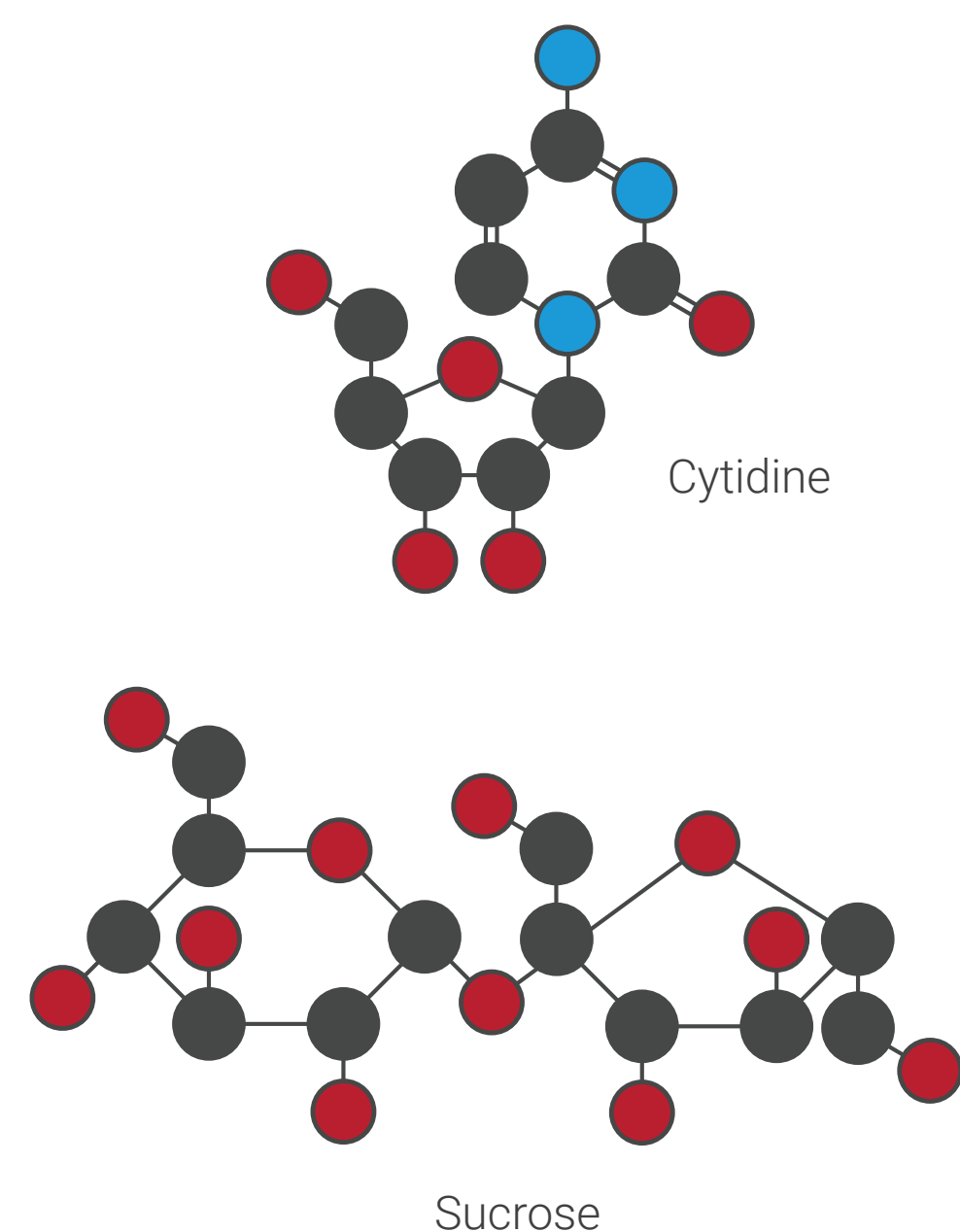
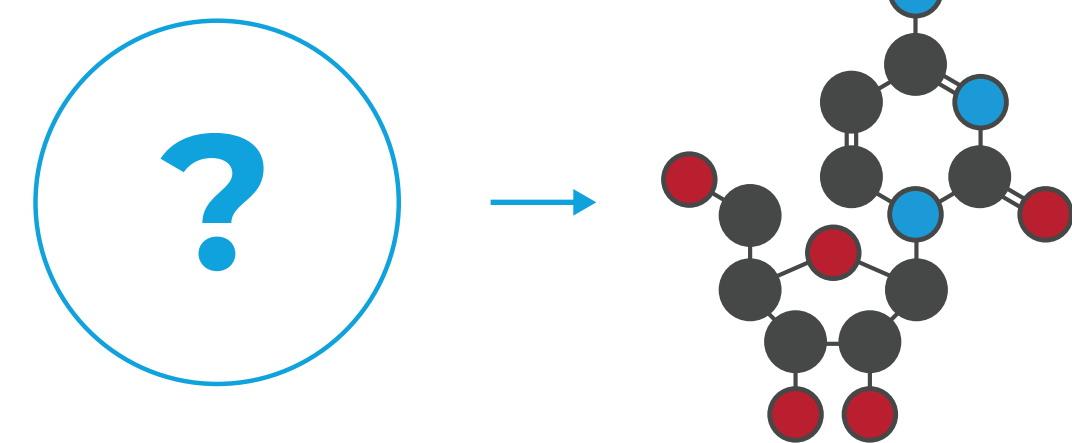


