第1卷 第3期
1993年9月

含 能 材 料
ENERGETIC MATERIALS

Vol. 1, No. 3
September, 1993

EFFECT OF INTRAMOLECULAR INTERACTION ON MOLECULE CONFORMATION STABILITY AND CRYSTAL PACKING OF POLYNITROCOMPOUNDS

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ABSTRACT In study of polynitrocompounds it is found that a dense crystal must not necessarily be constructed from dense molecules, and the main factors affecting the crystal structure are the electronic structure of their molecules. The correlation between the value of non-bonded intramolecular contact and the magnitude of the respective intermolecular contact seems to be unusual for this kind of compounds.

Alkoxydiazene-N-oxide and 1, 1, 4, 4,-tetranitrobutanediol-2, 3 derivatives were taken as examples in this study. The obtained results concluded that the intramolecular interaction can stabilize the crystal conformation, while the increase in the intermolecular contact decreases the crystal density.

KEY WORDS intramolecular interaction, polynitrocompounds, crystal packing.

1 INTRODUCTION

It is well known that the density of crystal compounds determines a variety of their important physico-chemical characteristics. In view of that, polynitrocompounds are of special interest.

Earlier we carried out a series of investigations directed to elucidating the correlation between the crystal structure of polynitrocompounds and their density that in some cases varied from 1.5 to 2.0 g/cm^3[1~3] for the compounds involving only the elements of the second period. We discovered a seemingly unusual correlation between the values of nonbonded intramolecular contacts on the one hand, and the magnitudes of the respective intermolecular contacts, on the other. A selfagreement between the contacts was established that shortening one kind of the contacts leads to elongation of the other[4~6]. This result is unexpected as it exceeds the limits of the classical works of Kitaigorodskii[7] who noted only the effect of geometrical parameters of the molecule on its crystal packing, not taking into account the nature and electronic structure of the molecule.

The obtained results led us to conclude that the density decrease in polynitrocompound crystal resulted from the increase in their intermolecule contact magnitude is con-

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nected with the increase in electrostatic repulsion between the molecules[5].

In further investigation of this relation we took an additional attenition to the shortening of intramolecular contacts and the effect of intramolecular electrostatic attraction or orbital interactions. These interactions stabilize the conformation of a complex overloaded molecule, and in their turn, determine the character of intermolecular interactions.

The present work, based on the comparison of the data of X-ray analysis of alkoxydiazene-N-oxide compounds and 1,1,4,4-tetranitrobutanediol-2,3 derivatives with qualitative consideration of orbital interactions within the framework of perturbation theory, as well as with the data of quantum-chemical calculations of the appropriate model compounds, traces the interrelation between all kinds of intramolecular orbital interactions and intermolecular interactions in crystals.

2 EFFECT OF SUBSTITUENTS ON ORBITAL INTERACTIONS IN MOLECULES OF ALKOXYDIAZENE-N-OXIDES

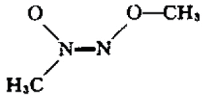
In the chemistry of power intensive compounds, alkoxydiazene-N-oxides attract our attention in view of the fact that, being isomers of nitramines, they have higher enthalpies of formation and higher thermostability.

Numerous X-ray studies of the compounds belonging to the class of alkoxydiazene-N-oxides[8~11] record a planar diazenoxide fragment in *Z*-configuration with attractive interaction between chemically nonbonded oxygen atoms. Construction of a molecule based on qualitative approaches to orbital interactions by using perturbation theory leads to the following for the fragment under consideration: a lone electron pair (LEP) on a nitrogen atom n (N) interacts with an σ-type LEP on an oxygen atom (an interaction in the plane of the N(O)—N—O group) (Fig. 1). Destabilization of an antibonding combination of LEP is greater than stabilization of a bonding combination. The antibonding LEP combination interacts with a vacant MO of the N—O polar bond. The σ^*-antibonding orbital is localized mainly on a positively charged atom of the N—O bond.

The n-σ^* interaction stabilizes *Z*-configuration of the fragment, since the occupied combined MO lies lower than the orbitals interacting due to partial overlap in the N—N region. In the case of *E*-configuration such an overlap is much smaller (Fig. 1).

Besides, there is an attractive interaction betweem the oxygen atoms lying at a distance less than 2.5 Å. In the case of two neighbouring LEP interaction, chemically nonbonded oxygen atoms of the same symmetry leads to formation of a bonding MO with an insignificant stabilization and to an antibonding MO with a considerable destabilization of the molecular levels (Fig. 2). When there is a vacant antibonding MO in the system, the antibonding LEP combination may interact with this vacant MO if they have the same symmetry and their energies are close.

An interaction between the levels occurs together with charge transfer from the antibonding region; as a result, the interaction of LEP becomes attractive. These arguments may be best confirmed by calculations of occupation between the interacting atom centres.

Calculations for molecule  were carried out in minimal basis set (STO-3G) by using the MONSTER-GAUSS-81 program with extensive geometry optimization. It follows from the calculations that the central four-atom fragment is a unified conjugated system with six π-electrons and attraction between the oxygen atoms. The high occupied MO has a π-character; it makes the greatest contribution to the positive element of the π-overlap occupation of oxygen atoms: the atomic coefficients are high and positive in their sign (Fig. 3).

