5)	1.415(6)		C-N(2)-N(5)	118.0(4)
N(3)-N(6)	1.397(5)		C-N(3)-N(6)	119.3(4)
N(1)-H(1)	0.91(5)	1.01(4)*	C-N(1)-H(1)	121(3)
N(2)-H(2)	0.64(6)	0.79(4)*	C-N(2)-H(2)	119(5)
N(3)-H(3)	0.77(6)	0.87(4)*	C-N(3)-H(3)	120(4)
N(4)-H(4)	0.82(4)	0.93(3)*	N(1)-N(4)-H(4)	105(2)
N(5)-H(5)	0.88(4)	1.00(3)*	N(2)-N(5)-H(5)	105(3)
N(6)-H(6)	0.90(4)	0.99(3)*	N(3)-N(6)-H(6)	112(2)

Nitrate anion

N-O(1)	1.206(5)	1.341(6)**	O(1)-N-O(2)	120.0(2)
N-O(2)	1.203(4)	1.262(4)**	O(2)-N-O(2)	120.1(5)

* Corrected for thermal motion with atoms moving independently.

** Corrected for thermal motion with oxygen atom riding on nitrogen atom.

Table 6. Interionic distances (up to 3.3A) and their e.s.d.'s.

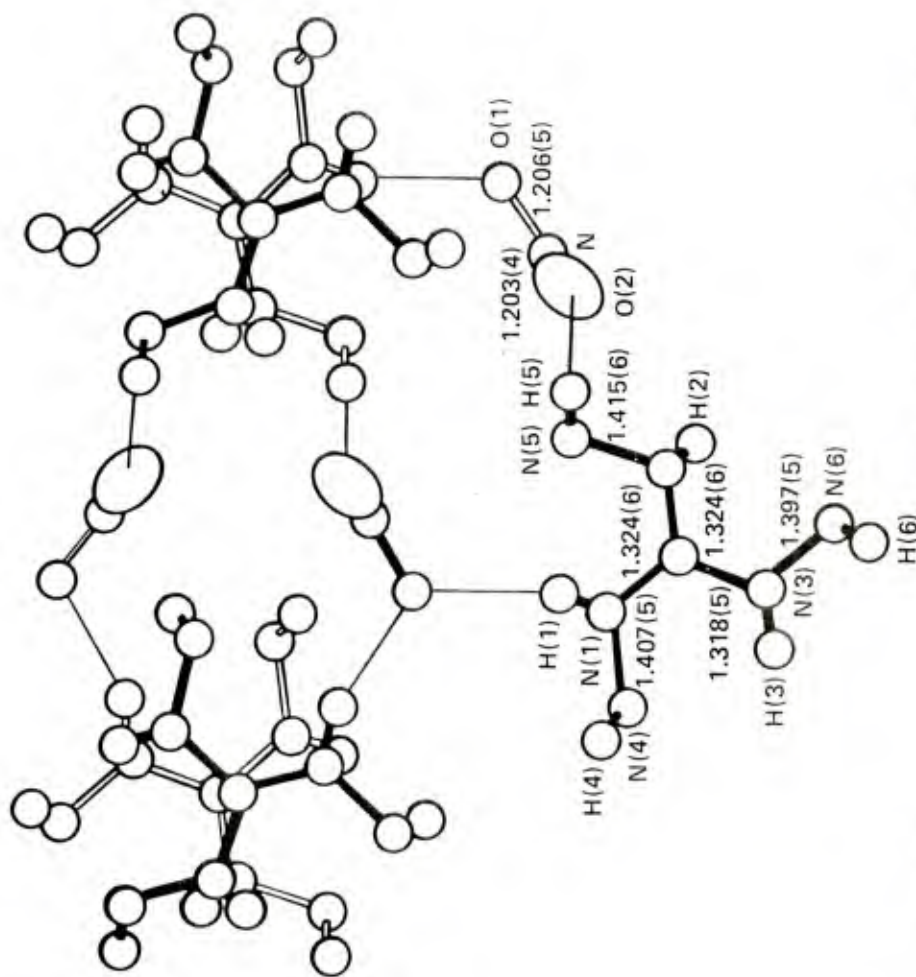
A) Hydrogen bonded interionic distances

	Distances (A)		Angles (°)
	N..O	H..O	N-H..O
(ii)N(1)-H(1)...O(1)	2.849(5)	1.98(5)	160(5)
(i) N(3)-H(3)...O(1)	2.880(5)	2.15(5)	160(5)
(iii)N(5)-H(5)..O(2)	3.103(5)	2.22(5)	178(4)
(iv)N(5)-H(5)...O(2)	3.103(5)	2.22(5)	178(4)