What can crystallography tell us?

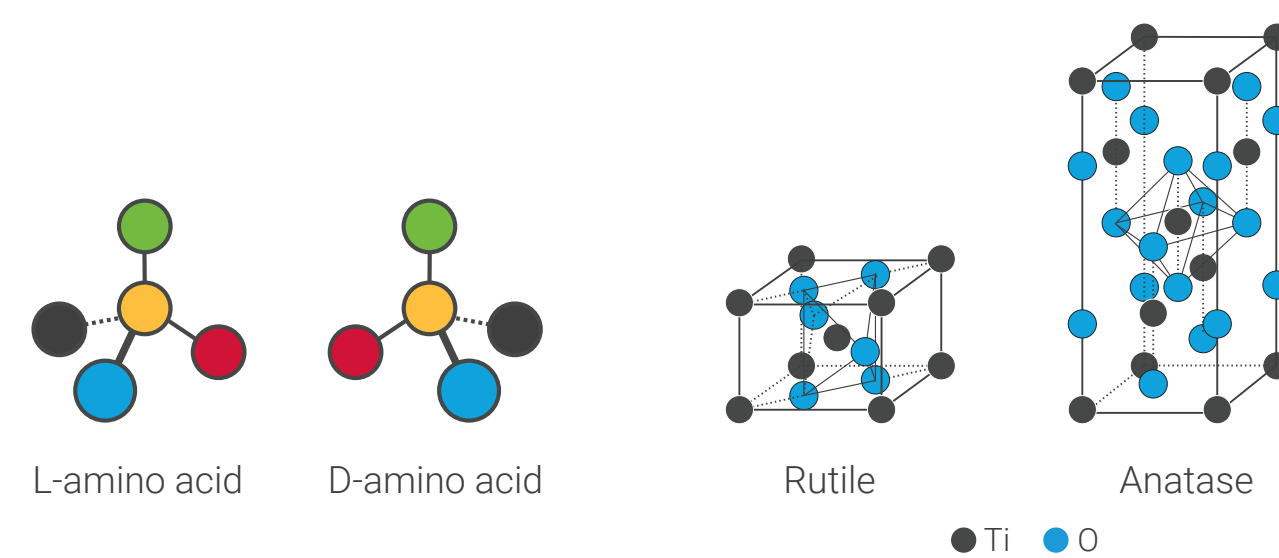
The three-dimensional (3D) structure of a molecule can be determined.



