

Glossary of terms – extension

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Diagrams

Ewald construction

Demonstrates the equivalence between the reciprocal lattice and the diffraction pattern. A crystal is placed in the center of a sphere with the radius of $1/\lambda$ (the Ewald sphere). The point through which the primary X-ray beam leaves the sphere defines the origin of the reciprocal lattice of the crystal. Bringing a reciprocal lattice point hkl into coincidence with the sphere, is equivalent to orienting the set of planes with indices (hkl) at the Bragg glancing angle θ with respect to the primary beam. In effect, each intersection of a reciprocal lattice point with the Ewald sphere defines when and where a Bragg reflection occurs.

Argand diagram

Complex numbers of the form $F=A+iB$ are represented on a plane (Argand plane), in much the same way as real numbers are represented on a line. If F is considered as a vector, then A corresponds to its component on the horizontal (real) axis, and B to its component on the vertical (imaginary) axis. The vertical axis is called "imaginary" because it has a unit of $i=\sqrt{-1}$, which is not a real number. The vector F has its length, or modulus, $|F|$ and an angle of inclination to the real axis, φ . An alternative expression for F is $F=|F|(\cos\varphi + i\sin\varphi)$. It can be rewritten using the Euler notation $F=|F|e^{i\varphi}$.

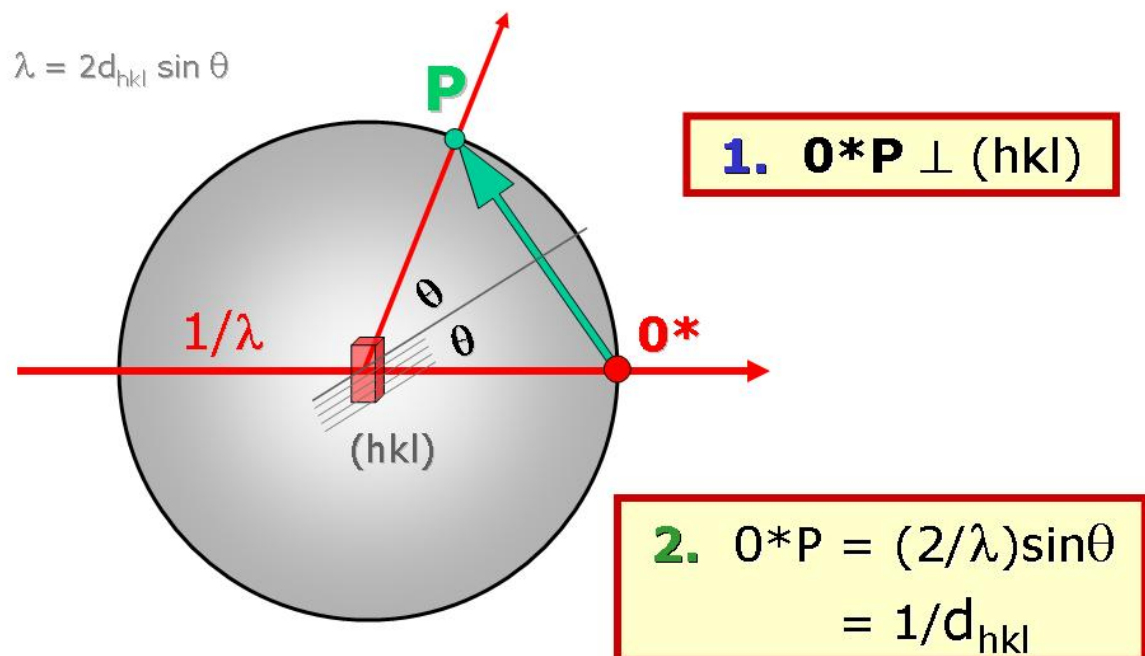
Harker diagram

A construction showing how the phase problem is resolved in the Isomorphous Replacement method. It is based on the vector equation $F_{PH}-F_H=F_P$ (*), where F_P is the native Protein structure factor (known experimentally as its modulus), F_{PH} is the analogous structure factor for the Heavy atom isomorphous derivative of the Protein crystal (also known from the experiment as $|F_{PH}|$), and F_H is an artificial structure factor calculated (as both the magnitude and phase) for the known