MS19-2-5 Thermal motion and position of hydrogen bonded to transition metals in coordination complexes studied with HAR combined with SHADE3 or NoMoRe
#MS19-2-5

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Abstract
Hirshfeld Atom Refinement (HAR) is a method which, based on X-ray data, yields more accurate positions of hydrogen atoms bonded to light chemical elements and – if data quality allows – also to heavy metals [1]. Nevertheless, treatment of hydrogen thermal motions is more problematic and HAR often yields ADPs which are N.P.D. or produces thermal ellipsoids with distorted shapes. Therefore, tools enabling estimation of hydrogen ADPs such as SHADE3 [2] or Normal Mode Refinement (NoMoRe) [3] are helpful. Transition metal (TM) hydride complexes are particularly challenging for X-ray crystallography. On the one hand, obtaining high quality data is hindered by problems such as high absorption and radiation damage. Access to neutron data which could be used as a benchmark is even more limited. On the other hand, using an advanced model of electron density such as HAR involves time-consuming calculations. This problem is even more exacerbated in the case of SHADE3 or NoMoRe, for which periodic wave function has to be computed.
In this contribution we present the results of HAR performed for five structures of TM (Fe, Nb, Rh and Os) and metalloid (Sb) hydride complexes for which both neutron and X-ray data were available in the CSD. Refinements were performed in three versions: (1) hydrogen thermal motions refined with HAR (usually isotropically, except the Fe and Rh complexes for which anisotropic refinement of C-bonded H atoms was possible), (2) H ADPs fixed at the SHADE3-derived values and (3) H ADPs obtained in the course of NoMoRe. The influence of the method of obtaining hydrogen thermal motions on the positions of hydrogen atoms derived by HAR, particularly TM-H bond lengths, will be analyzed. Changes of statistical parameters characterizing refined models will also be discussed. Differences between hydrogen ADPs obtained with various methods will be studied using the similarity index (S) [4]. For the Sb complex, for which neutron and X-ray data collection temperatures are the same, thermal motions derived from the neutron experiment and the three methods applied to X-ray data will be compared.
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HAR+NoMoRe crystal structure of the Rh complex.