What are the benefits of crystallography?



The molecular structure of an unknown compound can be visualized without prior information such as a chemical formula.

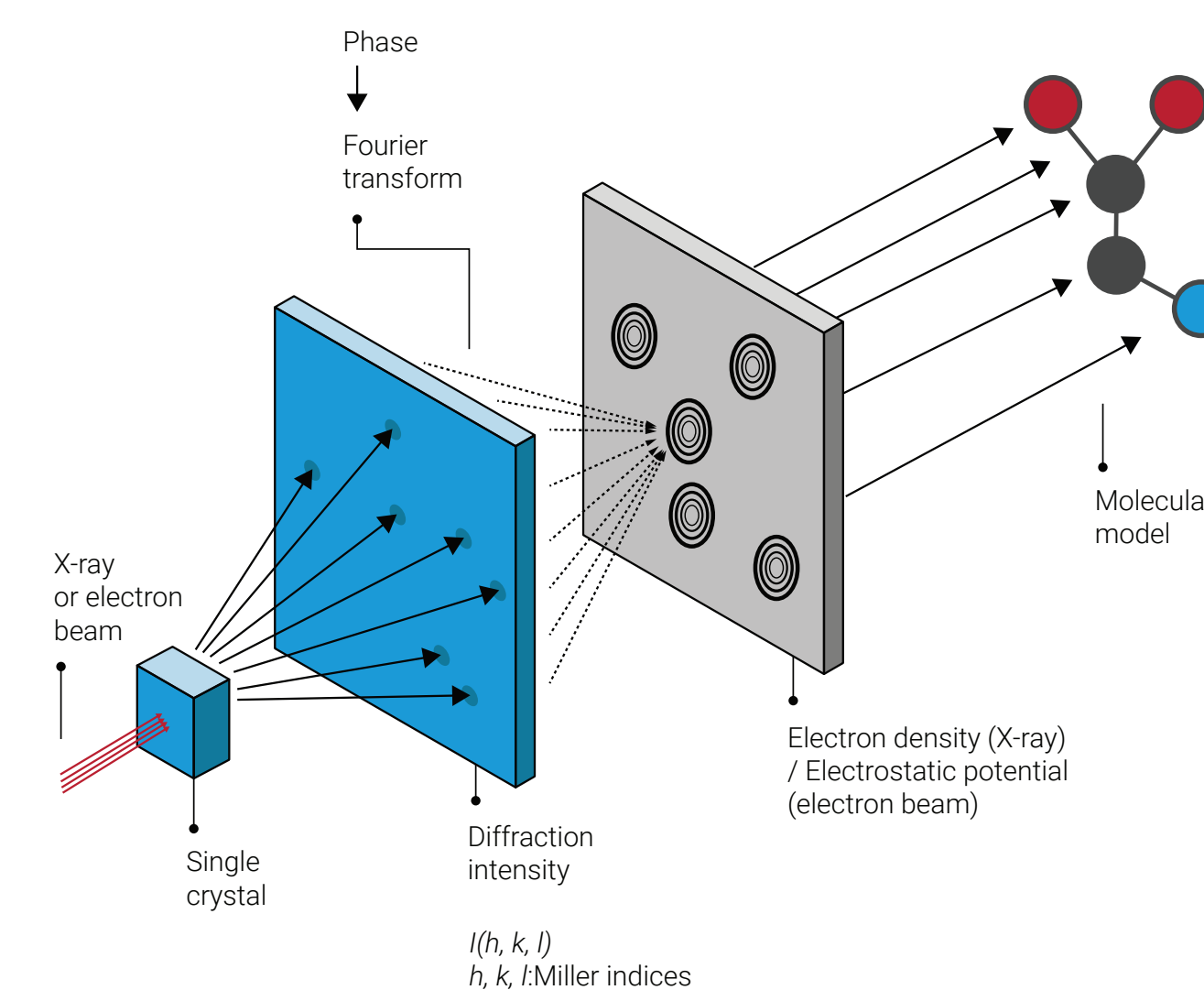


Chiral molecules can be distinguished.

