عنوان مقاله:
Study of Nitro Factor Dislodgement in Fox-7

محل انتشار:
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خلاصه مقاله:
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 NO2) 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 (-NO2) and amino (-NH2) 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.

کلمات کلیدی:
AIM, Scan, Dislodge, Fox-7