

**MS28-O3** Hirshfeld Atom Refinement for determining hydrogen positions in routine X-ray experiments**Keywords:** Hirshfeld Atom Refinement, hydrogen positions, hydrogen ADPs, X-ray crystallographyMagdalena Woinska<sup>1</sup>, Simon Grabowsky<sup>2</sup>, Paulina M. Dominiak<sup>1</sup>, Krzysztof Wozniak<sup>1</sup>, Dylan Jayatilaka<sup>3</sup>

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Locating hydrogen is a crucial problem in chemistry as hydrogen atoms often constitute the outer layer of molecules and therefore mediate in many important interactions and take part in a variety of reactions and processes. Neutron diffraction experiments are considered the best source of information about coordinates and thermal motions of hydrogen atoms in crystals whereas X-ray diffraction is still believed to be a much less reliable method in this respect. The presented work shows that applying Hirshfeld Atom Refinement (HAR) [1][2] for X-ray data analysis constitutes a significant improvement in comparison to IAM in terms of positional parameters of hydrogen atoms. Furthermore, HAR enables refinement of hydrogen anisotropic displacement parameters (ADPs) based solely on X-ray data, which cannot be achieved with IAM.

The analyzed results are based on HAR carried out for 81 high resolution X-ray data sets collected for organic compounds at temperatures not higher than 140 K. In the applied method aspherical atomic scattering factors are obtained from Hirshfeld partition of molecular density calculated on the BLYP/cc-pVDZ level of theory for a molecule surrounded by a cluster of charges and dipoles simulating the influence of a crystal environment. The X-H bond lengths (C-H, N-H, O-H) present in the investigated compounds are grouped into bond types defined in the work by Bruno & Allen [3] and their averaged values are compared to the neutron results. The difference between both means for individual bond types is usually within two and often even within one X-ray standard deviation. Moreover, precision of bond lengths obtained in HAR of X-ray data is similar to the neutron one, except bond lengths in water molecules for which HAR values are significantly more precise. These results remain the same if HAR is performed for data trimmed to the standard resolution of 0.8 Å, which makes the method suitable for refinement of data from routine X-ray experiments for well scattering compounds. Additionally, a short analysis of ADPs obtained from HAR will be presented.

## References

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