MS19 Experimental and theoretical advances in quantum crystallography

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Dynamic quantum crystallography – where are we now?
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Abstract
Nowadays we observe fast development of experimental diffraction techniques: new, strong X-ray sources and modern hybrid pixel detectors, enable 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]), thermal motion description still requires improvements. Anisotropic displacement parameters usually do not attract attention and are treated as a dustbin for all experimental errors (there are only few remarkable exceptions).
Within dynamic quantum crystallography we reinstate thermal motion to its rightful place. We enrich the analysis of thermal motion in crystals with information from periodic DFT calculations. As a benefit we obtain hydrogen atoms ADPs and accurate thermodynamic properties (heat capacity, entropy) for molecular crystals, which are still difficult to obtain for purely from theoretical calculations.
In this contribution the normal mode refinement (NoMoRe) approach[3,4]: current developments, applications[5,6], and future directions will be presented.

References
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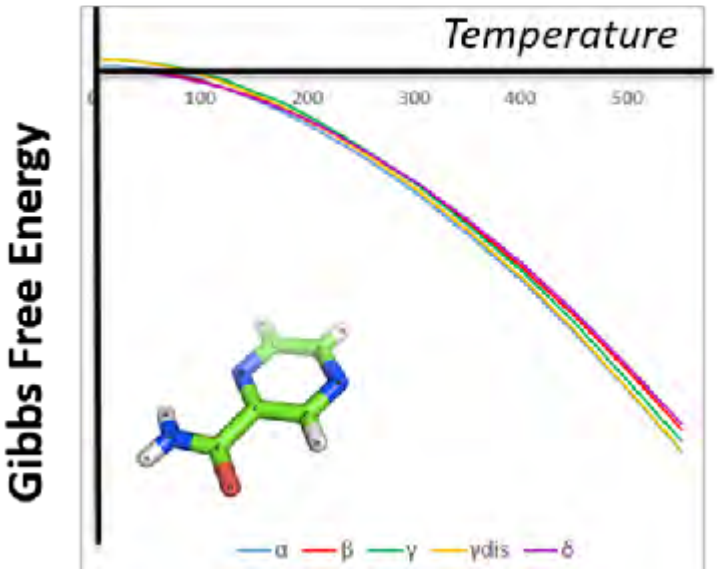
Free energies of pyrazinamide polymorphs.



Specific heat capacity estimated forα-glycine.