HIGH RESOLUTION SPECTROSCOPY AND DYNAMICS OF THE METHANE MOLECULE: CH_2D_2 ISOTOPOMER

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Methane is an important prototype for intramolecular dynamics [1] and of relevance in a variety of spectroscopic contexts [2]. We measured the infrared spectrum of CH_2D_2 at 78 K in the range 2800 - 6600 cm^{-1} with the Zürich high resolution (up to 0.0007 cm^{-1}) Fourier transform interferometer Bruker IFS 125 prototype (ZP 2001) equipped with an enclosive flow cooling cell. More than 75 vibrational bands were newly assigned and analyzed rovibrationally. Precise ($\sim$ 0.0001 - 0.0003 cm^{-1}) experimental band centers were combined with previously known band centers (93 altogether) and used as the initial information for the determination of the set of 9 "harmonic" ($\tilde{\omega}_\lambda$) and 41 quartic anharmonic (x_{λ_μ}) parameters, as well as 7 resonance interaction parameters. The derived set of effective Hamiltonian parameters reproduce the vibrational structure of the CH_2D_2 molecule up to 6600 cm^{-1} with a rms deviation of 0.54 cm^{-1}.

The data obtained were used then for estimating of "experimental" values of F_{ij}, F_{ijk}, and F_{ijkl} force constants of the methane intramolecular potential function. The comparison of these with the earlier experimental and *ab initio* results is discussed.

[1] R. Marquardt and M. Quack, J. Phys. Chem. A 108, 3166 (2004) (and references cited therein).
[2] O. N. Ulenikov, E. S. Bekhtereva, S. V. Grebneva, H. Hollenstein, and M. Quack, Phys. Chem. Chem. Phys. 7, 1142 (2005) (and references cited therein).