

3.11: Electron density map

A three-dimensional description of the electron density in a crystal structure, determined from X-ray diffraction experiments. X-rays scatter from the electron clouds of atoms in the crystal lattice; the diffracted waves from scattering planes h,k,l are described by structure factors \mathbf{F}_{hkl} . The electron density as a function of position x,y,z is the Fourier transform of the structure factors:

$$\rho(xyz) = \frac{1}{V} \sum_{hkl} F(hkl) \exp[-2\pi i(hx + ky + lz)] .$$

The electron density map describes the contents of the unit cells averaged over the whole crystal and not the contents of a single unit cell (a distinction that is important where structural disorder is present).

Three-dimensional maps are often evaluated as parallel two-dimensional contoured sections at different heights in the unit cell.

Units

Electron density is measured in electrons per cubic ångström, $\text{e } \text{\AA}^{-3}$.

Contributors

This page titled [3.11: Electron density map](#) is shared under a [CC BY 4.0](#) license and was authored, remixed, and/or curated by [Online Dictionary of Crystallography](#) via [source content](#) that was edited to the style and standards of the LibreTexts platform.