ROTATIONAL ANALYSIS OF THE VIBRATIONAL GROUND STATE OF DIMETHYL ETHER, CH_3OCH_3

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An effective rotational Hamiltonian[a] was used to analyze the rotational transitions in the vibrational ground state of dimethyl ether. Microwave[b] and mm-wave[c] measurements from the literature were combined with new measurements between 100 and 550 GHz in a global fit of all four torsional substates. Frequencies between 8 and 550 GHz were fit for transitions involving energy levels with J up to 40 and K_a up to 9. Only 22 spectroscopic parameters were necessary to fit 1499 frequencies to experimental precision (dimensionless standard deviation 0.67). The following parameters were determined in the least-squares fit: $\rho = 0.21665(19)$, $\beta = 8.426(27)$ deg., parameters equivalent to the rotational, quartic and sextic distortion constants, the internal energy tunneling parameters $\epsilon_{01} = -3.0392(43)$ MHz and $\epsilon_{02} = 0.0019(17)$ MHz and three tunneling constants related to the "rotational" constants.

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[a] P. Groner, submitted.

[b] F. J. Lovas, H. Lutz and H. Dreizler, J. Phys. Chem. Ref. Data (1979) 8, 1057-1107; J. R. Durig, Y. S. Li and P. Groner, J. Mol. Spectrosc. (1976) 62, 159-174.

[c] W. Neustock, A. Guarnieri, J. Demaison and G. Wlodarczak, Z. Naturforsch., Part A (1990) 45, 702-706.