substructure of the heavy atoms. To find the unknown phase of F_P (φ_P), we draw one circle with a radius of $|F_P|$ and another one using a new origin at $-F_H$ and a new radius of $|F_{PH}|$. The points where the two circles intersect, fulfill the equation (*). With one heavy atom derivative (SIR, Single Isomorphous Replacement), there are usually two such points, and the total lack of phase information is narrowed to a choice of two possibilities. For unique phase determination, another derivative is necessary (MIR, Multiple Isomorphous Replacement). This is equivalent to drawing, in an analogous way, a third circle, which will intersect the $|F_P|$ circle at only one of the former choices.

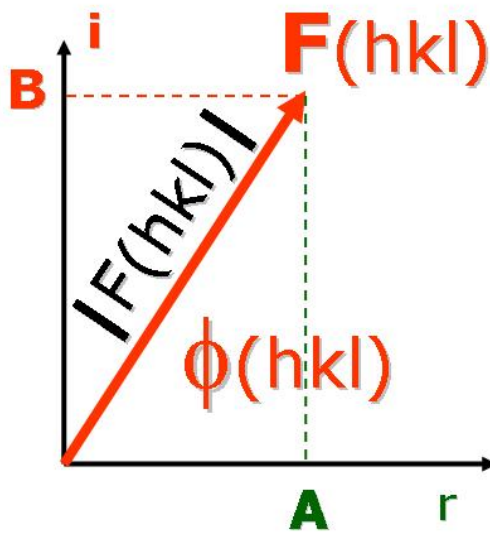
Ramachandran Plot

The conformational φ, ψ space of an alanylalanine dipeptide is searched and the results are plotted after Gopalasamudram Narayan Ramachandran on a diagram with the φ axis horizontal (from -180 to 180°) and the ψ axis vertical (from -180 to 180°). What is plotted is the energy of each conformer defined by a pair of φ, ψ angles. Usually, the isoenergetic contours (levels of constant energy) are represented by color, with light colors (white, yellow) representing high energy or impossible conformations, and dark colors (light to deep red) representing low energy (wells) or favorable conformations. Most of the Ramachandran plot area is light. There are only two prominent energy wells, one at about $\varphi=-60^\circ$, $\psi=-60^\circ$, and another at about $\varphi=-120^\circ$, $\psi=120^\circ$. A protein main chain with repeating φ, ψ angles from the first region will form an α -helix, and with repeating φ, ψ angles from the second region will form a β -strand.

Ewald Construction



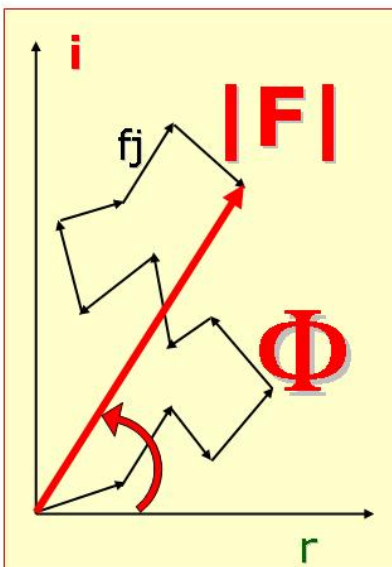
Argand representation of a complex number



$$\begin{aligned}
 \mathbf{F}(hkl) &= A + iB \\
 &= |F(hkl)| \cdot (\cos\phi + i\sin\phi) \\
 &= |F(hkl)| \cdot \exp(i\phi)
 \end{aligned}$$

