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## Quantum Chemical Study on Effects of Intermolecular Interactions in FOX-7 Clusters on the Dissociation of FOX-7

LI Xiao-dong, XU Zhe, YAN Xiang, LIU Lei, WANG Heng, WANG Jing-yu

(School of Chemical and Environmental Engineering, North University of China, Taiyuan 030051, China)

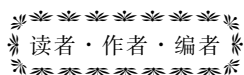
**Abstract:** Four kinds of gas clusters of 1, 1-diamino-2, 2-dinitroethene (FOX-7) were obtained by using RI-B2PLYP-D3 and PW6B95-D3 methods with dispersion correction density functional theory. On this account, the existing state of FOX-7 molecules in the crystal structures was simulated. The electron density difference of the neighboring molecules in the process of cluster formation was plotted, and the formation and origin of intermolecular interactions were explained from the point of view of electron density change. The effect of intermolecular interaction of condensed phase FOX-7 on the dissociation mechanism of FOX-7 was investigated. Results show that the intermolecular interactions are due to the partial intermolecular sharing of electrons formed by electron offsets in the FOX-7 clusters. The formation of intermolecular interactions also weakens the chemical bonds in some molecules, resulting in a change in the cleavage channel of FOX-7. Compared with the unimolecule state, the intermolecular interaction makes the cleavage activation energy of C—NO<sub>2</sub> bond in FOX-7 clusters reduce generally when PW6B95-D3 theory is used. Because of different angles of molecular interaction in different clusters, the process of nitro isomer has changed, compared with the unimolecule, the activation energy of nitro isomer channels of cluster II decreases by 210.9 kJ · mol<sup>-1</sup>, and the activation energy of nitro nitro isomer channel of cluster IV increases by 39.4 kJ · mol<sup>-1</sup>.

**Key words:** 1, 1-diamino-2, 2-dinitroethene (FOX-7); dissociation; clusters; intermolecular interaction; electron density differences

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含能共晶是不同含能分子通过氢键等相互作用力形成的具有稳定结构和性能分子晶体。含能共晶充分组合了单质含能分子的优点, 呈现出感度低, 综合性能优良的特点, 具有潜在的应用前景, 共晶研究已经引起国内外含能材料学界的高度关注。为推动含能共晶的研究和交流, 本刊特推出“含能共晶”专栏, 主要征稿范围包括含能共晶晶体设计与性能预测、含能共晶的制备、结构解析、性能等。来稿请注明“含能共晶”专栏。

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