

Some Unusual Applications of Crystallography

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Structure determination is a vital part of chemistry. The information about atom position and molecule geometry provides the basis for modelling, it proves the success of a new synthesis pathway. X-ray crystallography plays a major role amongst several ways for structure determination, including the unique features to determine the absolute chirality, or experimental access to the nature of electronic bonding. In my talk, I will present some of the less usual faces of crystallography. The combined analysis of anomalous signal and careful structure refinement with SHELXL at 2Å resolution led to the downfall of the model of ion transport in potassium channel proteins [1] - a model established since 1955 that has been taught in many biochemistry lectures. More recently, I changed X-rays for electrons. With electrons, single crystal structures can be determined from crystals less than 1 micrometer in size. Electron diffraction data show that ZSM5 grains, an industrially used class of zeolite catalysts, are single crystals and not intergrown [2]. I also constructed of a prototype electron diffractometer together with the company Dectris Ltd. With this machine I could extract the single crystal structure from a capsule of Grippostad, a drug against the symptoms of the cold. The possibility to decompose X-ray powder spectra into their single crystal structure components may place an end to many costly patent litigations [3, 4].

[1] D. A. Köpfer, C. Song, T. Gruene, G. M. Sheldrick, U. Zachariae, B. L. de Groot: "Ion Permeation in K⁺ Channels Occurs by Direct Coulomb Knock-On", *Science* (2014), 346, pp. 352-355

[2] T. Gruene*, T. Li, E. van Genderen, A.B. Pinar, J.A. van Bokhoven: "Characterization at the level of individual crystals: single crystal MFI type zeolite grains" *Chem. Eur. J.* (2017), 27, pp. 2384-2388

[3] T. Gruene* et al., "High-throughput Structural Chemistry with Electron Diffraction", manuscript in preparation.

[4] T. Gruene* et al., "An Electron Diffractometer with an EIGER detector for Structural Chemistry", manuscript in preparation.