CFEL SCIENCE

Colloquium

25th October 2013 - 14:00

CFEL, Building 99, seminar rooms I-III

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An overview of the modern phasing methods and of their perspectives

Modern *ab initio* phasing methods *(AB)* solved in practice the phase problem for crystal structures up to 200 non-H atoms in the asymmetric unit. They do not require prior structural information, but were demanding in terms of data resolution. Thus they were historically considered not suitable for protein phasing.

Molecular Replacement *(MR),* Isomorphous Derivative *(ID)* and Anomalous Dispersion Techniques *(AD)* are able to solve most of the structural problems in protein crystallography provided crystal of sufficient size and quality are available. Unfortunately many important substances are difficult to crystallize: this limitation encouraged the application of the synchrotron radiation to crystallographic problems. Data resolution improved and smaller limits to the size of the crystals could be settled.

An overview of the results today achievable via *AB, MR* and *AD* will be given. In particular it will be shown that:

a) Also *AB* methods are useful for phasing proteins. The techniques are particularly appealing since they are less demanding in terms of data resolution. Patterson, Direct Methods and *VLD (Vive la Difference)* methods will be shortly recalled.

b) The modern probabilistic approaches to *MR* and *AD* methods will be briefly illustrated and some applications will also be described;

Quite recently X-ray lasers new capabilities made scattering from single objects an experimental technique very appealing for phasing. Indeed it offers the possibility of making structural studies by using scattering from single non-crystalline particles or molecules. In this context the bases of the theory of the *confined structures*, related to the reciprocal-space oversampling method, will be described and the first applications illustrated.

Hosts: Henry Chapman + Francesco Stellato - Coherent Imaging Division