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Light-Atom Structures: Absolute Configuration Determination and Beyond

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The determination of the absolute configuration for light-atom structures is central to research in pharmaceuticals and natural-product synthesis [1]. In the absence of elements heavier than silicon, it is often problematic to make a significant assignment of absolute configuration. Traditionally, heavy-atom derivatives were prepared which have a stronger anomalous signal compared to the native compound. However, this is not always feasible. The assignment of the absolute structure of pure organic compounds has become somewhat easier with the advent of high-intensity microfocus sources [2], as the increased flux density improves the anomalous signal through improvements in counting statistics. In order to maximize the anomalous signal, X-ray sources with Cu anodes are usually used for the absolute structure determination. However, these data are usually limited to a maximum resolution of about 0.80 Å. High-brilliance microfocus X-ray sources with Mo targets enable the collection of high quality data beyond 0.40 Å within a reasonable amount of time. This allows not only a more accurate modelling of the electron density by using aspherical scattering factors, but also enables a reliable determination of the absolute structure, despite the significantly lower anomalous signal obtained with Mo Kα radiation. With the recently introduced liquid-Gallium-jet X-ray source unprecedented beam intensities can be achieved [3]. The shorter wavelength of Ga Kα compared to Cu Kα slightly weakens the anomalous signal of a typical light-atom structure. However, due to the shorter wavelength, the highest resolution for the liquid metal-jet source is typically at about 0.70 Å, compared to about 0.80 Å for Cu Kα. Hence, about 50% more unique reflections can be recorded. This clearly improves the structural model and the quality of the Flack parameter. Selected results on the absolute structure and charge density determinations for light-atom structures will be presented.

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