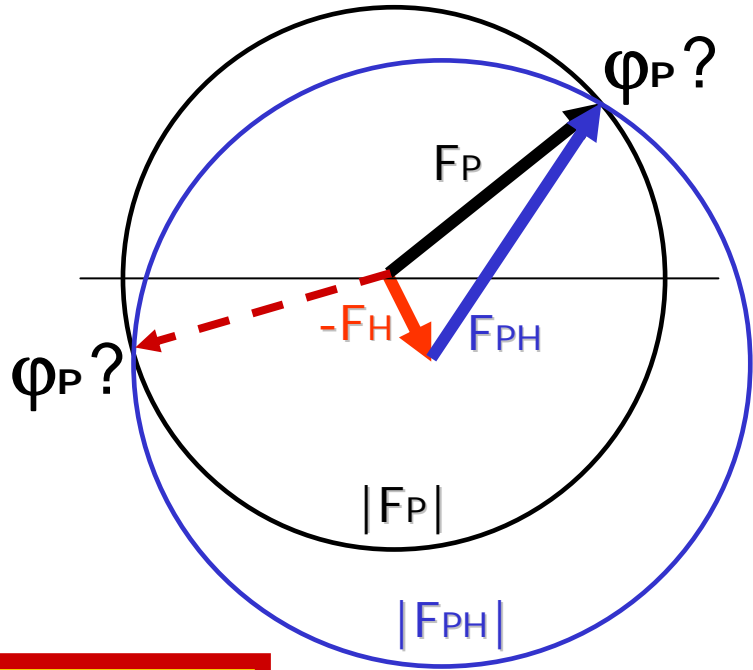
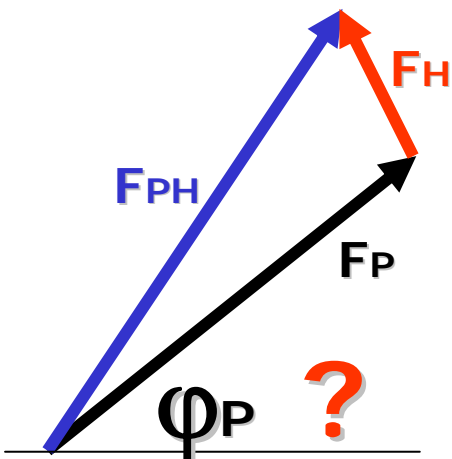
↑ ↑
magnitude *phase*

The Argand Diagram illustrates $F(hkl)$ as a Fourier summation in the complex plane



