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, e Å^{-3}.

Contributors