USING PROGRAM ERHAM TO ANALYZE HIGH-RESOLUTION INFRARED SPECTRA OF MOLECULES WITH INTERNAL ROTORS

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The effective rotational Hamiltonian for molecules with one or two periodic large-amplitude motions [a] implemented in program ERHAM has been adapted to enable prediction and least-squares fits of rotationally resolved lines in vibration-rotation spectra in the infrared region. The modified program is currently applied to assign the band of methyl formate at 925 cm^{-1} that has been measured at ETH in Zurich on the IFS125 Bruker prototype ZP 2001 FTIR spectrometer [b] at a resolution of 0.001 cm^{-1}. An external glass cell with an optical path length of 3 m contained the sample, and 150 interferograms were co-added. Right now it looks as if the splitting into A and E components were a little too small to be resolved sufficiently for positive identification.

[a] P. Groner, *J. Chem. Phys.* 107, 4483 (1997).
[b] S. Albert, M. Quack, *ChemPhysChem* 8, 1271 (2007)