MS29-P02 | On precision and accuracy of X-ray and neutron diffraction results for single crystals of glycine

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In our work, we aim at characterization and estimation of precision and accuracy of single crystal X-ray and neutron results obtained for high-quality crystals of α-glycine. As expected, the shorter the wavelength, the better resolution, and one can refine the structure of glycine with more details. That is why we used MoKα, AgKα and X-ray synchrotron radiation for our measurements. Even more, we also have obtained the structural data with neutron single wavelength radiation as relative diffraction lengths for hydrogen atoms are much higher in neutron diffraction than the corresponding atomic scattering factors in the case of X-ray diffraction. For those two distinct radiation sources, we collected the data at different temperatures ranging from 90 K to 295 K. Afterwards, we used different resolution limits ranging from full possible for each source down to 0.5 $Å^{-1}$. Finally, the fourth differentiating factor was the model used for refinement. We applied the simple IAM (Independent Atom Model) with isotropic treatment of hydrogen atoms, IAM with anisotropic thermal motion for hydrogen atoms, MM (Multipole Model) and finally a model allowing for the anharmonic motion for hydrogen atoms. What we find the most interesting, is the dependence of ADPs of all atoms within the glycine molecule on the resolution of the collected data. We would like to present detailed comparison of results from different techniques and different sources and interesting relation regarding thermal motion and finally ask a question, what should the standards of nowadays structure experiments look like.