

MS29-05 | ANISOTROPIC HYDROGEN ATOMS IN CHARGE DENSITY ANALYSIS

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In our recent experimental charge density studies, we noticed residual density close to hydrogen positions that could be modelled as anisotropic displacement. To justify this treatment, we collected neutron data for two benchmark structures and compared the derived anisotropic hydrogen displacement parameters to our refined parameters against the X-ray data, results obtained from the *SHADE*-server [1], the software *APD-Toolkit* [2] and from *HARt* [3]. The smallest deviations from the neutron values were achieved by the refinement of anisotropic hydrogen displacement parameters against the X-ray data. With that, the refinement of bond-directed quadrupole parameters turned out to be important. The main discrepancies were observed for hydrogen atoms that are attached to carbon atoms that were refined with Gram-Charlier coefficients. Furthermore, we investigated also the free refinement of the C-H bond distances after anisotropic refinement of the hydrogens. While *HARt* yields the most reliable C-H bond distances, it overestimated the hydrogen anisotropic displacement parameters [4].

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[3] Fugel, M., Jayatilaka, D., Hupf, E., Overgaard, J., Hathwar, V. R., Macchi, P., Turner, M. J., Howard, J. A. K., Dolomanov, O. V., Puschmann, H., Iversen, B. B., Bürgi, H.-B. & Grabowsky, S. (2018). *IUCrJ.* 5, 32–44.

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