Study of Nitro Factor Dislodgement in Fox-7

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Abstract

Since FOX-7 (1, 1-diamino-2, 2-dinitroethylene) is a relatively new energetic material, little is known about its physical and chemical properties. Therefore, first-principles quantum chemical calculations are used to predict the energies of atoms of FOX-7. Under gentle heating (thermolysis) is likely to cause hydrogen transfer between molecules, producing highly reactive chemical species. Conversely, rupture of a C-nitro bond (resulting in the production of NO_2) requires a large amount of energy, suggesting that this reaction is more likely to occur when the explosive has been subjected to shock or impact. The FOX-7 molecule consists of nitro (-NO_2) and amino (-NH_2) functional groups attached to a carbon (C-C) backbone. The close proximity of amino hydrogens to nitro oxygens has prompted speculation that the stability of FOX-7 is due to hydrogen bonding within the molecule. However, part of the increased stability can be attributed to other electronic effects. It is well known that the presence of amino groups tends to desensitize nitro-aromatic molecules to shock or impact initiation. In this research, based on scan calculations fox-7 did that. On the basis of calculations of the scan in order to dislodge fox-7 was operating Nitro. And check of the molecule energy changes accepted. This operating Nitro dislodge was carried out in two ways. So as a result we reached two independent. These two results help us properties of the fox-7 molecules and the same acetylene discovered.

Keywords: AIM, Scan, Dislodge, Fox-7.

1. Introduction

Fox-7 molecule (fig1) has numerous applications in the field of military weapons. This molecule has the closed formula $C_2H_4N_4O_4$. This Density is 1/885 g/cm^3 , molecular weight of 148/08 g , and the boiling point it to 238 degrees of Celsius. The name of this molecule in the naming method I.U.P.A.C. is "1, 1-diamino-2, 2-dinitroethylene". Fox-7 is a non-sensitive chemical compound. This property is very similar to the properties of explosives, which has great prominence in this field. The production of Fox-7 has been very expensive and it is not economical to commercial production. But according to its military applications, it has been very attractive for military research centers. This combination, the first time in the mid 90's was identified and synthesized in Defense Sciences Research Institute in Sweden. Since then it been has taken into a wide range of researches.
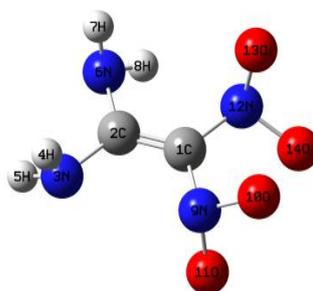
Fig 1. View Fox-7 structure.

2. Computational details

Depending on what theory of calculations is aimed, choosing the appropriate chemical model (based on method and pattern) could be different. Almost, nearly 300 kinds of the different patterns of family foundations have been created. That is merely for certain purposes. All calculations were calculated with Gaussian 03 software. In this study, we report new quantum chemical calculations for geometry optimization using Density Functional Theory (DFT) method B3LYP and valence double-zeta basis set augmented with both diffuse and polarization functions (aug-cc-pVDZ). The main aim of the present study was to theoretically investigate the property of transition state form of nitro scan in Fox-7 in order to understand its bond interaction behaviors. The major classification of bond interaction, in the framework of QTAIM has been proposed based on the sign of Laplacian of electron density ($\nabla^2\rho b$) and total energy density (Hb) evaluated at the Bond Critical Points (BCPs), fig 2. Hb is sum of the kinetic energy density (Gb) and electronic potential energy density (Vb) at a BCP.
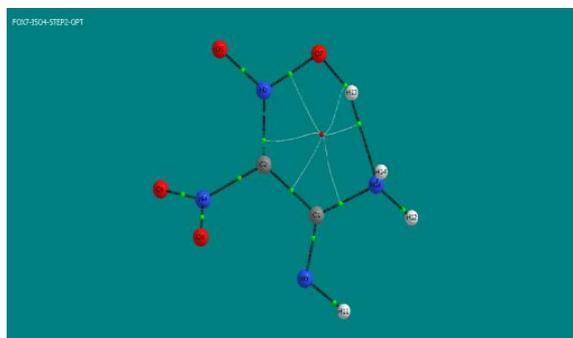
Fig 2. AIM image of Fox-7.

