HAR_NoMoRe – the future of a quantum crystallography refinement?

Helena Butkiewicz1, Anders Ø. Madsen2, Michał Chodkiewicz1, Anna A. Hoser1

Faculty of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland; Department of Pharmacy, University of Copenhagen, Universitetsparken 2, Copenhagen, Denmark

h.butkiewicz@o2.pl

Keywords: lattice dynamics, phonons, Hirshfeld Atom Refinement, thermodynamic properties

Ever since the first diffraction pattern for a single crystal was recorded, X-ray diffraction (XRD) has been developed into a widely used, powerful, and indispensable characterization method for structural analysis. Now, the theory and experiments are in a mature state, XRD diffractometers have new, strong X-ray sources and modern hybrid pixel detectors, enabling the collection of the diffraction patterns with accuracy and precision about which no one dreamed a few years ago. It requires state of the art models to extract all information present in collected experimental results as the intensity of the diffracted beam depends on both: electron density and thermal motion. Whereas much work was done with the electron density modelling (e.g. Hansen-Coppens multipole model [1], Hirshfeld atom refinement (HAR)[2, 3]), thermal motion treatment remains the same as it was a century ago. Therefore, we have developed a new method, in which instead of routine atomic displacement parameters (ADPs) refinement against single-crystal X-ray diffraction data, we refine frequencies from periodic ab-initio calculations4. We called such refinement Normal Mode Refinement (NoMoRe).

Herein we will present for the first time a new model that join those two worlds: the best description of the charge density model (HAR) and the best model to describe thermal motion (NoMoRe), Fig. 1. We will present how model works for exemplary compounds: urea, alanine, xylitol, naphthalene, glycine polymorphs.

![Figure 1. Schematic visualization of combination of HAR with NoMoRe.](image)