In search of anharmonic motion of H-atoms

S. Sutula[1], M. Malinska[1], L. Cañadillas-Delgado[2], O. Fabelo-Rosa[2], K. Woźniak[1]

[1] Department of Chemistry, University of Warsaw, Pasteura 1, 02-093 Warsaw, Poland,
[2]Institut Laue-Langevin, 71 Ave Des Martyrs, 38042, Grenoble, France

s.sutula@uw.edu.pl

Anharmonic movement is highly expected for the lighter atoms, as they are more influenced by the motion of their heavier parent atoms. However, because of low X-ray diffracting power of H-atoms, their motion is assumed as harmonic isotropic during routine structural studies or harmonic anisotropic during charge density studies with ADPs calculated in most cases. In this study we try to go one step further and check if it is possible to successfully refine H-atoms anharmonically.

For our study we performed neutron diffraction experiments on α-glycine ($P2_1/n$) high quality single crystals in 90 K and 200 K in ILL (Grenoble, France). With the high resolution of the data that we collected we tried to investigate whether anharmonic motion of H-atoms can be observed and modelled. Using Jana2020 we refined all H-atoms with Gram-Charlier coefficients up to the third level and then checked their 3D probability density function maps dependence on resolution. We performed Prince-Spiegelman test [1] to compare models with harmonic and anharmonic treatment of H-atoms to decide which model better fits the collected data, apart from simple comparison of refinement parameters like R_1, wR_2 and GooF.

At the end, to put H-atoms anharmonic motion refinements and observing changes in the model with varying resolution in perspective, we calculated lowest necessary resolution of the data collection according to Kuhs' formula. It has been shown by Kuhs [2], that most information of the anharmonic motion of atoms is contained within higher angle reflections intensities. Our results agree with this assumption and the provided formula.

[1] Prince, E. & Spiegelman, C. H. (2004). *International Tables for Crystallography Volume C: Mathematical, Physical and Chemical Tables*, Vol. edited by E. Prince, pp. 702–706. Dordrecht: Springer Netherlands

[2] Kuhs, W. F. (1992). *Acta Cryst.* **A48**, 80.

Keywords: anharmonic motion; hydrogen; neutron radiation; glycine

This work was supported by the Foundation for Polish Science, TEAM-TECH Core facility for crystallographic and biophysical research to support the development of medicinal products (co-financed by the European Union under the Regional Development Fund)