Crystal polymorphs can be identified.

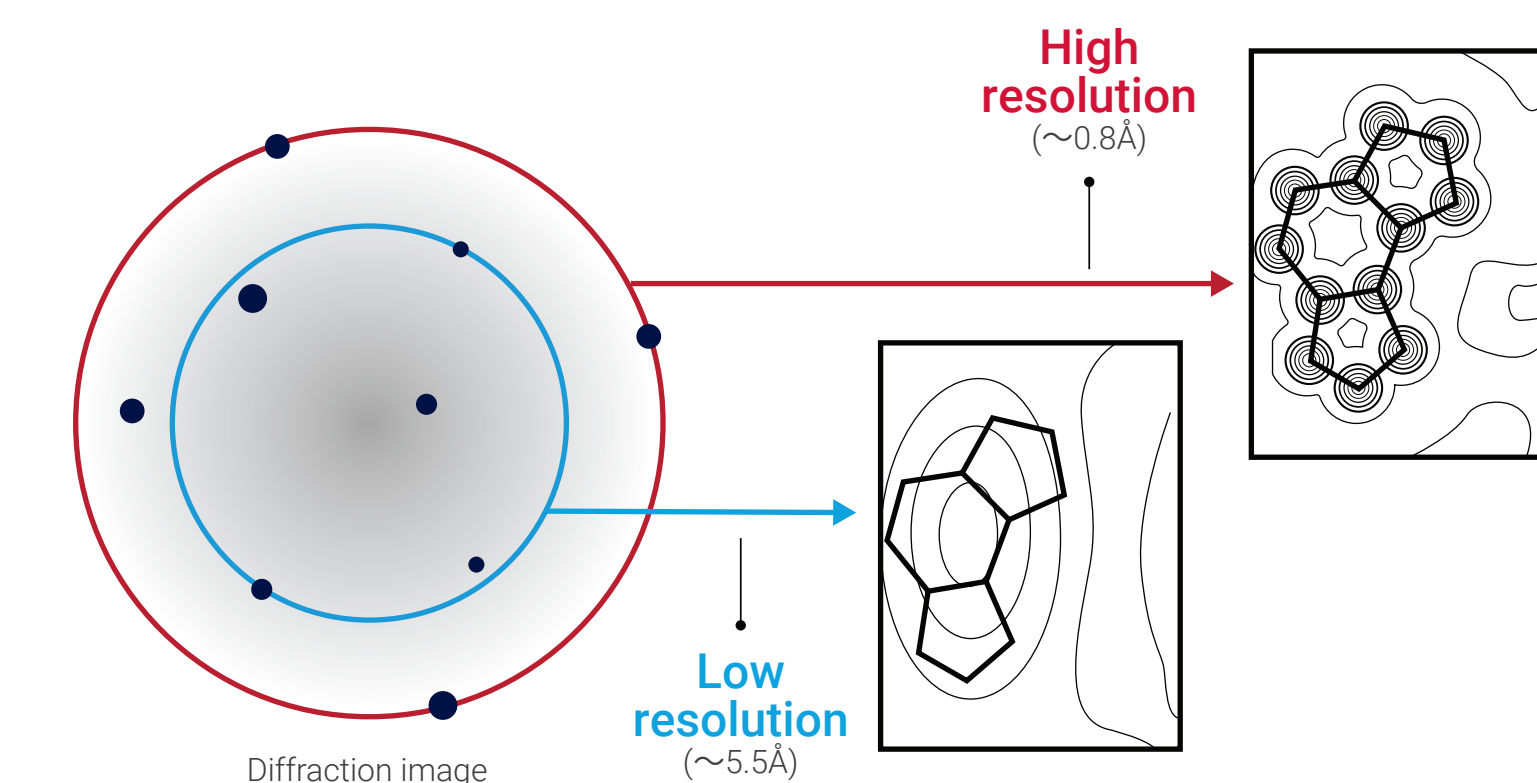
How does crystallography work?

