Anisotropic Displacement Parameters (ADPs) of Hydrogen Atoms. Can Invariom Modeling Contribute?

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Recently we have introduced invarioms (intermolecular transferable pseudoatoms) [1] and have shown that invariom modeling improves molecular geometry [2] for all atoms including hydrogens and overcomes the shortcomings of the independent atom model (IAM). Such modeling also improves the description of the thermal motion parameters as quantified with the Hirshfeld test.

To answer the title question we computed for a variety of small molecules hydrogen ADPs as described in [4], implemented in the XD [5] suite. In that procedure the internal displacements for all atoms are calculated by an *ab initio* methods, and then subtracted from the experimental data that also contain the external modes. The molecular C,N,O-skeleton is then fitted as a rigid body to the remains of the experimental ADPs. Finally these contributions are, together with the theoretical internal modes, assigned to the riding hydrogen atoms. These hydrogen ADPs are compared with results from an invariom structure refinement and to room temperature neutron data.

[1] Dittrich B., Koritsanszky T., Luger P., *Angew. Chem. Int. Ed.*, 2004, **43**, 2718. [2] Dittrich B., Huebschle C. B., Kalinowski R., Girnt, D., Luger P., *Acta Cryst. A*, *accepted.* [3] Hansen N.K., Coppens P., *Acta Cryst.*, 1978, **A34**, 909. [4] Flaig R., Koritsanszky T., Zobel D., LugerP., *J. Am. Chem. Soc.*, 1998, **120**, 2227. [5] Koritsanszky T., Richter T., Macci P., Gatti C., Howard S., Mallinson P.R., Farrugia L., Su Z.W., Hansen N.K., *XD*, Freie Universitat Berlin, Berlin, 2003.

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