In-house S-SAD and Se-SAD phasing with Cr Kα Radiation

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With the recent advances in X-ray technology, chromium radiation (2.29 Å) has become viable for in-house data collection and phasing. Chromium radiation appears to be well suited for measuring anomalous signals from weak anomalous scatterers such as sulfur, selenium, and calcium. In particular, the anomalous scattering strengths of sulphur (f''=1.14 e) and selenium (f''=2.28 e), the most common intrinsic and derivatized anomalous scatterers, are doubled when using Cr Kα radiation compared to those for Cu Kα radiation (1.54 Å, S: f''=0.56 e, Se: f''=1.14 e). Due to the difficulties in utilizing the K absorption edge of sulphur at 5.02 Å, limited access to X-ray beamlines and related transportation issues, it has become evident that Cr Kα radiation is very good choice for collecting sulphur anomalous data and a may be an alternative to a synchrotron beamline for collecting selenium anomalous data. This report shows examples of S-SAD and Se-SAD phasing from data collected on an in-house Cr source. To break the phase ambiguity inherent with SAD, the direct-methods procedure implemented in the program OASIS-2004 was employed. Phase discrimination using the product of the Sim and Cochran distributions leads to better initial phases and, consequently, to better electron-density maps.

Keywords: Cr radiation, S-SAD phasing, Se-SAD phasing