ROTATIONAL ANALYSIS OF THE VIBRATIONAL GROUND STATE OF ACETONE, CH_3COCH_3

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An effective rotational Hamiltonian[a] was used to analyze rotational transitions in the vibrational ground state of acetone. Microwave and mm-wave measurements from the literature[b] were combined with new measurements between 260 and 350 GHz and with new FT microwave frequencies in a global fit of all four torsional substates. Over 500 frequencies between 8 and 350 GHz were fit for transitions involving energy levels with J up to 34 and K_a up to 10. In one (preliminary) fit, 31 spectroscopic parameters were used to fit 555 frequencies to a dimensionless standard deviation of 1.25. The parameters determined in the least-squares fit were: $\rho = 0.0621754(64)$, $\beta = 25.8160(73)$ deg., parameters equivalent to the rotational, quartic and sextic distortion constants, the internal energy tunneling parameters $\epsilon_{01} = -763.436(83)$ MHz, $\epsilon_{1-1} = 0.1057(62)$ MHz, $\epsilon_{11} = 0.991(34)$ MHz, $\epsilon_{02} = 0.585(14)$ MHz and ten tunneling constants related to the rotational and distortion constants. This particular fit is not quite satisfactory because a number of transitions, including low K_c R-transitions, had to be excluded from the fit.

[a] P. Groner, J. Chem. Phys. 107, 4483 (1997).

[b] R. Peter and H. Dreizler, Z. Naturforsch. A 20, 301 (1965); J. M. Vacherand, B. P. Van Eijck, J. Burie and J. Demaison, J. Mol. Spectrosc. (1986) 118, 355; F. Oldag and D. H. Sutter, Z. Naturforsch. A (1992) 478, 527 (1992).