

Chemistry and crystal engineering

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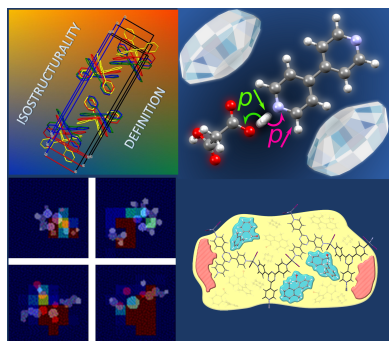
Keywords: crystal engineering; non-covalent interactions; editorial.

The **IUCrJ** theme of *Chemistry and crystal engineering* covers a broad range of topics and this is reflected in the articles published in **IUCrJ**. In 2022, Desiraju suggested that ‘the Holy Grail of crystal engineering is to answer the question: *Given the molecular structure of a compound what are all the possible crystal structures?*’ (Desiraju, 2022). It is interesting and instructive therefore to reflect on advances made towards this goal in recent years. While there is still a focus in crystal engineering to deepen our understanding of the influence of intermolecular interactions on crystal packing, increasingly the focus has moved to practical applications such as devices and materials with useful physical and chemical properties (Braga, 2023; Xiong *et al.*, 2024; Kasuya *et al.*, 2024; Xu *et al.*, 2024). Recent articles in the journal highlight developments both in methodology and techniques as well as a diverse range of classes of compounds being studied and of problems being tackled.

Studies on the nature of non-covalent interactions are highly topical (Biot & Bonifazi, 2020; Rajapaksha *et al.*, 2023) and are well represented in recent publications in the journal. These include the nature of π -hole interactions between iodide anions and quinoid rings which have been shown to be predominantly electrostatic (Milašinović *et al.*, 2023) while Carroll and co-workers used a crystalline sponge to isolate and characterize a family of biaryl alcohol guest molecules, showing that the orientation and molecular conformation adopted by the guest molecules is controlled by the intermolecular interactions (hydrogen-bonding, halogen-bonding and/or aromatic interactions) available at the guest exchange site (Carroll *et al.*, 2023).

Interesting questions remain, such as how far can a packing motif change while still being considered the same? This is the subject of a re-evaluation of the definition of isostructurality (Bombicz, 2024) which argues that consideration of symmetry and supramolecular interactions and their influence on the resulting crystal structure is required. The concept of similarity and isostructurality is key to the study of polymorphism (Subanbekova *et al.*, 2024; Jeziorna *et al.*, 2023) and even of the disappearance and reappearance of polymorphs (Sacchi *et al.*, 2024). A recent example of the value of such considerations is the study of the mechanism and kinetics of transforming polymorph C of the pharmaceutical ingredient ibrutinib to its halogen benzene solvates using a flow-through capillary mounted directly on a powder X-ray diffractometer (Jirát *et al.*, 2023). Four different transformation mechanisms were determined despite the isostructurality of three of the four solvated crystal structures. The influence of environmental factors on molecular packing is another area of ongoing interest. The increasing availability of diamond-anvil cells has promoted an interest in the effect of pressure on molecular packing. High pressure promotes some interactions over others and can force the molecules to adopt a particular conformation (Sacharczuk *et al.*, 2024) while pressure changes can induce migration of a proton to allow interconversion between a cocrystal form to an ionic salt (Patyk-Kaźmierczak *et al.*, 2024).

Crystallography may be said to have reached a mature phase as a science but new techniques and computational approaches are essential to allow researchers to tackle ever more complex problems. Recent developments in quantum crystallography hold great promise for improving the accuracy of key structural parameters. For example, Hirshfeld atom refinement (HAR) uses aspherical structure factors obtained from calculation to produce more accurate structural information such as more accurate hydrogen atom positions even in cases where the hydrogens are close to heavy elements (Capelli *et al.*, 2014; Wońska *et al.*, 2023). Zwolenik *et al.* (2024) applied



HAR to a molecular structure at high pressure and compared the result with an analysis of the same structure measured over a temperature range of 90 to 390 K.

Developments in machine learning and artificial intelligence will have an increasing impact on the nature of the questions that can be addressed using crystallography (Ekeberg, 2024; Billinge & Proffen, 2024; Zhu *et al.*, 2024). An intriguing example is recent work by Takiguchi *et al.* who devised a deep learning model to determine which of 20000 metal complexes extracted from the Cambridge Structural Database (CSD) are single-molecule magnets (SMM) with 70% accuracy (Takiguchi *et al.*, 2024). The latter article highlights the enormous value the CSD (Ferrence *et al.*, 2023) and other databases offer so it is encouraging to see the work being done by CODATA to ensure the interoperability of crystallographic data within the FAIR principles (findable, accessible, interoperable and reusable) (Brink *et al.*, 2024).

In conclusion, recent articles in the journal are evidence that crystal engineering concepts are well embedded in many aspects of chemical crystallography. Further advances in these themes are to be expected and will be welcomed in **IUCrJ**.

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