By irradiating a single crystal with X-rays or electron beams and analyzing the resulting diffraction pattern, atomic positions can be determined.



What kind of crystal should you select for measurement?

It is necessary to select a single crystal that yields high-resolution data, in which diffraction spots are clearly observed from the center to the outer region of the diffraction pattern.

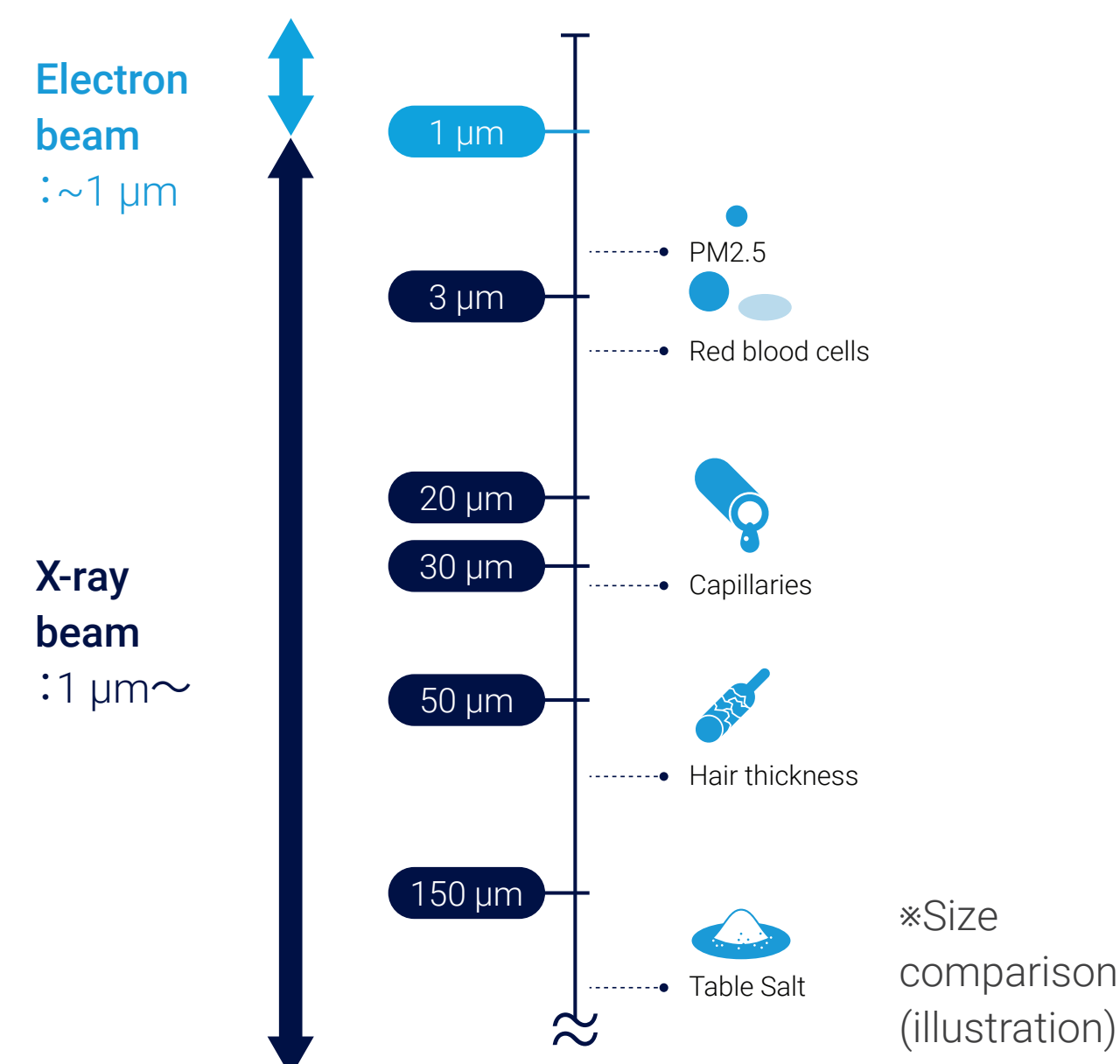


