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

ZHANG Lei<sup>1</sup>, ZHAO Yan-hong<sup>2</sup>, JIANG Sheng-li<sup>1</sup>, YU Yi<sup>1</sup>, WANG Xing<sup>1</sup>, ZHAO Han-yue<sup>1</sup>, LI Chong-yang<sup>3</sup>, CHEN Jun<sup>1,2</sup>

(1. CAEP Software Center for High Performance Numerical Simulation, Beijing 100088, China; 2. Laboratory of Computational Physics, Institute of Applied Physics and Computational Mathematics, Beijing 100088, China; 3. School of Materials Science and Engneering, Xiangtan University, Xiangtan 411105, China)

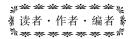
Abstract: Based on the first-principle software developed by ourselves, the thermodynamic stability, mechanical properties, and detonation performances of structure for hexanitrohexaazaisowurtzitane (CL-20) explosive with five crystallline phase, benzotrifuroxane(BTF) crystal explosive and CL-20/BTF 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  $\beta$ -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

CLC number: TJ55; O74; O641.12+1; O414

Document code: A

**DOI**: 10. 11943/j. issn. 1006-9941. 2018. 06. 001



## 《含能材料》"观点"征稿

为了丰富学术交流形式,及时传递含能材料领域同行们的学术观点和思想,《含能材料》开设了"观点"栏目。"观点" 栏目的来稿应观点鲜明、内容新颖、形式上短小精悍。欢迎含能材料各领域的专家积极来稿。来稿时请附个人简介及主要

《含能材料》编辑部