Qualitative construction of molecules with different substituents in a four-atom fragment, for example, with an electronegative σ-type substituents on the nitrogen atom, leads to lowering the bonding MO's and rising the antibonding MO's, hence the π-π^* interaction is decreased. If a π-donor is a substituent on a nitrogen atom, the multiple N-N bond is polarized, which leads to lowering the π^* (N—N) MO, i. e. the orbital interaction should increase. Analogously, if a π-donor happens to be an oxygen atom substituent in the diazenoxide fragment, the n-π^* interaction increases. The results of the MONSTER-GAUSS-81 program calculations confirm the qualitative analysis: an increase in the orbital interaction is followed by elongation of the N—N bond and shortening of the O⋯O distance; in this case the positive calculated occupation between the interacting atoms increaes. Charge distribution in the orbitals (Teble 1) of the four-atom fragment illustrates the substituent effect on the character of interaction. (The orbitals are classified with respect to plane of symmetry of the fragment). An increased attractive interaction between the oxygen atoms is explained by charge decrease on p_y-orbitals of these atoms and charge increase on p_y and p_x orbitals of the nitrogen atoms. Fig. 4 shows the dependence of N — N bond lengths on the O ⋯ O distance for the compounds[12,13] studied by X-ray technique at low temperature and theoretical calculations respectively.

It can be seen from both the experimental and theoretical data, the N — N bond length is inversely proportional to the distance between the oxyge atoms. An analogous experimental dependence was obtained for symmetric molecules (Fig. 5) (for the purpose of experiment geometric parameters of both the molecular fragments were previously averaged).

It should be noted that the above considerations on p-π^* and n-σ^* about the preferred Z-configuration over E-configuration are correct for the methylene-bis(nitrosohydroxylamine) anion as well.

Attractive interaction between oxygen atoms in molecules of alkoxydiazene-N-oxides is not an exception. Literature[14,15] reported on structural investigations of the molecules of 1,2-difluoroethylene and 1,2-difluorodiazene in which cis-configuration is preferred because of attractive interactions of lone electron pairs on fluorine atoms.

Thus the final molecular conformation makes a compromise of the two interactions; the repulsive interaction between chemically nonbonded atoms and the prevailing attractive interaction between orbital centres. The attractive interaction between oxygen atoms diminishes the charge distribution on these atoms, thus diminishing the electrostatic repulsion between the neighbouring molecules.

3 INTRAMOLECULAR INTERACTIONS IN MOLECULES OF 1,1,4,4-TETRANITROBUTANEDIOL-2,3 DERIVATIVES AND THEIR INFLUENCE ON THE CHARACTER OF INTERMOLECULAR INTERACTIONS

For synthesis of superdense compounds from complex strained molecules, a trinitroethylenic fragment is often used; a strained propeller conformation of a fragment with dihedral angels of ~80° between the nitrogroup planes is stabilized by n-π^*-orbital interactions between the occupied n-type orbitals of each nitrogroup with vacant π^*-orbitals on the neighbouring nitrogroups. The electrostatic attractive interaction between the neighbouring nitrogroup atoms $N^+ O^-$ of unlike charges acts into the same direction, i.e. towards enhancing the stabilization of the trinitroethylenic fragment conformation.

However, quite dense molecules with appreciable intramolecular interactions stabilizing the conformation of a molecule and reducing its molecular level are packed rather loosely in the crystal.

In this paper, an interrelation between intra-and intermolecular interactions involving an interaction of lone electron pairs is shown, exemplified by the structure of a rather dense fluorodinitromethyl fragment which is also quite often used in synthesis.

Crystallochemical analysis of the structures of 1,4-dihaloid-1,1,4,4-tetranitrodiols-2,3[17,18] shows that the conformation of the fragment is stabilized in the molecules by orbital interactions; both the lone electron pairs of the haloid atom interact simultaneously with the high MO's of the lone n-type electron pairs of both the nitrogroups in two interperpendicular planes. For the molecule geometry, the p-π^* interaction must lead haloid-oxygen atoms to approaching each other, as well as to shortening C—Hal and N—O bonds and lenghthening C—N bond. This geometry was observed in the experiment (Fig. 6). An additional confirmation of attractive interactions between the nitrogroup oxygen and haloid atoms was obtained by quantum-chemical calculations of a 2-chloro-2,2-dinitroethanol molecule. Optimization of geometric parameters and torsion angles of the molecule was carried out. The calculatded conformation of a separate molecule coincides with the experimental conformation of the molecular fragment. The calculations showed the HOMO to be a bond of n-type, with pairwise levels $MO_1(E_1=0.319H)$ and $MO_2(E_2=-0.311H)$ (Fig. 7). The oxygen atoms in nitrogroups and the chlorine atom make the greatest contribution into the positive occupation of π-overlap. On MO_1, AO $3p_x$ Cl^1 and AO p_y O^5 are in the phase; on MO_2, AO $3p_x$ Cl^1 and AO p_x O^3 are in the phase. The net calculated occupation between the interacting atoms Cl and O of the nitrogroups has a positive value. The p-π^* interaction in the haloiddinitromethyl fragment decreases the charge distribution in nitrogroups as compared to the molecule not involving a haloid atom; with increase of the haloid atomic number the orbital interaction increases, and the charge distribution on nitrogroups decreases respectively. Further, with increase of the haloid atomic number in a series of structures a shortening of the intermolecular O…O contacts is observed; all the intermolecular contacts are less than 3.3 Å, i. e. the electrostatic intermolecular repulsion in the crystal structure decreases. Hence in the calculation of the energy of the structure we must take into consideration, along with Van der Waals interaction, the electrostatic interaction that affects significantly the crystal density. However, this approach is too formal; it is necessary to examine the packing details. In the actual structure of 1,1,4,4-tetranitrobutanediol-2,3[16], the details of the molecular packing are the following (Fig. 8): two types of interactions are found between the nitrogroups of the two neighbouring molecules. First, this is an interaction between the lone electron pairs of the σ and π-type with a subsequent interaction with the vacant n-σ^* orbitals of the nitrogroups. Second, this is an interaction of the π-π^* type between the occupied orbital of one nitrogroup and the vacant orbital of another nitrogroup; the interaction gives rise to charge transfer. Quantum-chemical calculations for three pairs of the model dinitromethane molecules were carried out for those conformational ratios which were discovered in the structure of 1,1,4,4-dinitrobutanediol-2,3; as a result of this the criteria of estimation of the character of intermolecular orbital interaction were established. In the interaction of the LEP on the nitrogroups of two neighbouring molecules, the greater is the splitting of a twice degenerate HOMO, the stronger is the interaction between the orbitals of the nitrogroups; in the case of the interaction giving rise to charge transfer there is a total lowering of the localization of all the levels.