Resolution in X-ray crystallography $d = \lambda / 2\sin\theta$

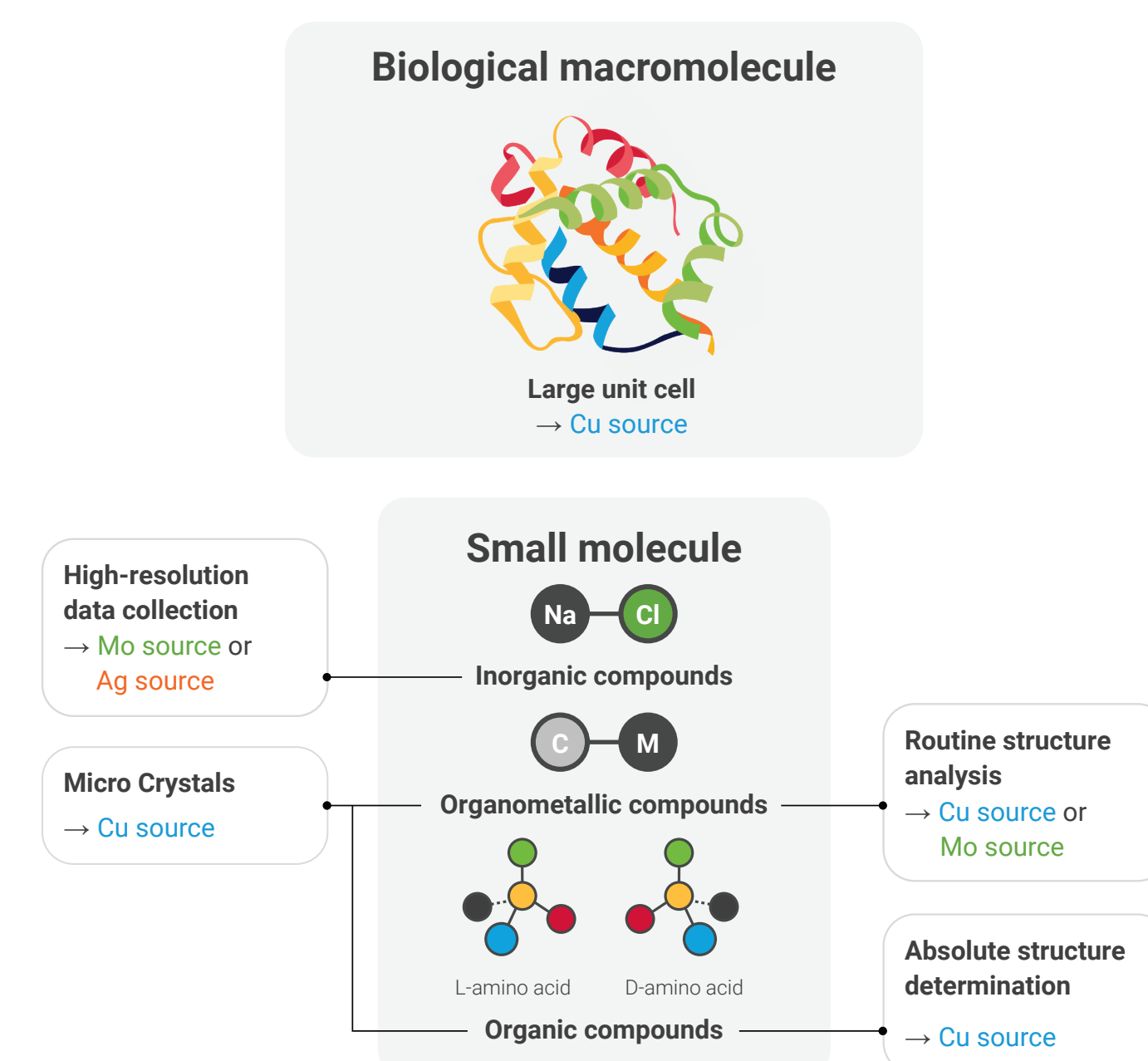
Toward the outer region of the diffraction pattern, the Bragg angle θ increases and the lattice spacing d decreases. A larger θ corresponds to higher resolution, allowing more accurate determination of individual atomic positions. In general, high-resolution data of around 0.837 Å are required for journal publication.

