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硝酸酯化合物生成热的分子轨道研究

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摘要 用MINDO/3, MNDO和AM1三种SCF-MO方法, 在全优化分子几何构型的基础上, 系统地计算研究了32个硝酸酯化合物的生成热, 与实验值相比, MNDO计算结果偏大很多; MINDO/3计算值与凝聚相实验值符合较好, 由于克服了MNDO法过高地估算原子之间Van der Waals核排斥能的缺点, AM1法给出了较满意的结果: 与七个气态实验值之间存在良好的线性关系(相关系数为0.992), 其间的平均绝对差值和平均差值分别只有10.28和-1.01kJ/mol。

关键词 生成热 分子轨道方法 MNDO 硝酸酯 MINDO-3 AMI

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The molecular orbital studies on heats of formation for nitrates

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Abstract The MINDO/3, MNDO and AM1 methods were used to calculate systematically the heats of formation for 32 nitric acid esters at their optimized mol. geometries. Compared to experimental values, the MNDO calculated results are much larger, and the MINDO/3 calculated results compare better the observed data in condensed phase. By correcting for the repulsive van der Waals energy among atoms the errors in MNDO were compensated and the AM1 calcns. give satisfactory results: there is a good linear relationship between AM1 calculated results and observed data in gas phase for 7 of the compounds, the linear correlation coefficient being 0.992. The average absolute difference and the average difference between the results are 10.28 and -1.01 kJ/mol, resp.

Key words FORMATION HEAT MOLECULAR ORBITAL METHOD NITRATE

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