In agreement with the qualitative examination of the attractive orbital interactions the calculations show the HOMO of the two molecules to be bonded with a positive occupation of the π-and σ-overlap: either of the nitrogroup orbitals themselves or of their projections. In our estimation, it is natural that the magnitude of interaction is more significant to charge transfer. Hence with the increase in the atomic number of haloid in 1,4-dihaloid -1,1,4,4-tetranitrobutanediol-2,3 the intramolecular orbital attraction is enhanced; however, the intermolecular orbital attraction is also enhanced and the intermolecular electrostatic repulsion is decreased. As a result, the increase of crystal density in this series is much greater than that shown in Table 2.

Quite different is the relation between the intra- and intermolecular interactions in the molecules of 1,4-dihaloid-1,1,4,4-tetranitrobutanediol-2,3 dinitrates, where an interaction between nitro- and nitrate-groups was discovered at 1,2-positions.

The geometric parameters in dinitrates of 1, 4-dihaloid-1, 1, 4, 4-tetranitrobutanediols-2,3 obtained in X-ray study shows distortion of super conjugation in haloiddinitromethyl fragment, as well as a possible n-π^* interaction between the 1,2-positions of the nitro- and nitrate-groups in the molecule with a short O…N contact of 2.72 Å. With increase of the haloid number this distance becomes shorter (2.85[F]; 2.80 [Cl]; 2.72 [Br])[19].

In full agreement with the experiment (Fig. 9), the calculations of the model molecules of 2-chloro-2,2-dinitroethanol nitrate with optimization of geometrical parameters show that the scheme of molecular levels distribution is determined mainly by intermolecular n-π^* orbital interactions between nitro-and nitrate-groups which destroy the super conjugation in the haloiddinitromethyl fragment. The high molecular level of the π-type decomposes into nonbonding sublevels of three nitro groups. Strained conformation of the molecule in the real crystal and in the calculation is stabilized by orbital interactions as the conformation calculated by means of the molecular mechanics program (MMX) changes considerably; the N…O distance is up to 4.2 Å. The n-π^* type interaction decreases the energy of the ground state of the molecule; this, in its turn, brings on a possibility of rise of intermolecular orbital interactions. In dinitrates, the intermolecular contacts are longer than in alcohols; mean values of the intermolecular contacts in the range of <3.3 Å increase with the increase of atomic number of the haloid.

There are some physical parameters that testify objectively to the correctness of our considerations. The first is the crystal density. In a row of alcohols, there is an increase in the crystal density significantly with the increase of haloid atomic number than expected from the calculations with the additive scheme. On passing from alcohols to nitrates (replacement of an alcohol group with a nitrate one), there is a sharp retardation of the density increase (Table 2). The compared structures have the same type of packing from centrosymmetric molecules. Secondly, this is a hypsochromic shift of n-π^* absorption band in the UV-spectra which was discovered in the study of the concentration dependence of this band for some polynitro- and nitrate compounds[20]. The results obtained show a "blue" shift of the absorption band in polycrystalline samples as compared to the solutions of these substances. The theory states that the energy gap for n-π^* and π-π^* transitions is determined by dipole-dipole and orbital interactions. The experimental value of the shift, 0.2~0.3eV or 1.88×10^4J/mol, allows us to conclude that the energy of the intermolecular orbital interactions, as well as the energy of dipole-dipole interactions shoud be included in the total energy of crystal structure since this energy accounts for the motif of molecule packing in a crystal.

4 CONCLUSIONS

Polynitrocompounds are a unique class of compounds and the rules affecting their crystal structure are mainly determined by the electronic structure of the molecule. A dense crystal must not necessarily be constructed from dense molecules; an additive scheme of building up a crystal volume suits well to the molecular crystal whose the structural energy is represented by Van der Waals energy. A contribution of coulomb energy to the structural energy of the polynitrocompounds is rather high. It is 20～40% of the total energy. We must also take into account the energy of the dipole-dipole and orbital intermolecular interactions.

