ROTATIONAL SPECTRUM AND LARGE AMPLITUDE MOTIONS OF 3,4-, 2,5- and 3,5-DIMETHYL-BENZALDEHYDE

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The microwave spectra of the 3,4-, 2,5- and 3,5-Dimethyl-Benzaldehyde (DMBA) molecules have been recorded for the first time in the 2-26.5 GHz frequency range, using the COBRA-FTMW spectrometer in Hannover, with an instrumental uncertainty of 0.5 kHz for unblended lines. The experimental assignments and fits are supplemented by *ab initio* quantum chemical calculations,conformational energy landscape, and dipole moment components. The analysis of the spectra for the three isomers are in progress. The latest results, including spectroscopic constants and large amplitude motion parameters, will be presented.

This investigation[a] follows the study of the spectra of the 4-Methyl-Benzaldehyde molecule[b]. The DMBA isomers belong to a similar series of molecules formally obtained by adding a second methyl group at the aromatic ring.

These molecules serve as prototype systems for the development of the theoretical model of asymmetric top molecules having C_s symmetry while containing two inequivalent methyl tops (C_{3v}), exhibiting different barrier heights and coupling terms to methyl internal rotation. Thus, the DMBA isomers represent benchmark species for testing the two-top internal rotors BELGI program written recently[c]

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[b] H. Saal, W. Caminati, I. Kleiner, A. R. Hight-Walker, J. T. Hougen, J.-U. Grabow, to be published.

[c] M. Tudorie, I. Kleiner, J. T. Hougen, S. Melandri, L. W. Sutikdja, W. Stahl, J. Mol. Spectrosc., 269 (2011), 211-225