NEXT LEVEL ACHIEVEMENT OF THE *XIAM* CODE IN MODELING MICROWAVE SPECTRA OF MOLECULES WITH VERY LOW TORSIONAL BARRIERS

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The *XIAM* code is one of the most frequently used programs to treat the microwave spectra of molecules with up to three methyl internal rotors. *XIAM* is user-friendly and fast, but often shows difficulties in dealing with low torsional barriers. An example is the case of *m*-methylanisole where the methyl group attached at the *meta*-position of the ring undergoes internal rotation with a barrier height of about 56 cm^{-1} for the *cis* conformer and 37 cm^{-1} for the *trans* conformer.[a] The standard deviation obtained with *XIAM* is much larger than the measurement accuracy for both conformers. Recently, the code has been modified, and two higher order effective parameters connected to the potential term $\cos(3\alpha)$ were implemented, which reduced the standard deviations of the fits to almost measurement accuracy.[b] The *XIAM*$_{mod}$ code also succeeded in modeling the microwave spectra of 3-fluorotoluene, 3,4-dimethylfluorotoluene,[c] and 4-methylacetophenone[d] with torsional barriers of 17 cm^{-1}, 32 cm^{-1}, and 22 cm^{-1}, respectively, to measurement accuracy.

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[b] S. Herbers, H.V.L. Nguyen, *J. Mol. Spectrosc.* **370**, 111289 (2020).
[c] K.P.R. Nair, S. Herbers, H.V.L. Nguyen, J.-U. Grabow, *Spectro. Chim. Acta A* **242**, 118709 (2020).
[d] S. Herbers, S.M. Fritz, P. Mishra, H.V.L. Nguyen, T.S. Zwier, *J. Chem. Phys.* **152**, 074301 (2020).