

硝酸甲与硝酸乙酯的结构、振动频率和热力学性质的密度函数理论(DFT)研究

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摘要 用密度函数理论(DFT)的BLYP和B3LYP方法,取6-31G,6-31G^{*},6-31G^{**},6-311G,6-311G^{*}和6-311G^{**}六种基组,对硝酸甲酯和硝酸乙酯的几何构型和红外振动频率进行了计算研究.

结果表明,B3LYP方法在采用极化基组(6-31G^{*},6-31G^{**},6-311G^{*}和6-311G^{**})时计算得到的结果均较好,适用于硝酸酯类化合物的研究.而BLYP方法无论采用何种基组均不适用;运用校正后的B3LYP/6-31G^{*}频率(校正因子0.975)计算得到的热力学性质(C^o_p,H^o和S^o)与实验结果较吻合。

关键词 [硝酸甲酯](#) [硝酸乙酯](#) [热力学性质](#) [密度函数理论](#) [几何异构](#) [振动频率](#)

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Density functional theory(DFT) studies on molecular geometries IR frequencies and thermodynamic properties of methyl and ethyl nitrates

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Abstract The BLYP and B3LYP density functional methods and a series of basis sets,6-31G,6-31G^{*},6-31G^{**},6-311G,6-311G^{*} and 6-311G^{**},have been used to calculate the molecular geometries and infrared spectra of methyl and ethyl nitrates.It is shown that BLYP method is not suitable for calculating the geometry and IR frequencies of organic nitrates no matter what kind of basis set is used. While B3LYP calculations produce satisfactory results when polarization bases(6-31G^{*},6-31G^{**},6-311G^{*}and6-311G^{**}) are used.The standard thermodynamic functions calculated using the B3LYP/6-31G^{*} frequencies scaled by 0.975 are in good agreement with the available experimental results.

Key words [METHYL NITRATE](#) [ETHYL NITRATE](#) [THERMODYNAMIC PROPERTIES](#) [GEOMETRICAL ISOMERISM](#) [FREQUENCY OF VIBRATION](#)

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