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# 硝胺及其甲基衍生物的从头计算研究 **3:** 甲硝胺及其同位素衍生物的谐性力场和振动光谱

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摘要 用TEXAS从头计算程序,取STO-4-21G基组,计算了甲硝胺的谐性力场和振动光谱.
直接理论计算的谐性力场经由其他分子转移来的经验校正因子校正后,提供了甲硝胺振动基频的预测.
预测值和甲硝胺分子在气相中的振动光谱实验值之间的平均偏差为31cm^-1.
为了获得更合适的气相甲硝胺振动力场和预测它的同位素衍生物的振动光谱,我们优化了一组新的校正因子,
使理论值和实验值的平均偏差减为8.9cm^-1.用这组校正因子得到的力场预测了三个同位素衍生物的振动光谱,
其同位素位移的理论预测值和实验值符合良好.

关键词 从头计算法 振动光谱 甲硝胺 谐性力场

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## Studies on nitramide and its methyl derivatives with ab initio calculations. pt. 3:the harmonic force field and vibrational spectra of n-methylnitramine and its isotopic derivatives

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**Abstract** The harmonic force field and the vibrational spectrum of N-methylnitramine have been calculated by TEXAS ab initio program using a 4-21G basis set. The directly computed theor. harmonic force field was scaled with empirical scale factors which were transferred from other mols. to provide a prediction of fundamental frequencies. The average deviations between prediction and experimental spectrum of N-methylnitramine in gas phase were 31 cm-1. A new set of scale factors was optimized to give better force field suitable for N-methylnitramine in gas phase and available for prediction of vibrational spectra of its isotopic derivatives These scale factors reduced the average deviations to 8.9 cm-1. The vibrational spectra of three isotopic derivatives of N-methylnitramine have been predicted with the force field resulting from the optimized set of scale factors, and are in good agreement with their experimental data in gas phase.

**Key words** AB INITIO CALCULATION VIBRATIONAL SPECTRUM METHYL-NITRAMINE

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