MOLECULES WITH A SIX-FOLD BARRIER: MICROWAVE SPECTRUM OF TOLUENE

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Recent progress in analysis and fitting of transitions in the toluene microwave spectrum characterized by $J \leq 30$, $K_a \leq 12$, and the free rotor quantum number $|m| \leq 3$ will be presented. The analysis was carried out using a new program which is specifically designed for six-fold barrier molecules, and allows the user to select almost any symmetry-allowed torsion-rotation term for inclusion in the fitting Hamiltonian. The program is based on the theoretical framework developed by Sørensen and Pedersen[a] in their application of the Longuet-Higgins permutation-inversion group G_{12} to the microwave spectrum of CH_3NO_2. In the analysis we have used the published and rather extensive unpublished data from previous studies as well as recent new measurements of the toluene microwave spectrum in the 8 – 18 GHz range. A rather successful fit of over 350 toluene microwave transitions in the abovementioned quantum number range has been achieved. The fit is close to the estimated experimental accuracy and includes more than thirty intertorsional m= +3 $\Leftrightarrow$ m= -3 transitions.

[a] G. O. Sørensen, T. Pedersen, *Studies in Physical and Theoretical Chemistry*, Elsevier, **23**, 219–236 (1983).