3. Results and discussion

3-1. FOX-7 scanning calculation of NO₂ factor and its dislodgement

 The scanning of optimized FOX-7 molecule was run with freezed angles of NO_2. Chart 1 shows that the beginning of the calculation in terms of zero energy molecule. In this state the distance of the NO_2 factor with molecule is 1.4 Å. Then scan with different stages of this energy is increased to 5.5. The slope of chart reduced and enhanced it with a very gentle slope will be the end when the reaches distances of 10 Å finds that most of the energy is equal to 102.5736 kcal/mol mode base compared to the base case. So the transition mode and product molecules will be equal.
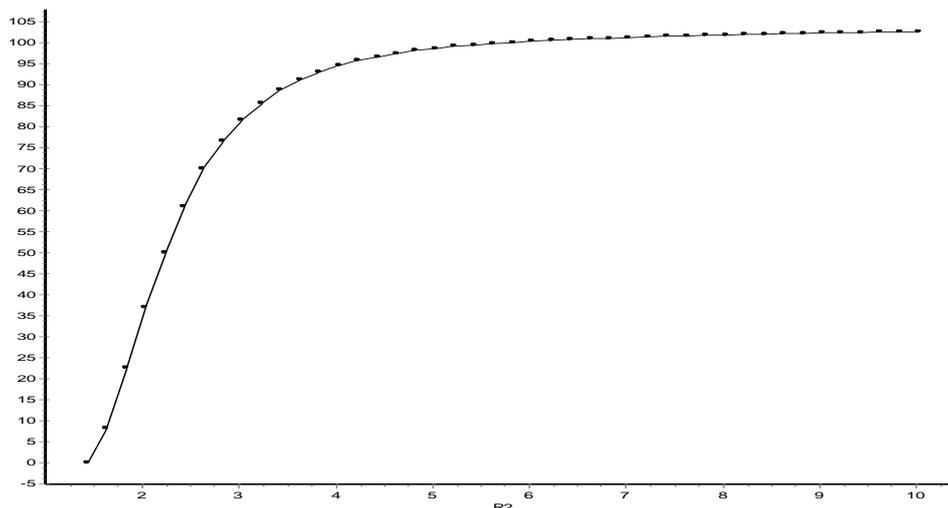
Chart 1. Potential energy surface diagram in the Fox-7 calculation scanning
(relative energy in kcal/mol)

3-2 The evaluation of hydrogen bonds in the Fox-7

The atoms of 1C and 9N placed under the command scan with 43 step of scan and distance of 0.2 Å. Then the angle of the 9N and 2N and 1C fixed and put the atoms we under scan, fig3. You must notice that in this case, unlike the previous mode the default scan is not considered completely.

View to be that alternative NO_2 After the initial stages Under the influence of the hydrogen bonds H5-O11 Gone to the back of the molecule and the distance molecules according to 0.2 Å added following up on the stage to 22 Step in.
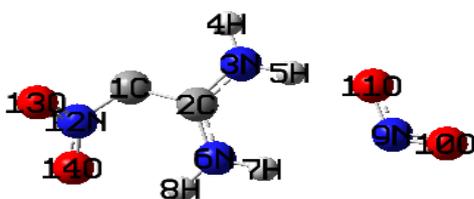
Figure 3: Distance of between the H_5-O_{11} bond by scan.
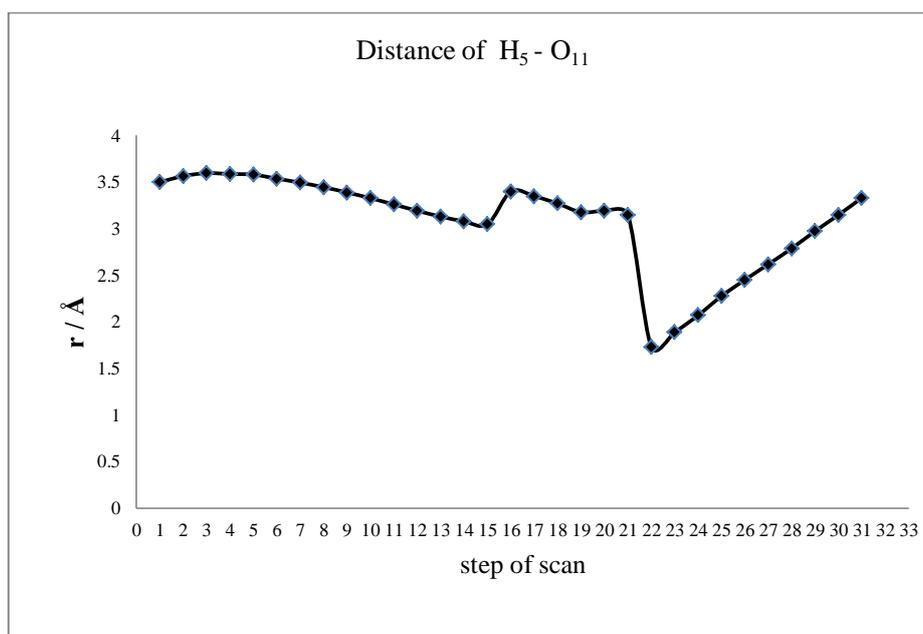
Chart 2: Distance changes of H_5-O_{11} at FOX-7 by scan.

