MICROWAVE AND INFRARED SPECTRA OF URETHANE

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The rotational spectrum of urethane ($H_2NCO_2CH_2CH_3$) was investigated in the frequency range 5–20 GHz using a MB-MWFT spectrometer. The accurate values of rotational, centrifugal distortion and quadrupole coupling constants were determined for the two most stable conformers. Previous MW results from the literature [1] have been revised for conformer I. Additional measurements in the frequency range 50–150 GHz are in progress, using a conventional absorption spectrometer. Also the nuclear spin-spin interactions are studied from additional hyperfine splittings observed in the MWFT spectra.
The Fourier transform infrared spectra of urethane have been recorded in the 1000–1900 cm^{-1} region at a 0.1 cm^{-1} resolution in a supersonic jet seeded with argon. Maximum absorption signals are obtained by controlling the temperature of the compound and the argon flow. Preliminary bands assignments are proposed on the grounds of FTIR spectra analysis, conformational equilibrium and *ab initio* harmonic frequencies. In order to confirm these assignments, higher level *ab initio* calculations of the total electronic energy and anharmonic frequencies within the adiabatic approximation [2], for each conformer, are presently under way.

1. K. M. Marstokk and H. Møllendal, Acta Chem. Scandinavia 53 (1999) 329.
2. M. Goubet, B. Madebene and M. Lewerenz, Chimia 58 (2004) 291.

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