The examples of intermolecular interactions of lone electron pairs on oxygen and haloid atoms in molecules of alkoxydiazen-N-oxide and in haloid-derivatives of 1,1,4,4-tetranitrobutanediol-2,3 presented in this review show that such interaction make the molecule dense, decrease charge distribution on the atomic orbital centres; this, in its turn, decreases the electrostatic repulsion of the neighbouring molecules and increases the density of the crystals more appreciably than that from the additive scheme.

The intermolecular orbital interactions between the high occupied orbital of one centre of the molecule and the vacant orbital of another centre of the molecule would give rise to charge transfer, thus lowering the total localization of the levels and causing inhomogeneity in the charge distribution on the nitro groups. All this, in its turn, enhances repulsive interactions between molecules and decreases intermolecular orbital interactions. This explains a sharp retardation of the growth of crystal density of 1,4-dihaloid-1,1,4,4-tetranitrobutanediol-2,3 with the increase of the haloid atomic number.

The investigated compounds were synthesized in the Institute of Chemical Physics in Chernogolovka: alkoxydiazene-N-oxides were synthesized by Zyuzin. 1,1,4,4-tetranitrobutanediol-2,3 and derivatives were synthesized by Fedorov; UV-spectra were studied by Leksina and quantum-chemical calculations were performed by Trofimova.

Table 1 Charge distribution in the orbitals of a four-atom fragment

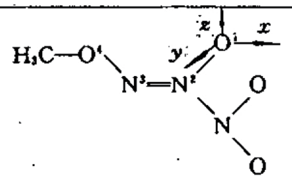
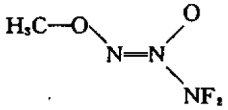
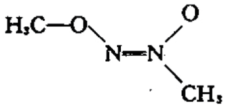
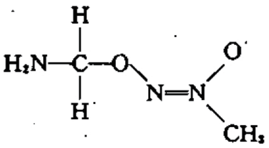
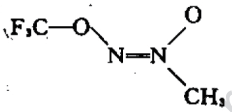
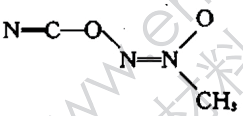
Molecules		O^1	N^2	N^3	O^4
	Σ	−0.1632	+0.1286	−0.0324	−0.1450
	2s	+0.0904	+0.5327	+0.2747	+0.1530
	p_x	+0.1310	−0.0429	+0.1900	+0.0069
	p_y	−0.5260	−0.2879	−0.2448	+0.0900
	p_z	+0.1412	−0.0774	−0.2548	−0.3967
	Σ	−0.1814	+0.1072	−0.0500	−0.1520
	2s	+0.0883	+0.5342	+0.2738	+0.1542
	p_x	+0.1000	−0.0636	+0.2002	−0.0022
	p_y	−0.5199	−0.2810	−0.2716	+0.0867
	p_z	+0.1500	−0.0863	−0.2551	−0.3922
	Σ	−0.2068	+0.0540	−0.0825	−0.1653
	2s	+0.0901	+0.5357	+0.2722	+0.1561
	p_x	+0.0601	−0.1199	+0.2127	−0.0204
	p_y	−0.4878	−0.2616	−0.3126	+0.0838
	p_z	+0.1298	−0.1044	−0.2561	−0.3865
	Σ	−0.2047	+0.0550	−0.0853	−0.1699
	2s	+0.0902	+0.5362	+0.2736	+0.1566
	p_x	+0.0603	−0.1195	+0.2112	−0.0218
	p_y	−0.4851	−0.2622	−0.3155	+0.0863
	p_z	+0.1288	−0.1037	−0.2573	−0.3920
	Σ	−0.1803	+0.0663	−0.0830	−0.1906
	2s	+0.0918	+0.5363	+0.2661	+0.1541
	p_x	+0.0607	−0.1305	+0.2357	−0.0354
	p_y	−0.4464	−0.2449	−0.3611	+0.0931
	p_z	+0.1125	−0.0987	−0.2263	−0.4040
	Σ	−0.1531	+0.0741	−0.0616	−0.1366
	2s	+0.0939	+0.5342	+0.2478	+0.1686
	p_x	+0.0615	−0.1430	+0.2738	−0.0330
	p_y	−0.4020	−0.2290	−0.4120	+0.1210
	p_z	+0.0924	−0.0922	−0.1733	−0.3949

Table 2 Crystal densities of the studied compounds

Compounds	ρ(g/cm^3)
$(NO_2)_2HCCH(OH)CH(OH)C(NO_2)_2H$	1.816
$F(NO_2)_2CCH(OH)CH(OH)C(NO_2)_2F$	1.945
$Cl(NO_2)_2CCH(OH)CH(OH)C(NO_2)_2Cl$	1.992
$Br(NO_2)_2CCH(OH)CH(OH)C(NO_2)_2Br$	2.369
$F(NO_2)_2CCH(ONO_2)CH(ONO_2)C(NO_2)_2F$	2.047
$Cl(NO_2)_2CCH(ONO_2)CH(ONO_2)C(NO_2)_2Cl$	2.013
$Br(NO_2)_2CCH(ONO_2)CH(ONO_2)C(NO_2)_2Br$	2.362

