

MS19-03 Resolution dependent scaling – a solution for problems in a multipole refinement? Regine Herbst-Irmer, Institute of Inorganic Chemistry, University of Göttingen, Germany
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In one of our recent charge density studies we were faced with some discrepancies when comparing the results of refinements against different data sets. We collected three data sets to high resolution at different temperatures (15 K and 100 K) and with different diffractometers (a Bruker TXS-Mo rotating anode equipped with INCOATEC Helios mirrors and an APEX II detector and an INCOATEC micro source with QUAZAR mirrors and an APEX II detector) on crystals of 9-diphenylthiophosphinoyl-anthracene. The refined monopole populations and kappa values especially for the phosphorus atoms differ at 100 K and at 15 K. Additionally, residual density remained around the phosphorus atoms for the two data sets at 100 K. The structure had first shown a typical shashlik-like residual density pattern close to the sulfur atom at all temperatures and close to phosphorus for the 100 K data sets. This could be explained as anharmonic motion and disappeared when Gram-Charlier anharmonic coefficients were introduced [1, 2]. Refinement of anharmonic motion to an even higher order did not help and led to unreasonable probability density functions. These two problems disappeared after 10 resolution dependent scale factors instead of just one were refined. The dependency of the scale factors against resolution will be shown. Possible explanations for these resolution and temperature dependent errors will be discussed.

- [1] Herbst-Irmer R., Henn J., Kratzert D., Stern D., Stalke D. (2009). *Acta Cryst.* **A65**, s109.
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MS19-04 Interrelations between crystal architecture, charge density and energy of uracil derivatives. Katarzyna N. Jarzemska, Radosław Kamiński, Krzysztof Woźniak, Paulina M. Dominiak, University of Warsaw, Pasteura 1, 02-093, Warsaw, Poland
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A comprehensive analysis of crystal packing and energetic features of the selected uracil derivatives is reported [1]. High quality X-ray diffraction data sets of the studied compounds were subjected to the TAAM procedure (Transferred Aspherical Atom Model based on the Hansen-Coppens formalism) with the use of the UBDB2011 databank [2], which gave results comparable both with the optimised and the neutron-diffraction-derived geometries. Furthermore, charge density data sets were collected and thoroughly analysed for the 6-methyl-2-thiouracil compound and for the 9-methyladenine : 1-methylthymine dimer. Most of the structures form hydrogen bonded layers kept together by π -stacking interactions. The only exception is 2,4-dithiouracil, which exhibits a rather complex 3D network based on N–H...S and C–H...S contacts. A deeper insight into the nature of crystal architectures was obtained through theoretical computations, concerning cohesive energy, dimer interaction energy, and molecule deformation energy evaluation. The balance between molecular layer stabilisation and their mutual interactions is essential for crystal growth, and thus it is reflected in crystal morphology and quality. Cohesive energy ranges from $-100 \text{ kJ}\cdot\text{mol}^{-1}$ for 2,4-thiouracil, to about $-140 \text{ kJ}\cdot\text{mol}^{-1}$ for uracil and 5-fluorouracil, and there is no significant correlation with the melting point temperature observed. Hydrogen bonded layers are more strongly stabilised one with another, when methyl substituents or sulphur atoms are present. Charge-density-derived interaction strengths were in a good accordance with the interaction energy calculation results. Furthermore, the energy calculations revealed the particular importance of properly determined positions of hydrogen atoms.

- [1] Jarzemska, K. N.; Kubsik, M.; Kamiński, R.; Woźniak, K.; Dominiak, P. M. (2012) *Cryst. Growth Des.*
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[2] Jarzemska, K. N.; Dominiak, P. M. (2012) *Acta Cryst.* **A68**, 139-147

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