Using lanthanide complexes for solving macromolecular structures

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Lanthanides exhibit numerous properties making them very attractive for solving macromolecular structures by X-ray crystallography. Their high Z number (Z = 57 for La, Z = 71 for Lu) make them good candidate for preparing heavy-atom derivatives. They all present a strong white-line in their L_{III} absorption edge (f'' ~ 30 e^-), which can be used for anomalous diffraction experiments. However, except for Ca-binding proteins, where they substitute for Ca, they are often difficult to incorporate into crystalline material without disrupting 3-D order. We have developed a method to introduce them into crystals by using lanthanide complexes originally developed for medical imaging. Since they do not make covalent bond to proteins they are generally used at quite high concentrations (100 mM and higher) to prepare derivative crystals either by soaking or by co-crystallization. Recently we developed new lanthanide complexes that establish stronger binding to proteins. Well-diffracting single crystals were obtained by co-crystallization with several proteins. However, in most cases crystalline precipitates are obtained from which powder-diffraction experiments exploiting anomalous diffraction could be undertaken.