MS29-P04 | TAAM: A RELIABLE AND USER FRIENDLY TOOL FOR HYDROGEN ATOM LOCATION USING X-RAY DIFFRACTION DATA

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The use of TAAM (Transferable Aspherical Atom Model) – a multipole model based approach - instead of spherical atom model in the structure refinement against X-ray data largely improves the X-H bond lengths.[1] A new method called Hirshfeld Atom Refinement (HAR) was shown to allow for accurate and precise estimation of the X-H bond lengths in small molecule by Woinska et. al.[2]. However, the computation cost for HAR is much higher than the TAAM refinement. The applicability of TAAM in determining the X-H bond lengths with accuracy comparable to neutron data was reinvestigated on the 81 organic molecule datasets used by Woinska et. al. A library called DiSCaMB has been developed to facilitate integration of the aspherical atom model into refinement programs.[3] The structures were refined using TAAM via DiSCaMB integrated with locally modified version of Olex2[4] and the X-H bond lengths thus obtained have been categorized and compared with the averaged neutron lengths as defined by Allen and Bruno.[5] The model related statistics comparison between IAM, HAR and TAAM will be highlighted.

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