

Poster Presentations

[MS45-P07] On The Quality Of Single Crystal X-ray Results.

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Although everything seems to be already well known in the field of routine structural single crystal X-ray analysis, even commonly used approaches should be critically reevaluated. In this communication, a detailed comparison of single crystal X-ray and neutron structural results will be presented. It will be shown how structural parameters, such as bond lengths and valence angles, are dependent on the 2θ diffraction angle. Accuracy and precision of structural data will be discussed. The commonly accepted checkcif benchmark parameters will be questioned. Some practical suggestions will be presented how to estimate and improve the quality of single crystal X-ray diffraction structural results. It appears that one can optimise measurements of diffraction data to get structural results comparable to those obtained by using single crystal neutron diffraction. Also a comparison of geometrical parameters obtained from routine low resolution and charge density high resolution single crystal X-ray studies will be presented.

Keywords: accurate geometry; quality of X-ray results, routine vs. high resolution data;