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硝化甘油与高分子黏合剂混合体系相互作用的理论

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Title: Theoretical Studies of Interreaction of Complex System Nitroglycerin Polymer Binder

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摘要: 运用MO PM3方法计算了硝化甘油（NG）与高分子黏结剂聚乙二醇（PEG）、端羟基聚丁二烯（HTPB）、缩水甘油叠氮基聚醚（GAP）、3 叠氮甲基 3 甲基环氧丁烷聚合物（AMMO）和3,3 双（叠氮甲基）环氧丁烷聚合物（BAMO）的混合模型体系的几何结构（聚合度n=1,2,3,4），由色散能校正电子相关近似求得其分子间相互作用能(ΔE)。结果表明，当n＝4时，5个混合体系的相互作用能为-49～-60kJ/mol。除GAP和BAMO以外，当n值增大时，混合体系的相互作用能增加。混合体系中，两个子体系的原子

Abstract: Geometrical structures of the supermolecular systems of nitroglycerin (NG) with polyethylene glycol (PEG), hydroyl terminated polybutadiene (HTPB), glycidyl azide polymer (GAP), poly(3 azidomethyl) 3 methyl oxetane(AMMO) and poly (3,3 bis (azidomethyl) oxetane) (BAMO) were optimized by the semiempirical molecular orbital theory PM3 method. Binding energies, after corrections for dispersion energies, were approximately obtained. The binding energies of five complex systems are -49kJ/mol to -60kJ/mol as polymerization degree n=4. When the polymerization degree increases, with the exception of NG with GAP and BAMO, the strengths of the intermolecular interactions of complex systems increase. In the complexes, the shortest intermolecular contacting distances

between two submolecules of the complexes are 0.270nm to 0.340nm.

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