GI-MS48-P05 | WANTED -- K-BETA!

Bodensteiner, Michael (University of Regensburg, Regensburg, GER); Mayer, Tobias (University of Regensburg, Regensburg, GER)

The Cu-K β wavelength (λ = 1.39 Å) has been known for a very long time, mostly as result of an unsuccessful alignment of the diffractometer optics. However, there are benefits and powerful features of this radiation that many crystallographers are not aware of. Compared to Cu-K α (λ = 1.54 Å) the amount of available data is increased by more than 35 per cent and the absorption significantly lowered. The latter is also true for a number of elements (Cu to Y) in comparison to Mo-K α radiation (λ = 0.71 Å). In addition, the diffraction power as well as the detective quantum efficiency is much higher for Cu-K β relative to Mo-K α . Another general advantage of K β radiation compared to K α is the absence of $\alpha 1/\alpha 2$ splitting at higher diffraction angles. This leads to a relative improvement of the $1/\sigma(I)$ at higher resolution. Our investigations have shown that in many cases almost identical or even better quality structures could be obtained by using Cu-K β compared to either Mo or Cu standard K α wavelengths. The presentation will show this at a number of examples and provide insight into the technical and refinement procedures within Cu-K β experiments.