

A Novel Mechanism of Thermal Decomposition of 1,2-Diamino-1,2-Dinitroethylene (FOX-7): New Insights from High-level Quantum Chemical Calculations

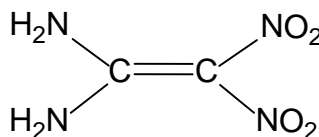
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1,1-diamino-2,2-dinitroethylene (DADNE, FOX-7) is a new promising high-performance insensitive energetic compound [1-2]. Kinetics and mechanism of thermal decomposition are crucial for understanding the sensitivity and performance of this species. However, even though the thermal decomposition of DADNE under various conditions has been intensively studied experimentally, there are still some contradictory assumptions concerning the initial reactions of its thermolysis. The C-NO₂ bond dissociation reaction, nitro-nitrite and nitro-aci-nitro isomerization have been widely discussed as possible primary channels of thermal decomposition of the title compound.



DADNE

The highly accurate CCSD(T)-F12 computations revealed that *none* of these reactions dominate the thermolysis of DADNE. On the contrary, we propose the two competing primary reaction channels which have never been discussed before. The rate-limiting step of DADNE thermal decomposition is the H-transfer from the amino group to a carbon atom yielding an amino-imino derivative of dinitroethane. Only a slightly higher activation barrier was found for cyclization to oxazete-N-oxide which is prone to fast subsequent molecular decomposition.

The calculated values of effective activation energy of DADNE decomposition are in perfect agreement with the experimental data available. We also compared the decomposition mechanism of the title species with the relevant case of triaminotrinitrobenzene (TATB), another insensitive high-energy compound which is widely used in applications.

[1] Latypov, N.V.; Bergman, J.; Langlet, A. et al. *Tetrahedron*, 54: 11525-11536, 1998.

[2] Jalovy, Z.; Ek, S.; Ottis, J. et al. *J. Energ. Mat.*, 31: 87-99, 2013.