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

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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_2 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^{-1}, and the activation energy of nitro nitro isomer channel of cluster Ⅳ increases by 39.4 kJ·mol^{-1}.

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