B) Non-hydrogen bonded interionic distances

	Distances (A)		Angles (°)
	N..O	H..O	N-H..O
(v)N(2)-H(2)..O(2)	3.268(6)	2.70(5)	150(5)
(v)N(2)-H(2)..O(2)	3.268(6)	2.70(5)	150(5)
(vi)N(4)-H(4)..O(2)	3.234(5)	2.50(5)	
(vii)N(4)-H(4)..O(2)	3.234(5)	2.50(5)	
(i)N(5)-O(1)	3.292(6)		
(ii)N(6)-O(1)	3.282(6)		
(viii)N(6)-H(6)-O(2)	3.348(5)	2.49(4)	158(3)
(ix)N(6)-H(6)-O(2)	3.348(5)	2.49(4)	158(3)
(ii)N(6)-O(2)	3.333(5)		

Triaminoguanidinium ion in positions: (6) $x, y, 3/4$; (ii) $\bar{x}, 1/2+y, 3/4$; (iii) $1-x, \bar{y}, 1/4$; (iv) $1-x, \bar{y}, 5/4$; (v) $1-x, 1/2+y, 3/4$; (vi) $x, 1/2-y, 1/4$ (vii) $x, 1/2-y, 5/4$; (viii) $x, y, 5/4$



Note: Atoms with closed bonds are at 3/4 c and atoms with open bonds are at 1/4 c. Hydrogen bonds indicated by single lines. Thermal ellipsoids scaled to enclose 50% probability.

Figure 2. Crystal structure projected on (001).

in adjacent layers with their central carbon atoms almost directly over each other. The closest intercation contact is 3.26Å (table 7) occurring between N(2) and H(5). The nitrate ions are stacked over each other in alternate layers. The closest interlayer cation-anion contact of 3.103Å occurs between O(2) and N(5) with an attendant weak hydrogen bond of 2.22Å between O(2) and H(5) of each adjacent layer (table 6). This results in weak hydrogen bonded chains of ions running parallel to the c axis.

Within a layer, each ion is surrounded by three oppositely charged ions. The interionic contacts (N...O) listed in table 5 are 2.849, 2.880, 3.268, 3.282, and 3.292Å. The shorter two distances have associated hydrogen bonds of 1.98 and 2.15Å for H(1)...O(1) and H(3)...O(1), respectively. These hydrogen bonds, which are somewhat stronger than the longer H(5)...O(2) bond, serve as connecting links within the network of adjacent sets of hydrogen bonded interlayer chains. These hydrogen bond lengths compare favorably with those observed in glycylglycine nitrate (ref. 10).

Each nitrate ion is involved with four hydrogen bonds: O(1) forms two 'in layer' hydrogen bonds, and each O(2) atom forms one hydrogen bond between adjacent layers of cations resulting in a three-dimensional network of hydrogen bonds.

Presently, it is not possible to explain definitively the burning rate behavior of triaminoguanidinium nitrate on the basis of its molecular or crystal structure. More data are needed before any burning rate formalism can be postulated. However, certain features of this structure stir the imagination and guide further research which may provide the data that will explain the burning rate behavior. These features are:

1. The anisotropic nature of the crystal with its weak interlayer cohesive forces parallel to the c axis and stronger interlayer forces parallel to the ab plane.
2. The possibility that the nitrate ion may be a rigid rotor hindered by the forces of hydrogen bonding.
3. The possibility of disorder in the nitrate.

Table 7. Interlayer ionic closest contacts and their e. s. d.'s.

	Distances(A)
*C-C	3.2813(7)
*N(2)-N(2)	3.2803(7)
*N(2)-H(5)	3.26(4)

* Triaminoguanidinium ion in adjacent layer

CONCLUSIONS

1. Triaminoguanidinium nitrate is a layered structure. Within each layer the predominant cohesive forces are electrostatic. Between layers, the dominant forces of cohesion are van der Waals' forces and hydrogen bonds.

2. The data presently available are insufficient and, therefore, any burning rate mechanism postulated at this time would be highly speculative and premature.

RECOMMENDATIONS

1. A determination of the charge distribution on the cation and anion should be undertaken using a semi-empirical SCF-MO treatment such as MINDO/3 (ref. 11) to ascertain to what extent ionic forces play in interlayer bonding.

2. A decomposition study of triaminoguanidinium nitrate should be initiated. The gaseous end products may provide the key to the burning rate mechanism.

3. A wide temperature range (liquid nitrogen temperature to melting point) DTA or DSC study should be initiated to verify the rigid body motion of the nitrate ion and to determine the onset temperature of free rotation (if any).

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