[1]李丽洁,陈树森,冉军鹏,等.不同结晶体系中PNMAIW对HNIW 转晶影响的理论研究[J].火炸药学报,2009,(4):1-5.

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不同结晶体系中PNMAIW对HNIW 转晶影响的理论研

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Title: Theoretical Study of the Effect of PNMAIW on HNIW Crystal Transition in Different Crystal Systems

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关键词: 物理化学; 分子模拟; HNIW; PNMAIW; 动力学; 键合能

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摘要: 为了从理论上揭示五硝基 乙酰基六氮杂异伍兹烷（PNMAIW）对六硝基六氮杂异伍兹烷（HNIW）转晶的影响，采用分子模拟的方法，设计了PNMAIW的稳定构型，分别研究了硝酸 水体系、乙酸乙酯 正己烷体系和乙酸乙酯 三氯甲烷体系中PNMAIW对HNIW转晶的影响。结果表明，PNMAIW存在4种稳定构型；由于PNMAIW与HNIW各面的键合能远大于溶剂和非溶剂与HNIW各面的键合能，因此，如果转晶体系中存在杂质PNMAIW，PNMAIW更容易接近HNIW的晶面，从而阻碍HNIW在溶液中的转晶。

Abstract: In order to reveal the effect of PNMAIW on the crystal transition of HNIW theoretically, the stability configuration of PNMAIW was designed by the methods of molecular modeling. The effect of PNMAIW on the HNIW crystal in the system of nitric acid/water, ethyl acetate/n hexane, and ethyl acetate/chloroform, respectively, was studied. The results show that PNMAIW has four stable structures. The bonding energy of PNMAIW to the surface of HNIW is much larger than that of the solvent and the nonsolvent to the surface of HNIW, so the exist of PNMAIW in the crystal transition system would inhibit the formation of ε

HNIW crystal.

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