Poster Presentation

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Temperature dependence of Uiso constraints in riding hydrogen treatments

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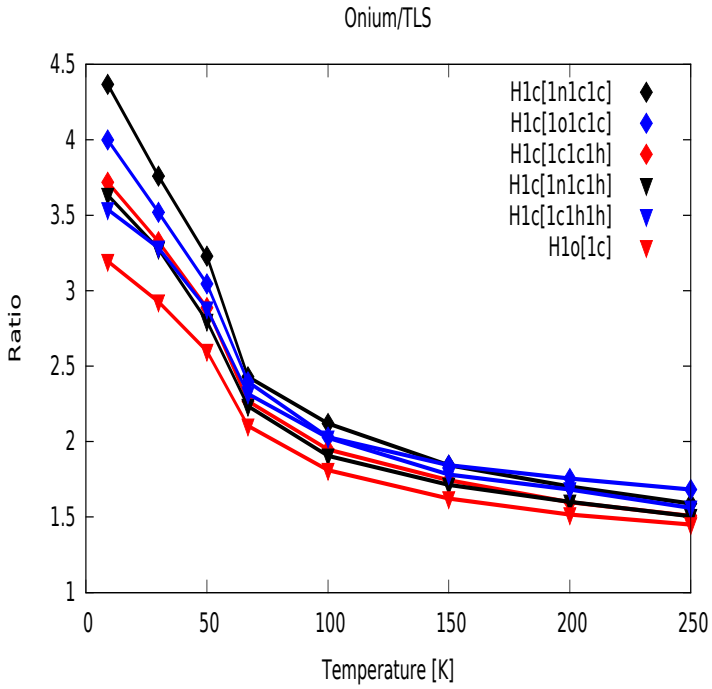
Anisotropic parametrisation of the thermal displacements of hydrogen atoms in single-crystal X-ray structure refinement is not possible with independent atom model (IAM) scattering factors. This is due to the weak scattering contribution of hydrogen atoms. Only when aspherical scattering factors are used can carefully measured Bragg data provide such information. For conventional structure determinations parameters of "riding" hydrogen atoms are frequently constrained to values of their "parent" heavy atom. Usually values of 1.2 and 1.5 times X-U_eq are assigned to H-U_iso in these cases. Such constraints yield reasonable structural models for room-temperature data. However, todays small molecule X-Ray diffraction experiments are usually carried out at significantly lower temperatures. To further study the temperature dependence of ADPs we have evaluated several data sets of N-Acetyl-L-4-Hydroxyproline Monohydrate at temperatures ranging from 9 K to 250 K. Methods compared were HAR [1], Invariom refinement [2], time-of-flight Neutron diffraction and the TLS+ONIOM approach [3]. In the TLS+ONIOM approach non-hydrogen ADPs from Invariom refinement provided ADPs for the TLS-fit. Hydrogen atoms in all methods were grouped and analyzed according to their Invariom name. We reach a good agreement of the temperature dependence of H-U_iso/X-U_eq. At very low temperatures the ratio H-U_iso/X-U_eq can be as high as 4, e.g. for Hydrogen attached to a sp3 carbon atom with three non-Hydrogen atom neighbors. Since all methods consistently show that the H-U_iso/X-U_eq ratio is temperature dependent, this effect should be taken into account in conventional structure determinations.

[1] *Jayatilaka D, Grimwood D J, Computational Science - ICCS. (2003), 142–151.,* ***[2]*** *Dittrich B, Hübschle C B, Pröpper K, Dietrich F, Stolper T, Holstein J J.,* ***[3]*** *Whitten A, Spackman A, Acta Cryst. (2006). B62, 875–888. Acta Cryst., B69, (2013), 91-104.*



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