MICROWAVE AND MILLIMETER-WAVE ROTATIONAL SPECTROSCOPY OF 3-METHYLCATECHOL

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The 3-methylcatechol is likely to be found in the atmosphere during biomass burning episodes. The molecule exhibits three large amplitude motions: the torsions of its two hydroxyl groups and the internal rotation of the methyl group. Microwave and millimeter-wave spectra were recorded. Their analysis was supported by quantum chemical calculations. The theoretical three dimensional torsional potential suggests the existence of three rotamers, of which only two were detected, confirming the results of Hazrah *et al.* [1]. The V_3 and V_6 coefficients involved in the internal rotation of the methyl group were determined by fitting one-dimensional potential curves. The rotational spectrum was investigated by using a coaxially oriented beam-resonator arrangement (COBRA)[2] pulsed jet Fourier-transform microwave (PJ-FTMW) spectrometer covering $2 - 20$ GHz at Chongqing university. The millimeter-wave spectrum (70-110 GHz) was recorded at 323 K using an amplified multiplication chain from Virginia Diodes Inc. and a new heated absorption cell designed for the study of semi-volatile organic compounds. The new microwave and millimeter-wave data was combined with the assignments published by Hazrah *et al.* to produce a new global fit.

[1] doi:10.1016/j.jms.2022.111715, A. S. Hazrah, M. H. Al-Jabiri and W. Jäger, Structure and conformations of 3-methylcatechol: a rotational spectroscopic and theoretical study, J. Mol. Spectrosc. 390, 111715 (2022).

[2] doi:10.1063/1.1147553, J.-U. Grabow, W. Stahl and H. Dreizler, A multioctave coaxially oriented beam-resonator arrangement Fourier-transform microwave spectrometer, Rev. Sci. Instrum. 67(12), 4072-4084 (1996).

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