GENERAL FITTING CODE – A NEW SPECTRAL ANALYSING TOOL

K. VÁVRA, K. LUKOVÁ, T. F. GIESEN, G. W. FUCHS, *Institute of Physics, University of Kassel, Heinrich-Plett-Strasse 40 D-34132 Kassel, Germany*

A new fitting program named "general fitting code" is being developed. The idea behind this program is to provide a platform that allows users to define and include their own Hamiltonian in an almost unlimited manner. GFC tries to combine the best features of AABS[1], SPFIT[2], XIAM[3] and offers additional usefull functionalities. The graphical part of GFC is written in the Python programming language and contains all necessary tools to analyse high resolution spectra – from smoothing and line fitting to Loomis-Wood or combinational diagrams and even simulating spectrum. The fitting core of GFC is written in the Julia programming language. GFC uses a slightly modified Gauss-Newton method. It was initially written to analyse a Corriolis perturbation in triatomic linear molecules and to analyse effects of the internal rotation on vibrationally excited states of an asymmetric top. The current abilities of GFC will be demonstrated on three molecules, (1) 2-iminopropanenitrile, (2) propylene oxide and (3) hydrogen thioperoxide. In the case of 2-iminopropanenitrile the potential barrier height parameters V_3 + V_6 were obtained by a simultaneous analysis of the ground and first torsionally excited state. Regarding propylene oxide, the ring breathing mode ν_{17} has been investigated and the potential barrier height V_3 was obtained based just on ro-vibrational transitions.

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[2] doi:10.1016/0022-2852(91)90393-O,H.M.Pickett, J.Mol.Spectrosc. **148**,371-377(1991)

[3] doi:10.1515/zna-1996-0807,H.Hartwig and H.Dreizler, Z.Naturforsch, 51a (1996) **923**

p-number: p147 **Submitted on Wed, 14 Jun 2023 19:11:24 +0200**