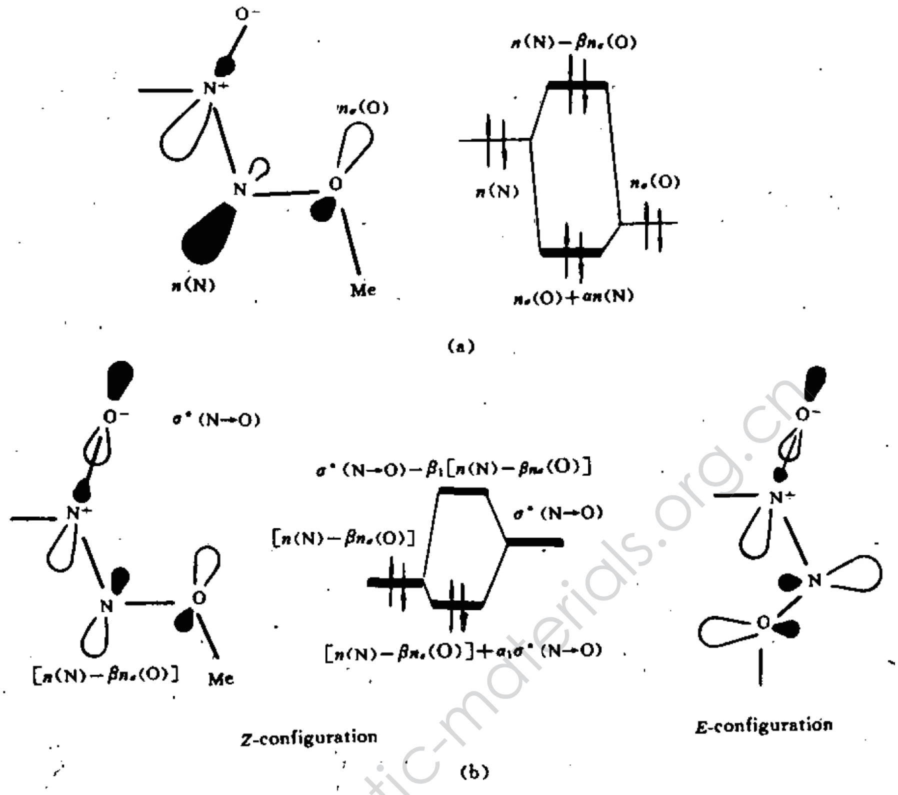


Fig. 1 Orbital interaction $n(N)-n_e(O)$ (a) and $[n(N)-\beta n_e(O)]-\sigma^*(N-O)$ (b) in a diazenoxide fragment. Two-level scheme ($\alpha,\beta,\alpha_1,\beta_1<1$)

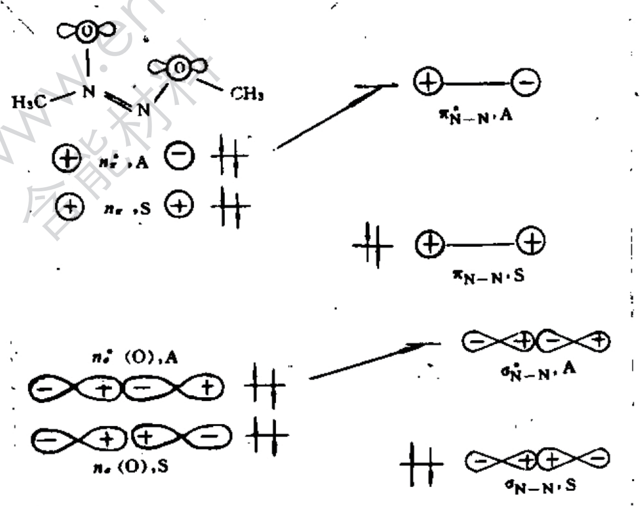


Fig. 2 Orbital interactions between lone electron pairs of two oxygen atoms in the diazenoxide fragment

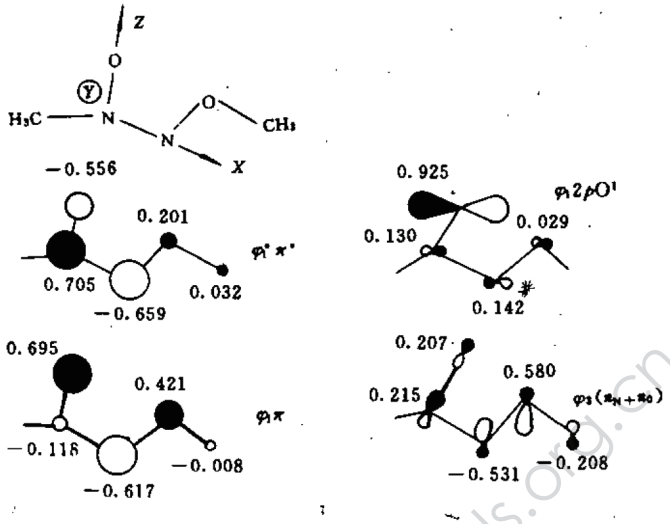
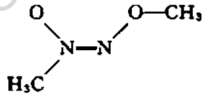


