

KN10 | ONE MILLION STRUCTURES AND COUNTING: THE JOURNEY, THE INSIGHTS, AND THE FUTURE OF THE CAMBRIDGE STRUCTURAL DATABASE

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This year marks a huge milestone in structural chemistry – the sharing of one million organic and metal-organic crystal structures. The creation of the Cambridge Structural Database (CSD) to collate and distribute these structures is truly a worldwide effort, with the CCDC curating and enhancing data from hundreds of thousands of crystallographers.

The beginnings of the CSD can be traced back to 1965 with J.D. Bernal and Olga Kennard, who had the vision and foresight to understand that the collective use of data would lead to the discovery of new knowledge. Their vision has certainly come to fruition today. Both the structures and the database itself have evolved significantly since then, as has its value to scientists worldwide.

Major advances in technology, new structure solution methods, extraordinary developments in computing, and significant advancements in chemistry have all had a dramatic effect on how the CSD has evolved. The growing size, complexity and diversity of the database coupled with the development of new ways to search and analyse the CSD has meant that new insights have been possible, and the data can be used in ways that would once have been unimaginable. This presentation will take a journey through the CSD, highlighting significant milestones in the development of the database and the science that it has enabled. It will conclude by exploring some future possibilities, how the CSD and the field of crystallography might evolve and asking what role structural data may play in the future with the sharing and analysis of the next million structures.