High Resolution Analysis of the FTIR spectra of CHF_3:
The ν_3 Fundamental Band and the Strongly Coupled Bands ν_2, ν_5, and $\nu_3+\nu_6$

I. B. Bolotova[a], O. N. Ulenikov[a,b,c], E.S. Bekhtereva[a,b,c], S. Albert[a],
S. Bauerecker[a,d] , H. Hollenstein[a] and M. Quack[a]

[a] Physical Chemistry, ETH-Zürich, CH-8093, Zürich, Switzerland,
[b] Tomsk Polytechnic University, Department of General Physics, 634050, Tomsk, Russia,
[c] Tomsk State University, Physics Department, 634050, Tomsk, Russia,
[d] Technische Universität Braunschweig, D-38106, Braunschweig, Germany

CHF_3 is a prototype molecule for the study of intramolecular energy flow [1-4]. Despite a long history [1-9] its rotationally resolved infrared spectrum is poorly understood due to numerous strong interactions. We have reinvestigated the IR spectrum of CHF_3 at highest resolution. Here we present the results of reanalysis of the ν_3 fundamental band and the $2\nu_3$-ν_3 "hot" band, located between a 600 and 900 cm^{-1}, previously investigated at lower resolution [7], as well as the strongly coupled triad of the states ν_2, ν_5, and $\nu_3+\nu_6$ previously measured and analyzed using FTIR supersonic jet spectroscopy [9] in the spectral region of 1100-1200 cm^{-1}.

The high resolution FTIR spectrum of CHF_3 has been measured with the Bruker 125 HR Zürich prototype spectrometer ZP2001 using a White cell, a 20cm cell, and a collisional cooling cell [1] in two spectral regions at room temperature. As a result of the analysis, transitions up to $J_{\max} = 58$ have been assigned for the ν_3 fundamental band, and $J_{\max} = 30$ for the $2\nu_3$-ν_3 "hot" band. About 6000 transitions with $J_{\max} \leq 70$ have been assigned for the bands ν_2, ν_5, and $\nu_3+\nu_6$. The new analysis results in a set of parameters which reproduce the initial experimental data with an accuracy close to the experimental uncertainties.

[1] S. Albert, K. Keppler Albert, H. Hollenstein, C. Manca Tanner, and M. Quack in **Handbook of High Resolution Spectroscopy**, Vol. 1, p.117-173; S. Albert, K. Keppler Albert, and M. Quack, Vol. 2, p.965-1019, M. Quack and F. Merkt eds., Wiley Chichester 2011.
[2] H. R. Dübal and M. Quack, *Chem. Phys. Lett.*, **1981**, 80, 439 - 444.
[3] H. R. Dübal and M. Quack, *J. Chem. Phys.*, **1984**, 81, 3779 - 3791.
[4] R. Marquardt, M. Quack, J. Stohner and E. Sutcliffe, *J. Chem. Soc., Faraday Trans.*, **1986**, 82, 1173 - 1187.
[5] G. Graner, and G. Guelachvili, *J. Mol. Spectrosc.*, **1984**, 107, 215 - 228.
[6] J. P. Champion, and G. Graner, *Mol. Phys*, 1**986**, 58, 475 - 484.
[7] K. M. Smith, G. Duxbury, D. A. Newnham, and J. Ballard, *J. Mol. Spectrosc.*, **2002**, 212, 6 -16.
[8] A. Amrein, M. Quack, and U. Schmitt, *Mol. Phys.*, **1987**, 60, 237 - 248.
[9] A. Amrein, M. Quack, and U. Schmitt, *J. Phys. Chem.*, **1988**, 92, 5455 - 5466.