

Crystallographic Literacy – American Crystallographic Association

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The American Crystallographic Association is developing a series of web-based lectures to help develop crystallographic literacy within the broader scientific community. The lectures are planned to be 5 to 10 minute discussions by experts in the field to help build knowledge of theory and best practices in crystallography. This presentation will highlight the direction and information that will be provided. The series will be a continuing project directed by the Education Committee and the ad hoc Crystallographic Literacy Group. The website will be live with some videos by the ACA Annual Conference.

An important aspect is the ability of dynamical refinement to determine the absolute structure of non-centrosymmetric crystals and thus the absolute configuration of chiral molecules. The physical effect behind this ability is not the resonant scattering like for x-ray diffraction, but the multi-beam interference. Hence, the limitations of absolute structure determination inherent to x-ray diffraction do not apply to electron diffraction. The determination of absolute structure is very robust and can be based on a simple comparison of the figures of merit of the two inverted models. The difference in the R1 values is typically several percent. Unlike for x-rays, the absolute structure can be equally easily determined for heavy-atom structures and light-atom structures [4,6].