Fig. 3 Distribution of high occupied and low vacant MO's

in a four-atom fragment of molecule



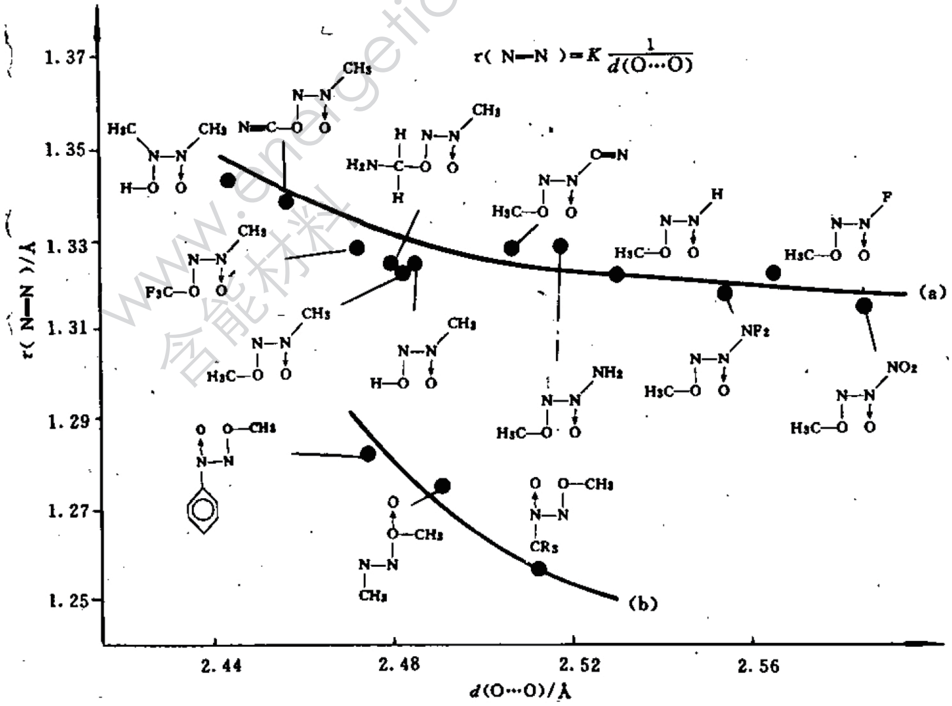


Fig. 4 Plot of N—N bond length as a function of O···O distance (Å) for asymmetric molecules; calculated (a) and experimental (b)

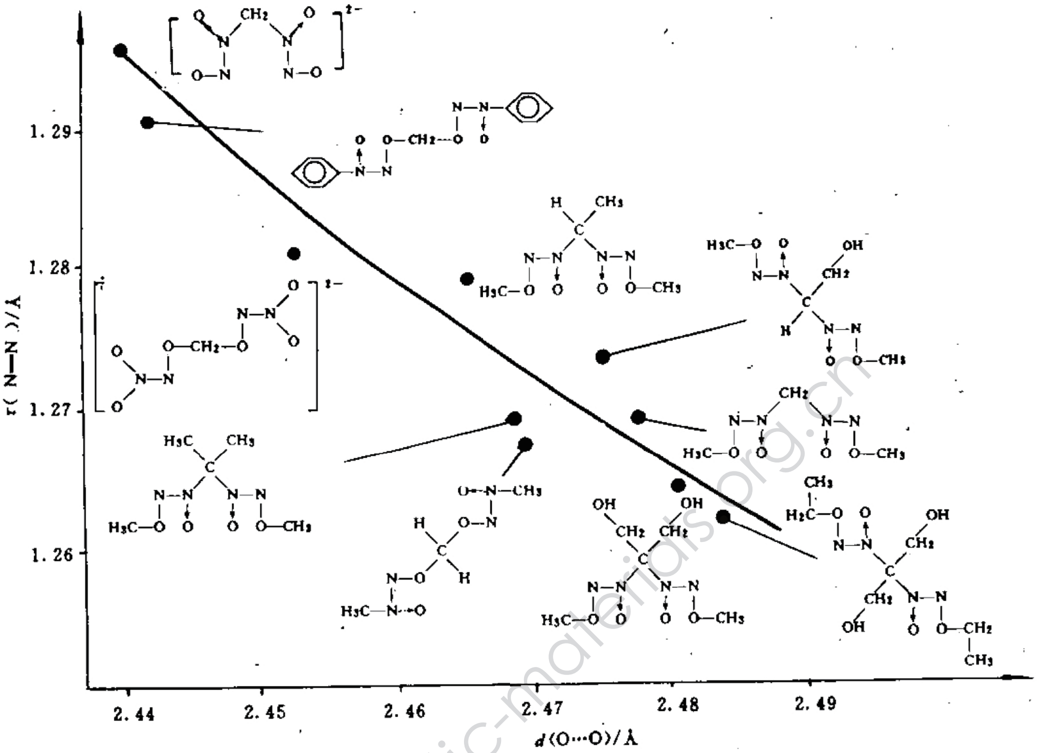


Fig. 5　Expermental plot of N⋯N bond length as a function of O⋯O distance (Å) for symmetric molecules

