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 modelisation of those reflections, which leads to the breakdown of Friedel’s law (i.e., $F_{hkl} \neq F_{-h-k-l}$). In order to account for the anomalous dispersion, a correction has to be applied to the atomic scattering factor of an anomalous scatterer. $F'_{hkl}$ describes the change in the amplitude, while $\Delta F_{hkl}$ represents the change in the phase angle. The dispersion corrections applied to the atomic scattering factor of an anomalous scatterer are given by $f'_{\alpha}$ and $\Delta f_{\alpha}$ as constants for a given wavelength.

Absolute Structure and Anomalous Dispersion

Absolute structure determination for an enantio-pure crystal is the determination of the spatial arrangement of a chiral molecule (absolute configuration). Due to the anomalous scattering, the diffraction from such a crystal shows a change in the phase and amplitude of interference-related reflections $F_{hkl}$ and $F_{-h-k-l}$. This causes small but measurable differences in the intensities of those reflections, which leads to the break-down of Friedel’s law. In order to account for the anomalous dispersion, a correction has to be applied to the atomic scattering factor of an anomalous scatterer. $F'_{hkl}$ describes the change in the amplitude, while $\Delta F_{hkl}$ represents the change in the phase angle. The dispersion corrections applied to the atomic scattering factor of an anomalous scatterer are given by $f'_{\alpha}$ and $\Delta f_{\alpha}$ as constants for a given wavelength.

Case Studies for Absolute Structure Determination

Case Study 1: Sucrose crystal, $C_{12}H_{22}O_{11}$, $a = 7.7189(2)$ Å, $b = 8.6428(2)$ Å, $c = 10.8085(3)$ Å, $Z = 102.999(1)$ Å, $T = 293 K$, $Z = 2$, $P_21_2_1_2_1$

Case Study 2: LARGER XYSULPHITE crystal, $a = 5.9744(2)$ Å, $b = 6.7921(2)$ Å, $c = 4.7144(6)$ Å, $Z = 100 K$, $Z = 4$, $P_2_1_2_2_1$

Conclusion

X-ray sources with Cu anodes are usually used for the absolute structure determination due to the high anomalous signal for Cu radiation. However, the data resolution from Cu sources is limited to 0.80 Å. Microfocus X-ray sources using energies higher than 8 kV such as the Mo-μs3 HB and the METALJET X-ray source, deliver data of high quality. Due to the shorter wavelength, a higher resolution can be achieved and, hence, more unique data are accessible. This allows for a more detailed description of the structural model using aspheric scattering factors, which also improves the precision of Flack parameter.