Chart 2 shows the reduce of distance between H_5 and O_{11} to 1.729 Å in 22nd step of the scan, that it is reveals intermolecular hydrogen bond.
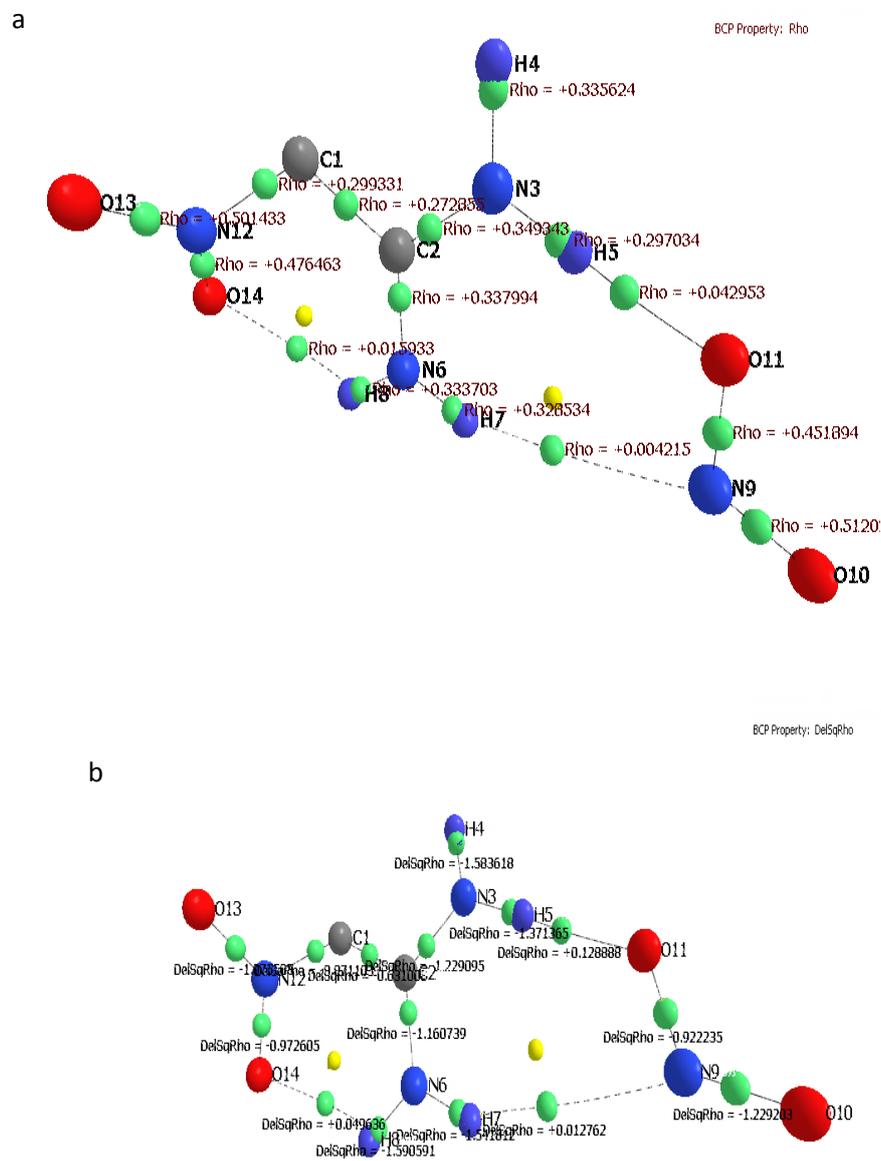
Figure 4: The AIM images of the 22th stage of the FOX7 molecules

a. Rho

b. ∇ ρ

The Figure 4 shows 22nd step of bond between C_1 and N_9 at Fox-7 after rotation of group N9 O10) ON_2 (O11, between H_5 and O_{11} the hydrogen bonds within the molecule elaborated by 10 -2 has been established, in the range Rho=0.042953, $\nabla^2\rho_b = +0.128888$.

3-3 The AIM calculations to compare the energy of atoms in FOX-7 and Dislodge isomer

In this case as well as in previous mode, FOX -7 and dislodge isomers and their TS by the AIM theory were studied and compared with ab initio methods, respectively. In the table 1 changes in atomic energy shown for the transition modes, initial materials and products. In this case, since the product has reached the highest level of energy to scan mode, so this have not the TS mode because the product and the TS will be same.

Table1: Atomic Energy for reactive and product in the conversion of FOX-7 to Dislodge isomer.

