# General Vibrational Spectroscopies with Wilson

Magnus Ringholm*, Dan Jonsson, and Kenneth Ruud

Centre for Theoretical and Computational Chemistry, Department of Chemistry, UiT The Arctic University of Norway, NO-9037 Tromsø, Norway, *magnus.ringholm@uit.no

We present an approach to simulate any elastic frequency-resolved vibrational spectroscopy where the incident lasers are in the infrared or ultraviolet/visible range, detuned from any electronic resonances, using a recursive scheme to identify the relevant contributions to the spectroscopic process. The approach is implemented in the computer program Wilson.

Wilson starts from the Liouville equation, identifies the terms that contribute to a user-defined elastic spectroscopic experiment involving molecular vibrations, evaluates these terms and renders the spectrum. The recursive nature of its routines means that all eligible experiments are treated on an equal footing and the only practical limitations are the computational capacity and the availability of the polarization property normal-mode derivatives that enter into the expressions that are identified. The program library OpenRSP[1], developed in our group, can calculate these derivatives in an analytic, recursive manner, allowing for a fully analytic *ab initio* treatment up to lineshape effects.

We will present some results from a pilot implementation to demonstrate the possibilities that this approach offers, and discuss some challenges and planned improvements.
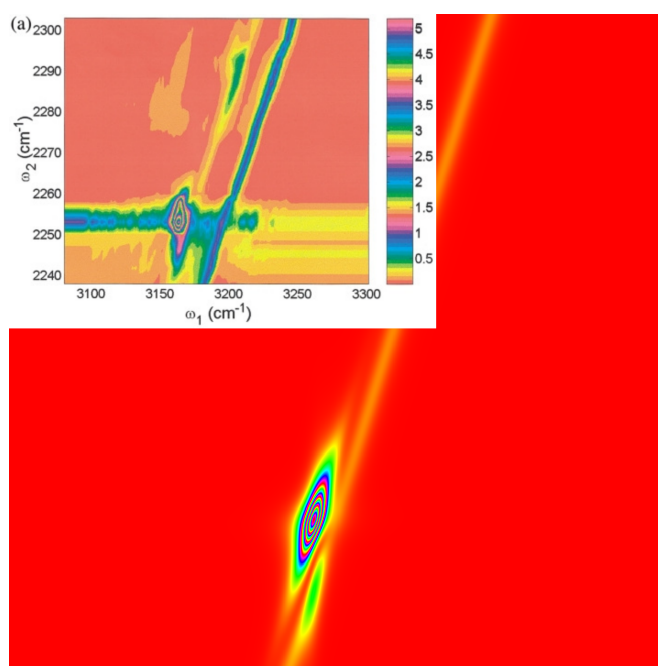


Fig.1 DOVE-FWM 2D-IR calculated spectrum of acetonitrile; experimental spectrum[2] with 8 mole% $C_6D_6$ admixture (inset)

[1] R. Bast, D. H. Friese, B. Gao, D. J. Jonsson, M. Ringholm, K. Ruud, A. J. Thorvaldsen, http://www.openrsp.org/
[2] W. Zhao, J. C. Wright, Phys. Rev. Lett. **84**, 1411 (2000)