

## 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 <sup>a</sup> 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<sup>-1</sup> that has been measured at ETH in Zurich on the IFS125 Bruker prototype ZP 2001 FTIR spectrometer <sup>b</sup> at a resolution of 0.001 cm<sup>-1</sup>. 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.

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<sup>a</sup>P. Groner, *J. Chem. Phys.* 107, 4483 (1997).

<sup>b</sup>S. Albert, M. Quack, *ChemPhysChem* 8, 1271 (2007)