GROUND STATE ROTATIONAL SPECTRUM OF METHYL CARBAMATE BETWEEN 79 AND 371 GHz

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The room temperature rotational spectrum of methyl carbamate, CH_3OCONH_2, has been recorded between 79 and 371 GHz with the Fast Scan Submillimeter-wave Spectroscopic Technique (FASSST) spectrometer. Methyl carbamate, a structural isomer of the amino acid glycine, has a methyl group internal rotor giving rise to A and E internal rotor states. 6000 new transitions belonging to the vibrational ground state have been assigned, about half of them belonging to the E state. A speedy spectroscopic assignment has been made possible by the integration of the two program packages CAAARS and ERHAM. CAAARS is a program suite for visual, interactive mouse-assisted line assignment of asymmetric rotor spectra using Loomis-Wood diagrams [a] and ERHAM is a program that solves the effective rotational Hamiltonian for molecules with two periodic large-amplitude internal motions [b] that can be applied also to molecules with only one internal motion. This Hamiltonian has been used to fit 28 spectroscopic parameters for the methyl carbamate ground state to the observed transition frequencies. The constants determined reproduce the observed line positions with a standard deviation of 0.082 MHz.

[a] I. R. Medvedev, M. Winnewisser, B. P. Winnewisser, F. C. De Lucia, E. Herbst, J. Mol. Struct. 742, 229 (2005).
[b] P. Groner, J. Chem. Phys. 107, 4483 (1997).