Improved thermal motion description for improved density models
Refinement of lattice dynamical models from periodic ab-initio calculations

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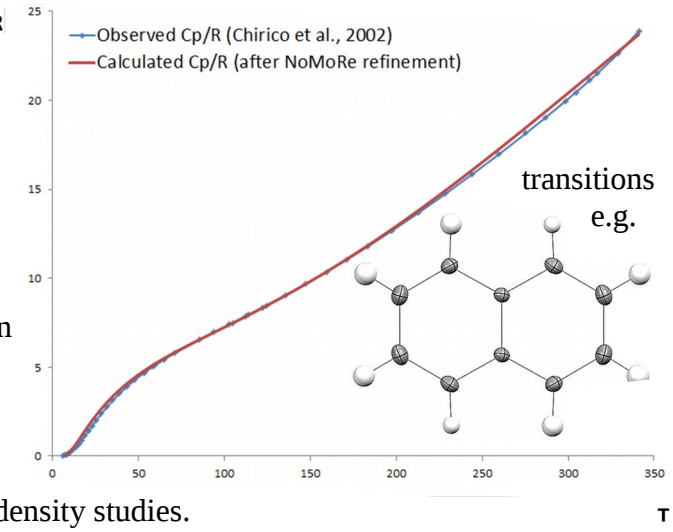
Meaningful results from charge density studies can be obtained only when both the electron density and the thermal motion is properly described. Herein, we would like to present a new modeling approach, which improve thermal motion description [1].

Our recent calculations of Debye-Waller factors based on periodic *ab-initio* calculations for various molecular test systems [2] has prepared the ground for proposing the refinement of quantum-mechanically derived normal modes of vibration against diffraction experiments. As opposed to the standard approach using independent atomic motion, some of the advantages and possibilities that emerge are:

1. A physically reasonable picture of the molecular motion in the crystal.
2. Refinement against data obtained at multiple temperatures in a common model.
3. Modeling thermal diffuse scattering.
4. Reduction of the number of model parameters.
5. Anisotropic motion of H atoms.

The approach is computationally expensive, but may prove useful for electron density studies, studies of thermal effects in crystals, i.e. studies of thermochromic and thermoelectric compounds, solid-state phase-transitions e.g. as well as to derive thermodynamic properties such as free energies, of polymorphic crystals.



We will introduce the method as implemented in our program NoMoRe and present some first results for a range of systems of increasing complexity: Urea, L-alanine, naphthalene and xylitol, including first applications of the proposed model of thermal vibration to charge density studies.

1. Hoser, A. A. and Madsen, A. Ø. (2015) Acta Cryst. A, submitted.
2. Madsen, A. Ø., Civalleri, B., Ferrabone, M., Pascale, F. & Erba, A. (2013). Acta Cryst., A69, 309–321