MS29-P03 | Comparison of Different Strategies for Modelling Hydrogen Atoms in Charge-Density Analyses

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The quality of five approximation methods to model anisotropic displacement parameters (ADPs) for hydrogen atoms was investigated in a comparative study based on two model compounds [1]. Hydrogen atom parameters and structural properties derived from our collected neutron data sets of these compounds were compared with those obtained from the SHADE-server [2], the software APD-Toolkit [3], the results from Hirshfeld atom refinement conducted in the OLEX2 GUI (HARt) [4], and the results of anisotropic hydrogen refinement within XD2016 [5]. Surprisingly, the refinement of anisotropic hydrogen displacement parameters against the X-ray data yielded the smallest deviations from the neutron values. The refinement of bond-directed quadrupole parameters turned out to be vital for the quality of the resulting ADPs [6].

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