Improved thermal motion description for improved density models Towards Dynamic Quantum Crystallography: SHADE3

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Meaningful results from charge density studies can be obtained only when the density is properly deconvoluted from thermal motion. Hydrogen atoms, due to their low scattering power for X-ray diffraction, are particularly difficult to describe. Herein, we would like to present new approaches which improve the H atoms thermal motion description.

We present a major update of the SHADE server http://shade.ki.ku.dk. In the newest version of the server, besides that all options of estimating H-atom ADPs which were offered by SHADE2 are still available, two new methods for estimating hydrogen ADPs are present. The first of them combines the original TLS analysis with input from periodic ab-initio calculations. The second allows the user to input experimental information from spectroscopic measurements or from neutron diffraction experiments on related structures and utilise this information to evaluate hydrogen ADPs. Tools to setup the ab-initio calculations and to derive the internal motion from the calculations are provided. We test the new server on a range of compounds where neutron diffraction data are available. The results are in most cases significantly better than previous estimates, and for strong hydrogen bonds in proton sponges the ab-initio calculations become crucial.

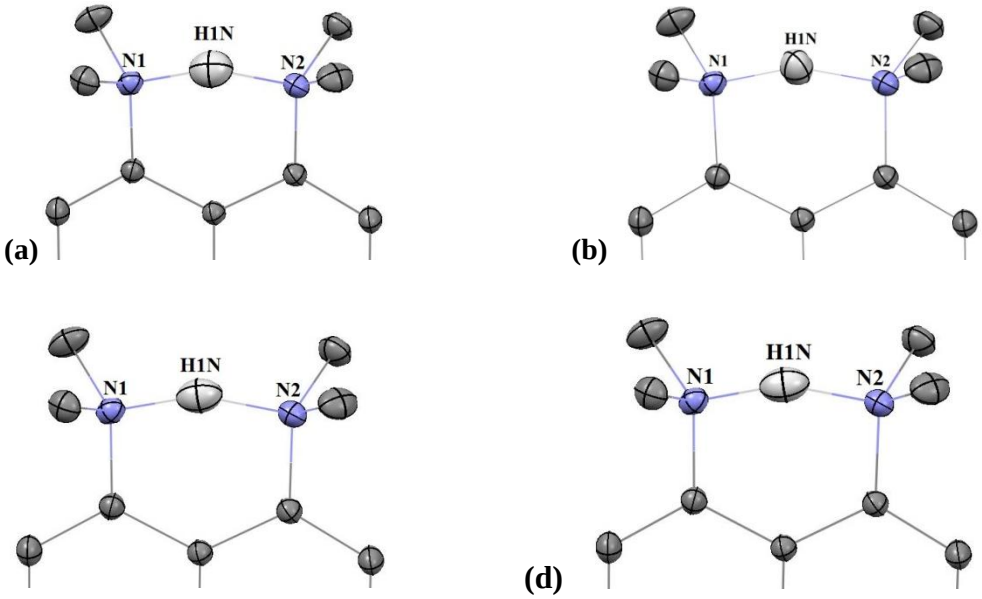

Figure 1 ORTEP representation of ADPs at 50% probability level for the N-H...N hydrogen bond in proton sponge 1. H1NN ADPs were obtained by: **(a)** neutron measurements **(b)** SHADE2 **(c)** SHADE3 with frequencies from the literature, **(d)** and the SHADE3 program with internal msds transferred from similar proton sponges.