Which should you choose, X-rays or electron beams?

X-rays should be the first choice unless sample size is too small, select electrons for samples up to 1 micron and X-rays for everything else.

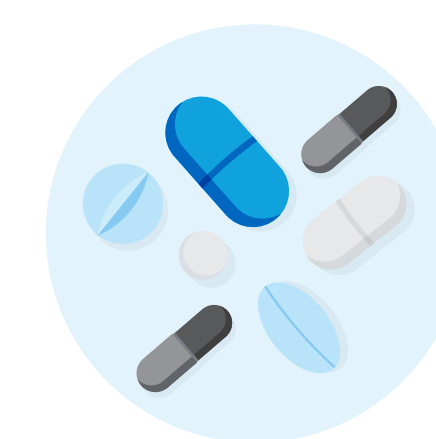


How do you choose the appropriate X-ray source?



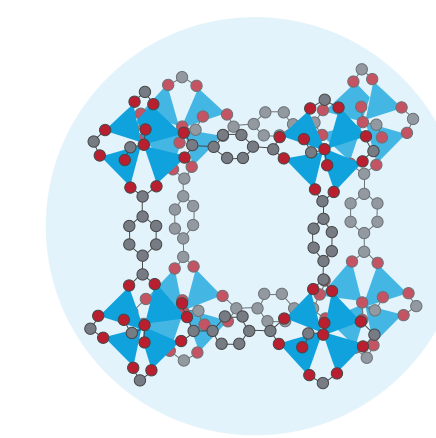
*For specialized applications such as high-pressure experiments, Ag radiation may also be used.

Where is crystallography used?



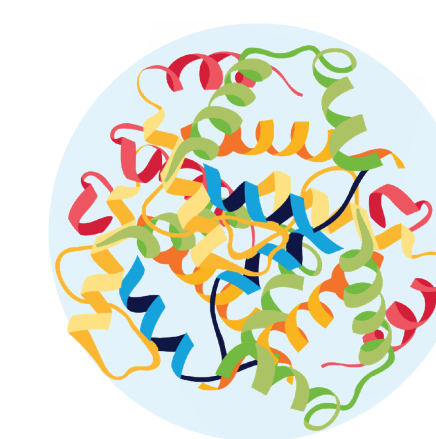
Pharmaceuticals

In the development of new drugs, accurately determining the three-dimensional structure of the active ingredient is essential. Single crystal structure analysis reveals bonding modes and differences between optical isomers, helping optimize drug efficacy and reduce side effects.



Functional materials

In many functional materials, performance is directly determined by crystal structure. Single crystal structure analysis allows atomic-level determination of atomic positions, bonding modes, and molecular or ionic arrangements. For example, in MOFs (metal-organic frameworks), it clarifies the connectivity between metal ions and organic ligands and the pore structure, supporting the design of functions such as gas adsorption, separation, and catalysis.



Life sciences

The functions of proteins are closely related to their three-dimensional structures. Single crystal structure analysis supports drug discovery and disease research.



Novel battery materials

Improving battery performance and developing new materials require detailed structural analysis. Single crystal structure analysis reveals material properties and electrical conductivity at the atomic level.

Rigaku's Crystallography Instruments



XtaLAB mini II



XtaLAB Synergy Series



XtaLAB Synergy-ED



Learn more at
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