

Phasing in the Home Laboratory

Cheng Yang, James W. Pflugrath, and Joseph D. Ferrara

Rigaku Americas Corp., The Woodlands, TX 77381

Many examples of S-SAD and Se-SAD phasing have been reported with diffraction data collected away from absorption edges with copper radiation (1.54 Å) as well as at the K absorption edge of selenium with synchrotron radiation (0.979 Å). Chromium radiation (2.29 Å) has been available for in-house data collection for a few years now, and a number of successful SAD experiments using Cr radiation have been published by several groups. However, Cr radiation has not been fully utilized despite being ideally suited for measuring anomalous signals from weak anomalous scatterers such as sulphur, selenium, calcium, and other atoms commonly found in protein crystals.

We explore why softer x-rays generated by a Cr anode may be better than a synchrotron source. Beam stability, radiation damage, and mechanical issues are less of a problem with in-house experiments. The human psychology of travel and use of an unfamiliar experimental station may also be avoided with an in-house system. This is a cost effective method of single crystal x-ray diffraction data collection and structure determination that is especially useful when time is of the essence and synchrotron time is unavailable due to shutdowns and maintenance. In the end the tortoise may win the race.

With the addition of Cr radiation to the crystallographer's toolkit, in-house x-ray sources can routinely provide at least two wavelength options. This report also discusses the results of phasing by combining diffraction data from both Cu and Cr-collected data sets.