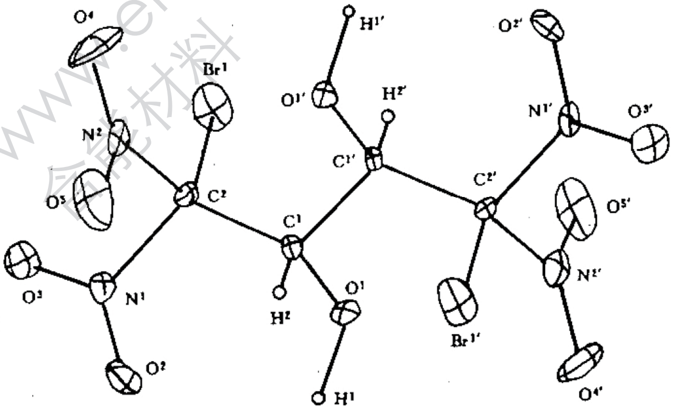
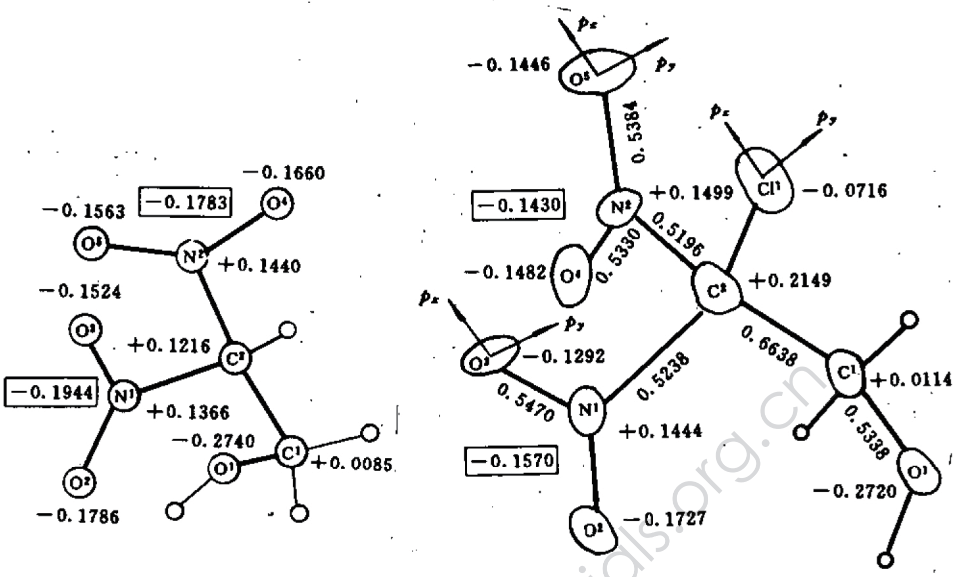


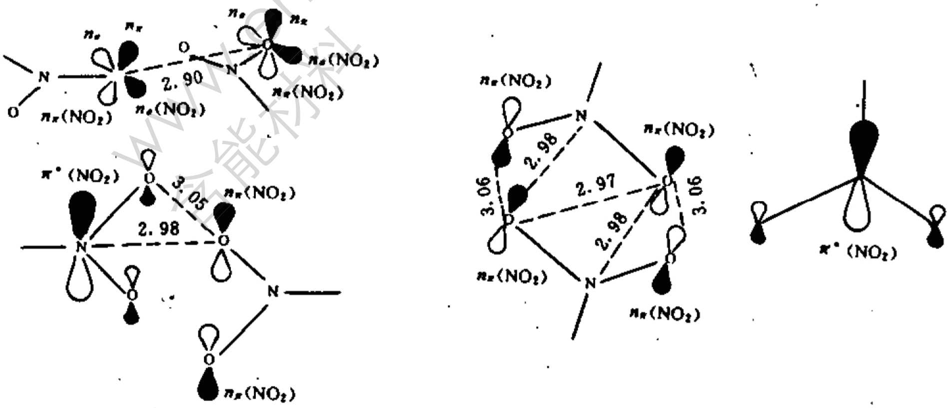
Fig. 6　Structure of a 1,4-dibromo-1,1,4,4- tetranitro-butanediol-2,3 molecule.

In molecules of 1,4-dihaloid-1,1,4,4-tetranitrobutanediol: r(C—N)=1.549～1.558(8)(Br); 1.533～1.550 (4) (Cl); 1.535～1.540 (4) (F); 1.502～1.504(3) (H) Å, r(C—Hal) =1.866(5)(Br)[1.91]; 1.707(2) (Cl)[1.76]; 1.319(2)(F) Å, r(O⋯Hal)=2.92(Br); 2.78(Cl); 2.49 (F) Å



(a) (b)

Fig. 7 Electronic parameters for molecules of 2,2-dinitroethanol (a) and 2-chloro-2,2-dinitroethanol (b) (total charge on nitrogroups is given in brackets; for structures RC(NO$_2$)$_2$CH(OH)CH(OH)C(NO$_2$)$_2$R the mean values of O⋯O intermolecular contacts: R=Br, r=3.053 Å; R=Cl, r=3.089 Å; R=F, r=3.086 Å; R=H, r=3.106 Å



(a)

(b)

Fig. 8 Variants of orbital interactions between the nitrogroups of the neighbouring molecules for the structure of 1,1,4,4-tetranitrobutanediol-2,3 (a) and 1,4-dichloro-1,1,4,4-tetranitrobutanediol-2,3 (b)

