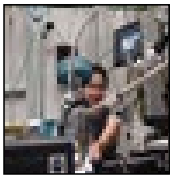
OPEN ACCESS Freely available online

Journal of Advanced Chemical Engineering

Crystallographic Data and Model Quality – Beyond 0.8 Å and Independent Atom Model



Maura Malinska

University of Warsaw, Poland

Abstract

Commonly, the Independent Atom Model (IAM) of electron density is used in the case of routine X-ray data analysis. However, this model does not give a quantitative description of electron density distribution because atoms are assumed to be neutral and spherical. The aim of the project is using new methods that have been developed for reconstruction of electron density against CuKα X-ray diffraction data. These methods are Bond-Oriented Deformation Density Model (BODD), Our study showed agreement between results after refinements against MoKα and CuKα data. Observed systematic errors for CuKα data are; systematically higher ADPs of heavy atoms and less density information in residual density maps and fractal dimension plots. It stems from the amount of the information available in CuKα data. Undoubtedly, the use of described methods results in more precise and accurate final structures comparing to the IAM structure. As expected HAR and TAAM methods are more precise and accurate than BODD, while BODD is faster and more user-friendly. HAR and TAAM results are similar, however, for HAR refinement we recommend to estimate the ADPs of hydrogen atoms with the aid of the SHADE server.

Biography

Maura Malinska has completed her PhD in 2014. She is the assistant professor at University of Warsaw, Poland. She has 48 publications that have been cited over 800 times, and her publication H-index is 16.

Citation: Maura Malinska, *Crystallographic Data and Model Quality – Beyond 0.8 Å and Independent Atom Model*, International Conference on Crystallography and Structural Chemistry| Barcelona, Spain | August 31, 2020