MS45 What is inside the black box?

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You have the molecular structure – are you out of the black box?
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Abstract
There are several techniques a crystallographer may apply occasionally as a black box: using the software of data collection and structure solution, or the physical chemistry of nucleation at crystal growth, etc.; but being lucky enough to have the molecular structure – are you ready and can you sit back? You have to explore how the crystal structure is constructed from the molecules, how the crystal structure and the macroscopical properties are related to each other. Understanding the rules, the hows and whys of crystal architecture, offers often challenges, and this way is often flanked by pitfalls. I will speak about the relation of chirality and crystallizability, surprizing stoichiometry, long uncovered crystal symmetries and pseudo-symmetries, week intramolecular interactions which completely change crystal properties, ways and reasons of solvent inclusion. Selected examples prove that understanding of crystal architecture is not necessarily straightforward.

Figure 1 Challenges offered by the exploration of crystal architecture.