MOLECULAR BEAM INFRARED SPECTRUM OF THE FIRST C-H STRETCHING OVERTONE REGION OF NITROMETHANE

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The first C-H stretching overtone region of nitromethane has been measured using a bolometer detected molecular beam machine with a resonance cavity. Nitromethane is an almost free rotor with a very low torsional barrier in the ground state. The purpose of this study is to find out whether the low 6-fold barrier of the ground state will turn to a much higher 2-fold barrier in the first stretching vibrational overtone of nitromethane with 2 quanta of stretching vibrational energy.[b] This might happen, if the vibrational energy would stay localised in one bond long enough compared with the period of internal rotation.

The spectrum of nitromethane has been measured in the wavenumber region 6047-6055 cm^{-1} with a resolution of 5MHz. As the rotational temperature is very low, only levels with the internal rotation quantum number m=0 and m=1 should be significantly populated. The spectrum has been assigned using ground state combination differences. Using a rigid rotor program the band center and the rotational constants have been obtained for the m=0 state. The analysis of the m=1 state is in progress.

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