MS28-O5 Improved thermal motion description for improved density models: towards Quantum Dynamic Crystallography

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Meaningful results from charge density studies can be obtained only when density is properly deconvoluted from thermal motion. Herein, we would like to present new approaches and models which improve thermal motion description. First approach is devoted to accurate estimation of hydrogen atoms ADPs. A major update of the frequently used in charge density studies SHADE server (http://shade.ki.ku.dk) will be presented. In addition to the options offered by SHADE2, the newest version offers two new methods. The first method combines the original TLS analysis with input from periodic *ab-initio* calculations. The second method utilizes input from experiment on related structures to evaluate ADPs of H atoms. In the second approach, we propose to utilize information obtained from harmonic frequency periodic *ab-initio* calculations at the Γ point, in the refinement of single crystal X-ray or neutron diffraction data. Our approach has many advantages. By refining frequencies for given normal modes we are obtaining lattice dynamical description, which is closer to reality than simple model with ADPs and we are obtaining better deconvolution of thermal motion from charge densities. The frequencies, which are obtained after the refinement, enable the calculation of thermodynamic properties. We also demonstrate that it is possible to significantly reduce the number of parameters used in refinement, with only a small increase of wR2. We will introduce the method and present some first results for four model systems including first applications of proposed model of thermal vibration to charge density studies.

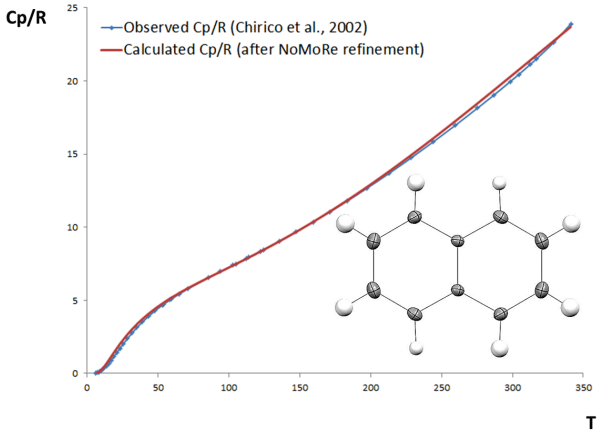

Figure 1. Estimated heat capacity for naphthalene after refinement compared with heat capacity from calorimetric measurements

Keywords: thermal motion, ab-initio calculations

MS29. Quasi crystals and aperiodic materials

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MS29-O1 Statistical description of icosahedral quasicrystals

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The atomic structure of icosahedral quasicrystals is modeled most frequently by using 6D description [1,2]. Within this approach, 3D polyhedra are considered as atoms stretched to multidimensional objects in perpendicular space. By projecting the objects (called atomic surfaces or occupation domains) on physical space, the real atomic structure is obtained. The refinement, however, is to be performed in real space. At the same time, it is rather difficult to adjust the 6D model during that process.

We show the alternative to the abovementioned method, *i.e.* the statistical description [3]. Here, the structure modeling can be done in physical space only with no need to lift the atomic structure to high dimensions. We replace atomic surfaces by statistical distribution of atomic positions with respect to the periodic reference lattice. The atomic structure is investigated by modeling this distribution.The statistical approach was already used for structure refinement of many decagonal phases [4]. It was also used to derive the structure factor of icosahedral quasicrystals based on 3D Penrose tiling [5].

In this talk, the details of structure modeling of icosahedral quasicrystals using the statistical description will be shown. The examples of atomic decoration of the Ammann rhombohedra will be considered and the application of the derived structure factor to the refinement procedure will be discussed.

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Keywords: icosahedral quasicrystal; structure modeling; statistical description; Average Unit Cell; diffraction pattern