Theoretical Study on Thermodynamic Stability and Detonation Performance of CL-20 and Its Cocrystal

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Abstract: Based on the first-principle software developed by ourselves, the thermodynamic stability, mechanical properties, and detonation performances of structure for hexanitrohexaazaisowurtzitane(CL-20) explosive with five crystallline phase, benzotrifuroxane(BTF) crystal explosive and CL-20/BTF cocrystal explosive were studied. Results show that the electrostatic attraction effect of weak hydrogen bonds makes the intermolecular binding energy of CL-20/BTF cocrystal increase by 39% compared with that of hydrogen-free BTF crystal, which improves thermodynamic stability of cocrystal structure and significantly changes its mechanical properties, such as bulk modulus and sound speed etc. Although the BTF/CL-20 cocrystal and pure BTF crystal have the similar density, but due to the oxygen balance coefficient of the cocrystal has been optimized, so its detonation velocity and detonation pressure are improved by about 11% and 5%, respectively. Compared with the β-CL-20 crystal, the density and oxygen balance of the cocrystal are decreased, the detonation pressure and detonation velocity relatively decrease by about 15% and 6%, respectively. Design of a new type of insensitive cocrystal explosive should avoid the molecule with extremely weak strength covalent bonds and structure with characteristic peaks of high density vibration spectrum, thermodynamic stability effect of hydrogen bond on the molecular space packing should be effectively used, and the hydrogen element content should be moderately controlled to protect the high energy density of explosives.

Key words: hexanitrohexaazaisowurtzitane(CL-20); cocrystal; molecular interaction; macroscopic physical properties; detonation performance

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