[MS10-P05] Internal modes of anisotropic displacements of hydrogen atoms from the invariom database. J. Lübben[a] and B. Dittrich[b].

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In 2006 A. Madsen introduced the SHADE web server [1]. It allows to estimate the anisotropic displacement parameters of hydrogen atoms (H-ADPs) in single crystal X-ray diffraction studies of the charge density: An internal average contribution of hydrogen-atom motion from Neutron diffraction is combined with the rigid-body motion of the whole molecule, which in turn is obtained from a TLS fit [2] to the ADPs of the non-hydrogen atoms. The invariom database [3] provides an alternative source of information on the additive internal modes of H-ADPs than Neutron diffraction, since computations of scattering factors involve calculation of infrared (IR) frequencies for each model compound, and IR frequencies can be converted into atomic displacements. A local coordinate system needs to be taken into account in the process. We assume that internal contributions to the displacements in a rigid molecule are invariant in different molecules, because the electron density is also transferable. This hypothesis is tested and we present a comparison of an application of estimated ADPs on glyine [4] with the results of an earlier study [5] of H-ADPs on this molecule. We also use so- generated hydrogen ADPs in an investigation of the charge-density distribution of a dipeptide, where the effect of including H-ADPs on invariom-refined bond distances and their effect on bond-topology in a free multipole refinement is studied.

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