

## Experimental Phasing with Powder Data

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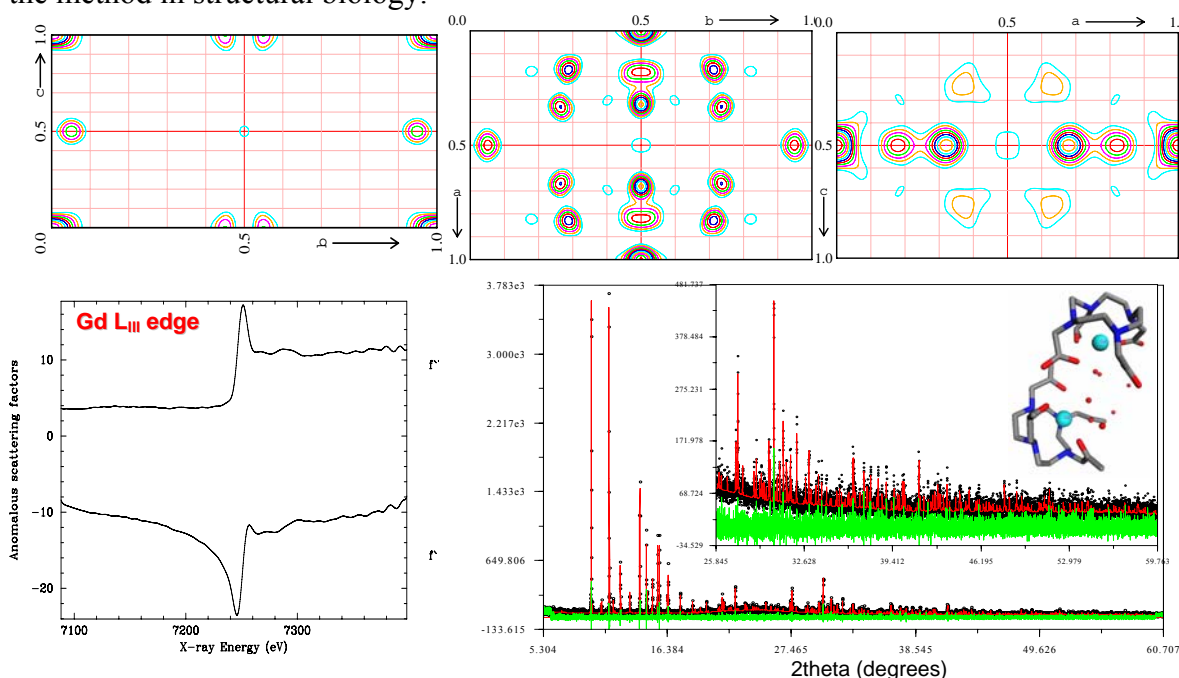
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X-ray diffraction is amongst the most important methods for obtaining information about the structure of proteins and thereby gain insight into fundamental biological and biochemical mechanisms. Determination of protein structures is currently dependent on the availability of good quality and sizeable single crystals. On the other hand, polycrystalline materials have been extensively employed for structural studies of materials where single crystals are unavailable. The strategy we develop in this area is associated with novel methods for powder diffraction data collection and interpretation. Examples which will be presented include the experimental phasing of the Gd-HPDO3A complex [1] and hen egg-white lysozyme tetragonal derivative crystals with lanthanide complexes [2]. The issues which will be discussed demonstrate the power and the future applicability of the method in structural biology.



**Figure 1:** *Upper:*  $w = 1/2$  Harker sections of Patterson maps for Gd-HPDO3A crystals. Levels are contoured in  $1\sigma$  steps. *Lower-Left:* Anomalous scattering factors around the Gd- LIII absorption edge (7.246 keV). *Lower-Right:* Pawley refinement ( $Rwp = 5.23\%$ ,  $\chi^2 = 1.4643$ ) of the powder data collected at 7.209 keV ( $\lambda \sim 1.719 \text{ \AA}$ ). In total 611 intensities contribute to the profile to  $1.72 \text{ \AA}$  resolution. The lower solid line shows the difference profile. *Inset1:* Magnification of the powder data in the  $25.8^\circ$ - $59.7^\circ$   $2\theta$  range. *Inset2:* Schematic representation of the GdHPDO3 conformation. The grey, blue, red and light blue colours correspond to C, N, O and Gd atoms respectively.

### References

- [1] K. Kumar et al., Inorg. Chem. **33**, 3567-3575 (1994).
- [2] É. Girard, M; Stelter, J. Vicat, R. Kahn, Acta Cryst. **D59**, 1914-1922 (2003); É Girard, E. Pebay-Peyroula, J. Vicat, R. Kahn, Acta Cryst. **D60**, 1506-1508 (2004).