Theoretical Studies for THz Spectra of CL-20/HMX Cocrystal

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Abstract：The improvement of physicochemical properties of explosives by the way of cocrystallization has become a research hotspot in the field of energetic materials, the formation of cocrystal explosive is mostly driven by the intermolecular interactions, and their energy level transitions are located in the detection range of THz spectra. In this work, taking hexanitrohexaazaisowurtzitane(CL-20)/cyclotetramethylenete-tranitramine(HMX) cocrystal as the model system, the THz spectra of cocrystal components β-HMX, CL-20, and CL-20/HMX cocrystal were theoretically studied by combining the methods of molecular dynamics simulation and quantum mechanics. The assignment and analysis of vibration modes for characteristic peaks were carried out. The response of different intermolecular interactions in THz spectra was confirmed. Results show that compared with the cocrystal components CL-20 and HMX, the new characteristic absorption peaks of CL-20/HMX cocrystal located at 0.25, 0.49, 1.1, 1.47, 1.73, 2.27 THz and 3.7 THz respectively are found. Among them, the absorption peaks at 1.1, 1.47 THz and 1.73 THz are caused by intermolecular C—H···O hydrogen-bond, whereas the absorption peak at 1.73 THz is mainly assigned as the heterogeneous intermolecular hydrogen bonds.

Key words：hexanitrohexaazaisowurtzitane(CL-20)/cyclotetramethylenete-tranitramine(HMX) cocrystal；Terahertz(THz) spectrun；hydrogen bond

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