

高能体系分子间相互作用研究: 含NNO~2和NH~2混合物

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摘要 以abinitioHF/6-31G^{*}计算求得NH~3+NH~2NO~2的两种优化构型, 经MP4电子相关能校正和Boys-Bernardi方案校正基组叠加误差求得精确的分子间相互作用能。还用PM3方法计算研究TATB(均三氨基三硝基苯)分别与HMX(奥克托金)和RDX(黑索金)的混合体系, 经色散能校正电子相关近似地求得分子间相互作用能。结果表明, NH~3与NH~2NO~2之间的最大结合能为-38.32kJ/mol; 分子间相互作用增强了N-NO~2

键强度; TATB与HMX, RDX的结合能远大于石墨与HMX或RDX的结合能,

表明TATB对HMX和RDX的润湿和钝感作用较石墨更强。

关键词 [从头计算法](#) [氨](#) [亚硝酸铵](#) [均三氨基三硝基苯](#) [奥克托金](#) [黑索金](#) [结合能](#) [分子轨道方法](#) [混合炸药](#)

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A study on the intermolecular interactions in energetic systems: The mixtures containing NNO~2 and NH~2 groups

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Abstract Two fully optimized geometries of NH~3+NH~2NO~2 are obtained using the ab initio method at the HF/6-31G^{*} level, and the accurate intermolecular interaction energy is calculated using the MP4 electron correlation correction and the basis set superposition error correction by the Boys-Bernardi "counterpoise" protocol. In addition, the PM3 method is employed to study the intermolecular interactions of TATB (1, 3, 5-triamino-2, 4, 6-trinitrobenzene) with HMX (ocotogen) and RDX (hexogen). The intermolecular interaction energies with approximation of electron correlation correction by the dispersion energy are given. The computed results indicate that the greatest binding energy of NH~3+NH~2NO~2 is -38.32kJ/mol. The intermolecular interactions can strengthen the N-NO~2 bond. The binding energies of TATB with HMX or RDX are much larger than those between graphite and HMX or RDX. Therefore TATB can wet and desensitize HMX (or RDX) better than graphite.

Key words [AB INITIO CALCULATION](#) [AMMONIA](#) [HMX](#) [BINDING ENERGY](#) [MOLECULAR ORBITAL METHOD](#) [COMPOSITE EXPOLOSIVES](#)

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