$$F(hkl) = \sum f_j \exp[2\pi i(hx_j + ky_j + lz_j)]$$

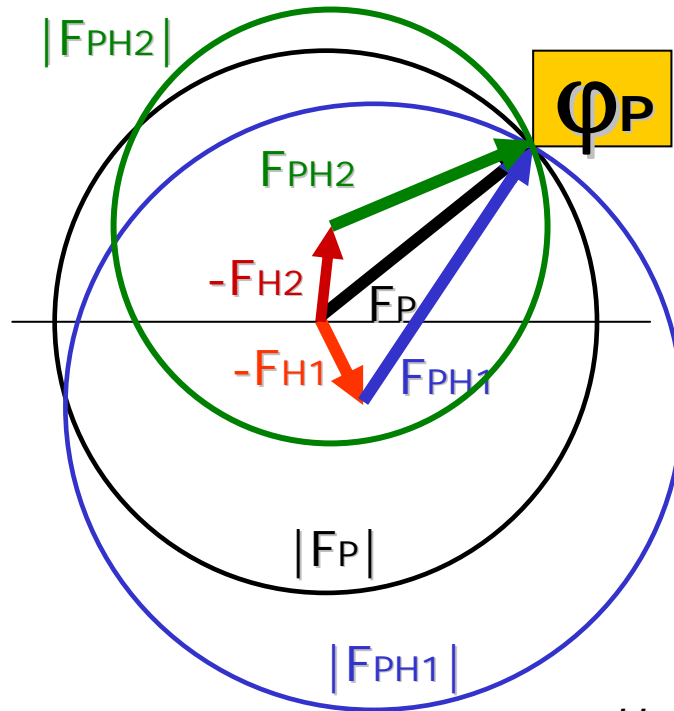
Isomorphous replacement SIR



$$F_{PH} = F_P + F_H$$

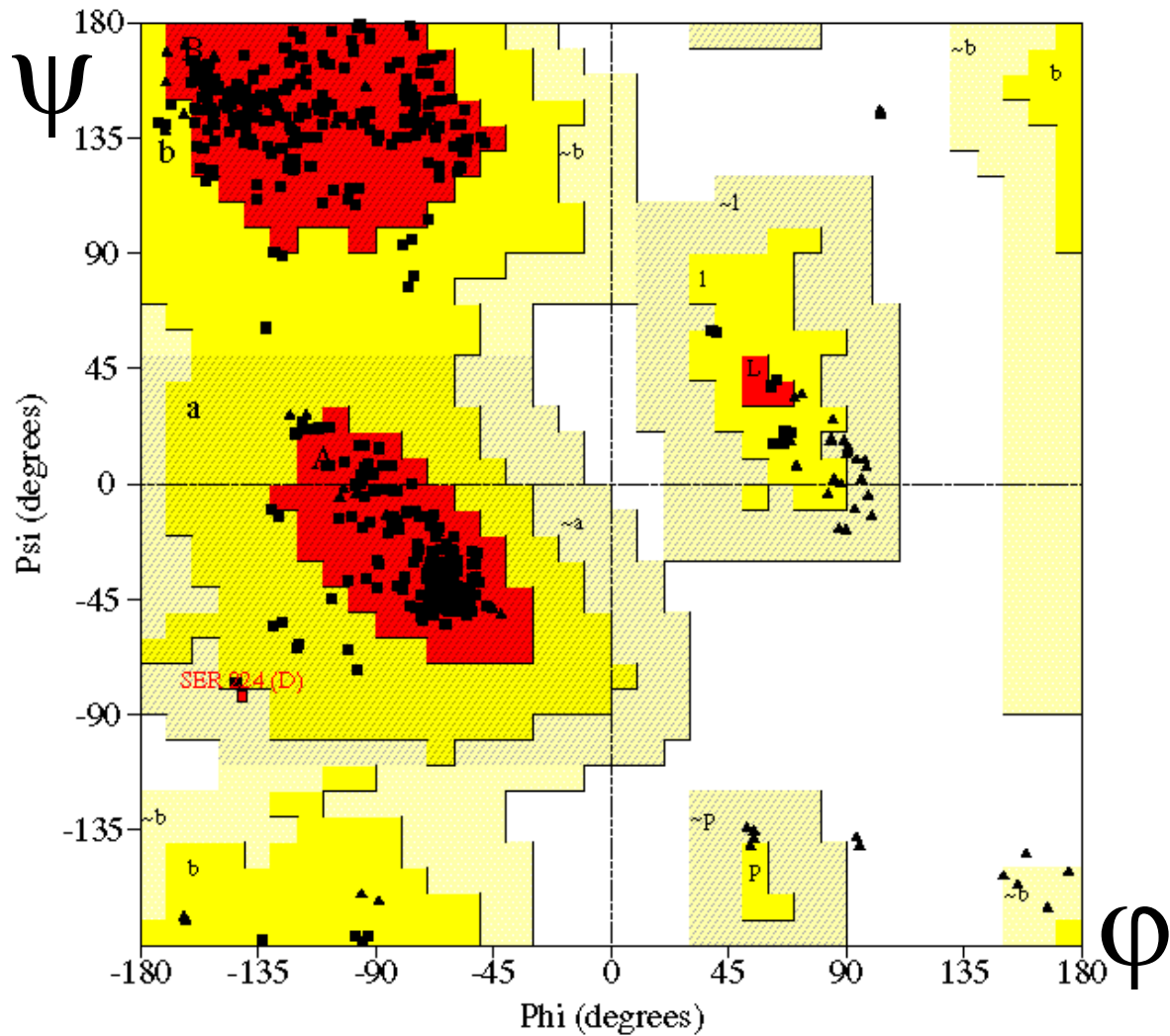
Harker diagram

Isomorphous replacement MIR



Harker diagram

Ramachandran Plot



Methods for the solution of the phase problem

SIR/MIR Isomorphous Replacement

MR Molecular Replacement

MAD Multiwavelength Anomalous Diffraction

SAD Single-Wavelength Anomalous Diffraction

Direct Methods

Heavy-Atom Method

Trial-and-Error

Multi-Beam Diffraction

Famous names in crystallographic terms

Bravais

Fourier

Hermann-Mauguin

Laue

Bragg

Ewald

Harker

Patterson

Bijvoet

Friedel

Wilson