

High resolution analysis and quantum dynamics of fluoroform ^{12,13}CHF₃

I. Bolotova¹, S. Albert¹, S. Bauerecker², E. Bekhtereva^{3,1}, Z. Chen¹, C. Fabri¹, H. Hollenstein¹, M. Quack^{1*}, O. Ulenikov^{3,1}

¹Physical Chemistry, ETH Zürich, Vladimir-Prelog-Weg 2, 8093 Zürich, Switzerland, ²Physical Chemistry, TU Braunschweig, Hans-Sommer-Strasse 10, 38106 Braunschweig, Germany, ³Institute of Physics and Technology, Tomsk Polytechnic University, Lenin av. 30, 634000 Tomsk, Russia

The spectroscopy of ¹²CHF₃ has been the basis for the study of time independent and time dependent quantum dynamics for a long time [1-9]. There have also been substantial efforts concerning the *ab initio* potential hypersurface ([10, 11] and references cited therein). We present a survey of our recent analyses ranging from the Terahertz (Far infrared) spectral range to about 3000 cm⁻¹, with particular emphasis on the pure rotational (FIR) spectra measured at the infrared beamline of the Swiss synchrotron Light Source (SLS), ν_3 fundamental (700 cm⁻¹ range), the ν_2 , ν_5 , $\nu_3+\nu_6$ polyad (1200 cm⁻¹ range), the $\nu_4/2\nu_3$ dyad (1400 cm⁻¹), the $2\nu_4$ (*A*₁ and *E*) dyad and results on the ¹³CHF₃ isotopomer including the ν_1 fundamental. The implications for the study of intramolecular vibrational energy redistribution (IVR) will be outlined with particular emphasis on ¹³C isotope effects.

[1] a) S. Albert, K. Keppler Albert, H. Hollenstein, C. Manca-Tanner, and M. Quack *Fundamentals of Rotation-Vibration Spectra*, Vol. 1, pp. 117-173; b) S. Albert, K. Keppler Albert, and M. Quack *High-Resolution Fourier Transform Infrared Spectroscopy*, Vol. 2, pp. 965-1019; c) M. Quack *Fundamental Symmetries and Symmetry Violations from High-Resolution Spectroscopy*, Vol. 1, pp. 659-722 in *Handbook of High Resolution Spectroscopy*, M. Quack and F. Merkt eds., Wiley Chichester (2011).

[2] H.-R. Dübal, M. Quack, *Chemical Physics Letters*, **1981**, 80, 439; H.-R. Dübal, M. Quack, *Journal of Chemical Physics*, **1984**, 81, 3779.

[3] R. Marquardt, M. Quack, J. Stohner, E. Sutcliffe, *J. Chem. Soc., Faraday Transac.*, **1986**, 82, 1173.

[4] A. S. Pine, J. M. Pliva, *Journal of Molecular Spectroscopy*, **1988**, 130, 431.

[5] J. Segall, R. N. Zare, H.-R. Dübal, M. Lewerenz, M. Quack, *Journal of Chemical Physics*, **1986**, 86, 634.

[6] A. Amrein, M. Quack, U. Schmitt, *Molecular Physics*, **1987**, 60, 237.

[7] A. Amrein, M. Quack, U. Schmitt, *Journal of Physical Chemistry*, **1988**, 92, 5455.

[8] M. Quack, *Annual Review of Physical Chemistry*, **1990**, 41, 839.

[9] T. Carrington Jr., L. Halonen, M. Quack, *Chemical Physics Letters*, **1987**, 140, 512.

[10] T. K. Ha, M. Lewerenz, R. Marquardt, M. Quack, *Journal of Chemical Physics*, **1990**, 93, 7097.

[11] R. Marquardt, M. Quack *Global Analytical Potential Energy Surfaces for High-Resolution Molecular Spectroscopy and Reaction Dynamics*, Vol. 1, pp. 511-550 in [1].