How can you obtain the crystal structure of a crystalline compound from the experimental diffraction data?

The determination of a crystal structure is called solving a structure. When using X-rays, the aim is to find the electron density (if X-rays are used) for every point in the unit cell. Once the electron density is found, it is an easy task to obtain the positions and nature of each atom in the unit cell.

The electron density is usually expressed as $\rho(\mathbf{x})$ where $\mathbf{x}$ is a vector pointing to a location inside the unit cell. The unit is given in electron/Å^3.

$$\rho(\mathbf{x}) = \frac{1}{V}\sum_{\mathbf{h}} F(\mathbf{h}) \exp(-2\pi \mathrm{i}\mathbf{h}\mathbf{x})$$

This equation shows that the electron density can be obtained from the full set of structure factors $F(\mathbf{h})$. The structure factor is a complex magnitude and fully characterise the unit cell content

$$F(\mathbf{h}) = \sum_i f_i(\mathbf{h}) \exp(2\pi \mathrm{i}\mathbf{h}\cdot\mathbf{x_i})$$

The magnitude $f_i(\mathbf{h})$ is the **atomic scattering factor** and is tabulated for each atom. The sum encompasses all atoms at position $\mathbf{x}_i$ inside the unit cell.

Thus, each structure factor consists of an **amplitude** and a **phase**. The good news is that the amplitudes can be obtained from the experimental measurements of all the diffracted beams. The bad news is that the phase cannot be retrieved experimentally.

Since the discovery of crystal diffraction, specialists have invented many methods for retrieving phases. We shall not deal with those historical methods but we will mention a very powerful algorithm that solved the phase problem in most cases, *i.e.* the **charge flipping algorithm**. To learn more about this, you can refer to the question dealing with the charge flipping algorithm.

Once the phases are retrieved and combined with the magnitudes of the structure factors, it is straightforward to obtain the electron density (top relation) of the unit cell and thereby determine the atomic positions in the unit cell.