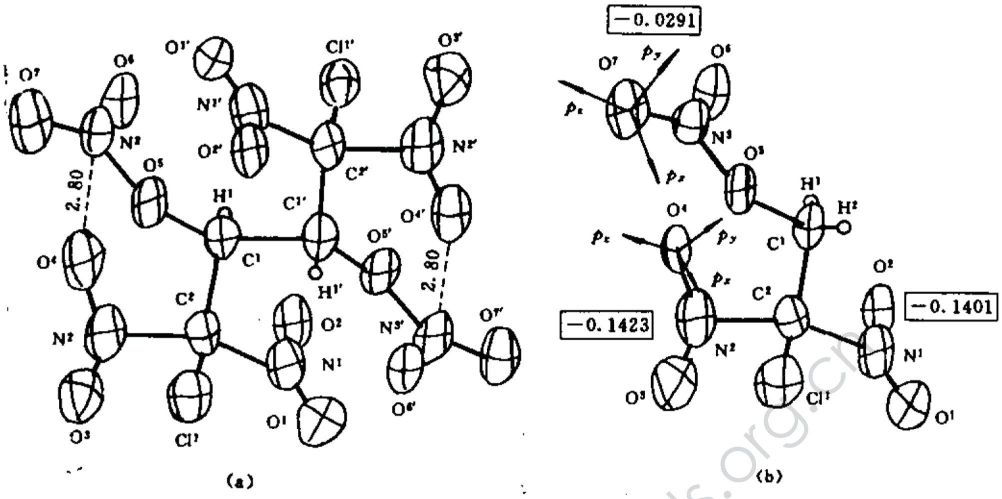


Fig. 9　Molecule of 1,4-dichloro-1,1,4,4-tetranitrobutanediol-2,3 nitrate (a) and electronic parameters of 2-chloro-2,2-dinitroethanol nitrate molecule (b). (In molecules of 1,4-dihaloid-1,1,4,4-tetranitrobutanediol-2,3 dinitrates a short O⋯N contact is shortened with increase of the haloid atomic number: 2.85(F); 2.80(C1); 2.72(Br). *ab initio* calculations r (O⋯N) = 2.757 Å, MMX r(O⋯N) = 4.20 Å)

REFERENCES

1 Atovmyan L O, Gafurov R G, Golovina N I, Eremenko L T. Dokl. Akad. Nauk SSSR, 1978, 241(5): 1080

2 Andrianov V I, Atovmyan L O, Gafurov R G, Golovina N I, et al. Zhurn. Strukt. Khimii, 1980, 21(5): 108

3 Atovmyan L O, Golovina N I, et al. Izv. Akad. Nauk SSSR, Ser. Khim., 1985 (5): 1023

4 Zhitomirskaya N G, Eremenko L T, Golovina N I, Atovmyan L O. Izv. Akad. Nauk SSSR, Ser. Khim., 1987(3): 576

5 Golovina N I, Atovmyan L O, et al. Zhurn. Strukt. Khimii, 1990, 31(1): 126

6 Atovmyan L O, Golovina N I, et al. Zhurn. Organ. Khimii, 1988, 26(9): 1848

7 Kitaigorodskii A I. Molekul. Kristally. Moscow: 1971.

8 Atovmyan L O, Golovina N I, Zyuzin I N. Izv. Akad. Nauk SSSR, Ser. Khim., 1987(6): 1309

9 Cherepinskii-Malov V D, Mukhamedzyanov A S, Andrianov V G, Marchenko G A. Zhurn. Strukt. Khimii, 1983, 24(1): 164Z

10 Hickmann E, Hadicke E, Rether W. Tetrahedron Lett., 1979(26):2457

11 Marchenko G A, Chertanova L F, Stryuchkov Yu T, Buzykin B I. Izv. Akad. Nauk SSSR, Ser. Khim., 1987(8):1777

12 Marchenko G A, Chertanova L F, Antipin M Yu, Stryuchkov Yu T, et al. Dokl. Akad. Nauk SSSR, 1987,294(5):1169

13 Chertanova L F, Marchenko G A, Kovalenko V I, Stryuchkov Yu T. Izv. Akad. Nauk SSSR, Ser. Khim., 1988(11):2516

14 Epiotis N D. J. Amer. Chem. Soc., 1973,95(10):3087

15 Sheppard W A, Sharts C M. In: Organic Fluorine Chemistry. New York: W. A. Beniamin Inc., 1969.

16 Fedorov B S, Golovina N I, Barinova L S, Trofimova R F, Arakcheeva V V, Atovmyan L O. Izv. Akad. Nauk SSSR, Ser. Khim., 1991(4):830

17 Fedorov B S, Golovina N I, Barinova L S, Arakcheeva V V, Trofimova R F, Atovmyan L O. Izv. Akad. Nauk SSSR, Ser. Khim., 1991(10):2372.

18 Fedorov B S, Golovina N I, Arakcheeva V V, Shilov G V, Atovmyan L O. Izv. Akad. Nauk SSSR, Ser. Khim., 1992(3):671

19 Fedorov B S, Golovina N I, Arakcheeva V V, Barinova L S, Trofimova R F, Galkin P V, Atovmyan L O. Izv. Akad. Nauk SSSR, Ser. Khim., 1992(3):664

20 Golovina N I, Leksina L N, Trofimova R F, Atovmyan L O. Zhurn. Strukt. Khimii, 1988,29(2):172