The Microwave Spectra of m-Xylene and m-Xylene-d_{10}. Determination of the Low Methyl Internal Rotation Barrier

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The rotational spectra of m-xylene, $(CH_3)_2C_6H_4$, and of m-xylene-d_{10}, $(CD_3)_2C_6D_4$, have been recorded between 6 and 26.5 GHz using pulsed beam Fourier transform microwave spectroscopy. The clue for the assignment of the internal rotation multiplets was the inertial defect derived from the A_1A_1 species transitions.

The rotational constants for m-xylene and m-xylene-d_{10} are A = 3572.1117(1) MHz / 2896.1195(17) MHz, B = 1761.8621(1) MHz / 1446.0236(15) MHz, C =1197.3943(2) MHz / 988.2357(7) MHz, the barrier to internal rotation of the two methyl groups are V_3 = 53.7(16) J/mol / 39.8(5) J/mol, their moments of inertia were assumed to be I_α = 3.14 uÅ^2 / 6.28 uÅ^2.

Key words: Rotational Spectra; Low Methyl Internal Rotation Barriers; Two Top Molecules; Molecular Beam Fourier Transform Microwave Spectroscopy.