With our powers combined... The CSD and its applications across structural science

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Abstract

Following a vision that the collective use of data would lead to new knowledge and generate new insights Dr Olga Kennard established the Cambridge Structural Database (CSD) in 1965, a step which transformed modern crystallography. Today over one million structures are shared through this resource and the database is something the entire scientific community can be proud of. It is thanks to this community's exemplary data sharing practices, as well as the thoughts of visionaries in the field, that this collection of data exists.

The CSD and the accompanying software are now used by scientists worldwide working in over 70 countries, and the knowledge derived from the structural data contained in the database has underpinned fundamental chemical discoveries and played a key role in designing new materials from drugs to pigments and beyond.

This talk will look at some of the research that the CSD has enabled and highlight the knowledge and insights that have been derived from this collection of data. It will explore how the database has evolved over the years and how researchers have used it for a range of different purposes, from rationalising the geometries of macromolecules, to predicting intermolecular interactions, and even to understanding the surface chemistry of crystals themselves.