Poster Presentations

[MS10-P06] Can one use invarioms to place hydrogens for refinement against X-Ray data?

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Accurate hydrogen atom positions are essential for the interpretation of crystal structures, but X-Ray data are not optimal for determining them. Neutron diffraction determines proton positions precisely [1], but does not include any information about the electron distribution. The introduction of invarioms [2] provides a golden opportunity to obtain more information about hydrogen atom positions and the corresponding electron density distribution. It is also possible to obtain this information from quantum mechanical calculations [3], but the quantum mechanical computations are inconvinient for molecules that are too large and complex.
The invariom classification [2] provides a more detailed description of hydrogen atoms and their environments than is normally employed in molecular force-fields. We will show how invarioms can be used to derive improved force-field parameters for the precise positioning of hydrogen atoms in crystal structures of small molecules and macromolecules. We hope that this will lead to more efficient treatment of hydrogen atom positions in programs such as SHELXL [4] andCRYSTALS [5] that provide restrained refinement of hydrogen atoms.

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[5] Cooper, R. I., Thomson, A. L. & Watkin, D. J. (2010). *J. Appl. Cryst.*, **43**, 1100-1107.

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