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Thematic course: About some primary reactions of thermolysis of 1,1-diamino-2,2-dinitroethylene (FOX-7) revealed by DFT calculations. Part 1.

Direct hydrogene transfer to nitro group

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Abstract

Primary thermolisys reactions of 1,1-diamino-2,2-dinitroethylene (DADNE, FOX-7) which is one of perspective energetic materials are considered. Recently synthesised, it has some suitable detonation characteristics: high thermal stability, low sensitivity to blow and friction. So it has been intensively studied, especially with respect to its thermal stability. Some competing reactons of first thermolysis stage have been investigated: nitro group abstraction, rearrangment of nitrogroup to nitrite group, transfer of oxigen and hydrogen on vicinal carbon atoms. In present work the hydrogen transfer on oxigen atom of nitrogroup, which is one of possible first stage reactions of FOX-7 thermolysis is considered by means of quantum chemistry methods. Reaction modelling is performed in gas phase with DFT PBE/cc-PVDZ method. It was shown that beside well-known reaction path there is low activation barrier (34,8 kcal/mole) direct hydrogen transfer, which is conducted by confornmational change of hydrogen atom going it oppisite direction of disappearing aminogroup. Without the conformational change this transfer is impossible due to atoms being close and N-H bond is stronger than N-O so reverse reaction takes place without activation. As a result of this route at the first stage an aggresive acid product is formed and then could cause decay of DADNE molecules. This acid could further transform causing secondary products arising (e.g. two-base acid, water etc.) playing part in secondary thermolysis reactions of FOX-7.

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