Atom	ISO1	TS	E(TS)–E(ISO1)
C1	-3.7701622068E+01	-3.7751825522E+01	-0.05020346
C2	-3.7414757731E+01	-3.7449779212E+01	-0.03502148
N3	-5.5425596835E+01	-5.5403276635E+01	0.02232020
H4	-3.7517740534E-01	-3.9919254926E-01	-0.024015143
H5	-4.2284729496E-01	-4.1646917809E-01	0.0063781169
N6	-5.5425077539E+01	-5.5404425063E+01	0.02065247
H7	-4.2284710726E-01	-4.1928444481E-01	0.0035626624
H8	-3.7508551017E-01	-3.8755992537E-01	-0.012474415
N9	-5.4435340541E+01	-5.4214594699E+01	0.22074585
O10	-7.5486034902E+01	-7.5439160678E+01	0.04687423
O11	-7.5510598824E+01	-7.5448159448E+01	0.06243938
N12	-5.4435601055E+01	-5.4578731975E+01	-0. 14313092
O13	-7.5486092961E+01	-7.5466943595E+01	0.01914937
O14	-7.5510673757E+01	-7.5483459822E+01	0.02721393
AIM Total energy	-598.4273535		-598.26286275
Ab initio	-598.4273557		-598.2635020
a.u. Δ(AIM- Abinitio)	0.0000022		0.00063925
kcal/mol	0.0013805		0.40113544

On the basis of the following form, In turn of the Fox-7 molecule into a state scanning and separating the NO_2 factory group, nitrogen atoms (N_9) in this factory group the greatest will increase energy and because the oxygen attached to this factory group will increase a lot of energy, so the NO_2 factory group isolated from the carbon atom to a lot of instability appeared.

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While nitrogen atoms (N_{12}) in the vicinity of the NO_2 factory group with reduce energy and in the absence of these factor into the consistency group finds. Of course, this decrease and increase the sustainability of the show that finally dislodge the NO_2 factory groups causing instability and instability in the molecule will be and return to the initial mode tends to molecules.

(ISO₄)

(ISO₁)
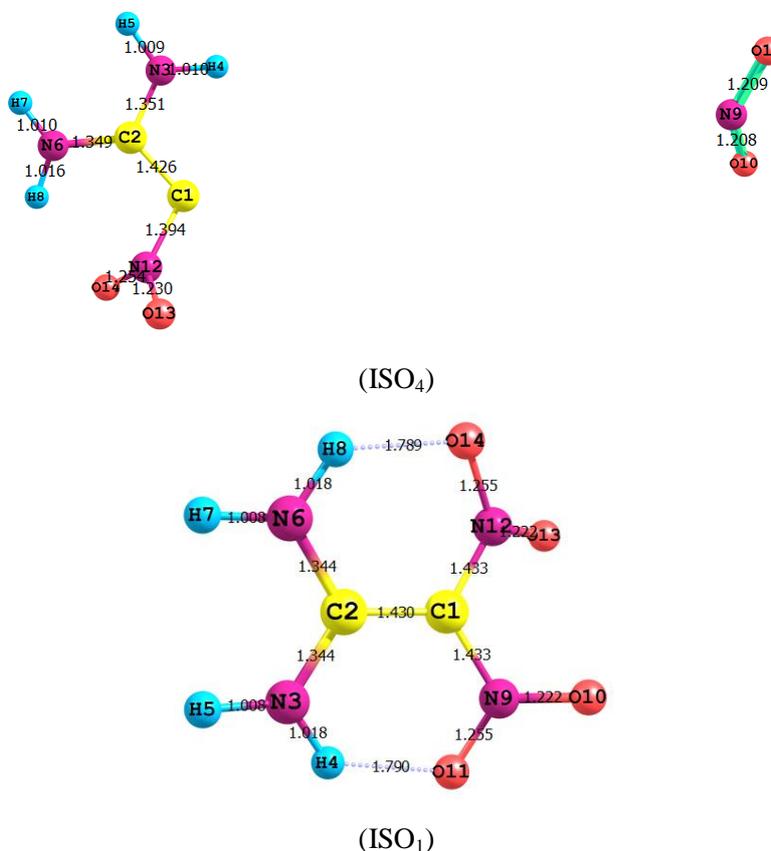
Figure4. The geometric product specifications and reactive in the conversion of Fox-7 to Dislodge isomer, the length of the link by Angstrom and according to their degree of bond angles

4. Conclusion

Comparison between molecules of Fox-7 and isomer Dislodge showed that dislodge a NO_2 factor group cause a lot of instability in the molecule. -The study of the molecule under 22 and 232 stages of calculations of the scan. We observe that the alternative NO_2 back completely gone molecule And Completely under the influence of the hydrogen bonds between the H5-O11-H7, and from now on the length of will be added to the side of the bond. Intermolecular hydrogen bonds so therefore in this calculation are the main role of this molecule in sustainability has played.

Acknowledgment

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