Absolute Configuration Determination for Light Atom Structures using Low Power Microfocus X-ray Sources

J. Graf¹, H. Ott², T. Stuerzer², M. Ruf³, B. Noll³, M. Benning³, C. Michaelsen¹, B. Dittrich⁴

The determination of the absolute configuration for light-atom structures has become central to research in pharmaceuticals and natural products synthesis. In the absence of elements heavier than silicon, it is often problematic to make a significant assignment of absolute configuration, especially for smaller crystals.

Besides the introduction of new mathematical methods to evaluate the Bijvoet differences, the assignment of the absolute structure for light atom compounds has become easier with the advent of high-intensity microfocus sources, as the increased flux density improves the anomalous signal through improvements in counting statistics.

In this presentation, we will be reviewing the current performance levels of different low power microfocus X-ray sources, such as the I μ S and the METALJET X-ray source. Further, we will be discussing the main features of the newest generation of the I μ S. We will be presenting selected results to demonstrate the impact of these modern microfocus X-ray sources on the data quality for applications in chemical and biological crystallography.

¹ Incoatec GmbH, Geesthacht, Germany

² Bruker AXS GmbH, Karlsruhe, Germany

³ Bruker AXS Inc., Madison (WI), USA

⁴ Heinrich-Heine-Universität Düsseldorf, Germany