FAKULTÄT FÜR CHEMIE

universität wien

Einladung zum Vortrag von

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MIT Department of Chemistry's X-ray Diffraction Facility, Cambridge, MA, USA

"Single-Crystal X-Ray Diffraction: Structure Determination for Chemistry and Pharmaceutical Research"

Although widely regarded as one of the most powerful tools of three-dimensional structure elucidation, single-crystal x-ray diffraction has its limitations. The need for a high quality single crystal is perhaps the most obvious weakness, however a more subtle yet serious issue is the lack of understanding about the method itself. Because the final product of a crystal structure determination gives rise to a beautiful photorealistic rendering of the atomic model that looks just like a photograph of the molecule, scientist and laypersons alike tend to uncritically believe what they see, thus overestimating the powers of the method. The most fundamental misunderstanding probably lies in the circumstance that x-ray diffraction is not a spectroscopic method. That means one does not record individual responses from atoms or functional groups but rather the Fourier transformation of the complete electron density function in the unit cell. Also commonly ignored is the fact that a crystal structure is the spatial and temporal average over the whole crystal and the full duration of the diffraction experiment, which gives rise to challenges such as twinning or disorder. Powerful as the method may be, crystal structure determination is complex and not usually trivial. In order to learn the most from a given diffraction experiment, one has to thoroughly understand the method and one has to carefully and skillfully perform every step of structure determination. By means of case studies, this presentation will briefly introduce the method and outline some of the typical pitfalls of single-crystal structure determination.

Mittwoch, 11. April 2018, 14:00 Uhr
Seminarraum 2 der Fakultät für Chemie
Währinger Straße 42, 1090 Wien

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