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, \((\text{CH}_3)_2\text{C}_6\text{H}_4\), and of m-xylene-d_{10}, \((\text{CD}_3)_2\text{C}_6\text{D}_4\), 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 \(V_3 = 39.8(5)\) J/mol / \(39.8(5)\) J/mol, their moments of inertia were assumed to be \(I_z = 3.14\,\mu\text{Å}^2 / 6.28\,\mu\text{Å}^2\).

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