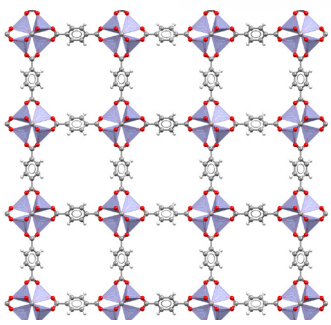
What's Up: CCDC Newsletter

October 2019

2019 has been a busy year for CCDC! As we approach the end of the summer and head into the new academic year, we'd like to share some of the great work that's been happening here at CCDC.

Software developments

As we approach our 4th release of 2019, here's a summary of just some of the new features in our software this year...



1. The launch of Polyhedral display in Mercury, allows users to visualise metal organic structures using polyhedral representations.

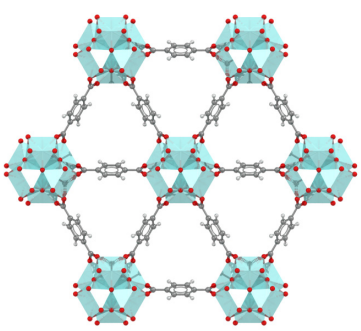
2. Python 3 compatibility now available with Python 3.6 as default for 2020.

3. Support in the CSD Python API for all types of **3D query** available in ConQuest.

4. Extension of the CSD-CrossMiner database to include nucleic acid containing structures from the PDB. Searching these structures was augmented by the addition of new, nucleotide specific feature definitions.

5. Seamless, flexible searching of CSD data and PDB data, allowing for the easy the extraction of data driven insight from mining of 3D information, including ligands with specific structures/similar structures, patterns of interactions between protein binding sites, waters, metals and small molecules, and geometric patterns within small molecules bound to proteins.

6. Molecular interaction maps in the **CSD Python API**, enabling automated generation of interaction maps for protein binding sites and small molecules.



7. Polymer expansion in Mercury, allowing for easy and rapid expansion and exploration of coordination structures of metal organic polymers, and the generation of high-quality figures.

KEEP AN EYE OUT FOR OUR NEXT RELEASE COMING-UP IN NOVEMBER!

Scientific advisory board

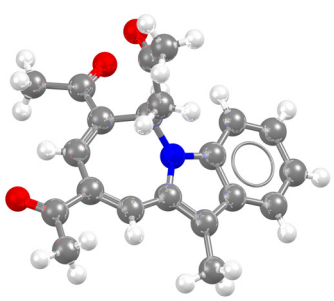
As we move into the 2020s the need for comprehensive, high quality structural data combined with deep domain expertise to fully leverage the latest technologies such as AI is becoming more important than ever. The opportunities to discover and develop new materials computationally means that a vast number of concepts can be evaluated before moving to expensive physical experimentation and development. Therefore in July we were pleased to

announce the formation of a new Scientific Advisory Board comprising globally leading scientists to help drive our growth in new and exciting areas. Read more.

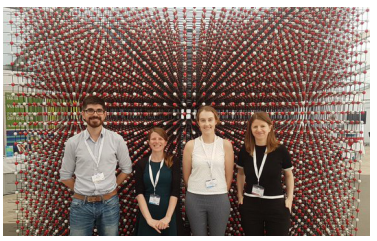
Our latest update saw 14,673 new entries added within the CSD, bringing the total size to 1,023,815 entries and 1,006,180 unique structures!

Reaching a million!

This year has been a huge milestone for CCDC with the CSD hitting over one million structures In June. This is an achievement the whole community should be proud of! Scientists from around the world working across many different fields of research regularly deposit their structures in the CSD, and our team of deposition Coordinators and Scientific Editors work hard to ensure consistent accuracy and quality of the data we provide. Find out more about CSD One Million and what it means for structural science.



Events



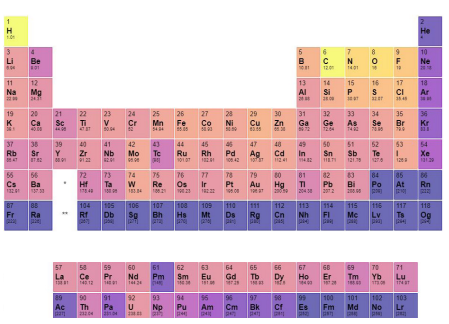
We've had a packed conference and events calendar this year!

Some main highlights include our successful European UGM and the series of CSD One Million celebration events that we have so far held at the ACA, the ECM and the ACS. We are very thankful to all the speakers that gave excellent presentations at these events, in particular, the one million symposium held at the ACS in August, what a great couple of days! We'll be providing a full report of the content and discussions from the symposium in the coming weeks.

Our final celebratory event will be held at AsCA in December. Keep an eye out for further details of this and more upcoming events.

IYPT 2019

CCDC have partnered with the British Crystallographic Association to celebrate the year of the international periodic table the way we know best: with crystal structures.

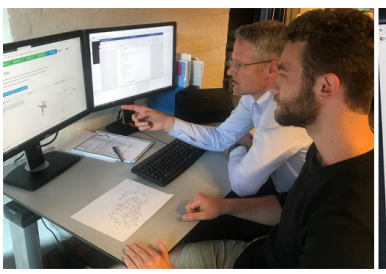


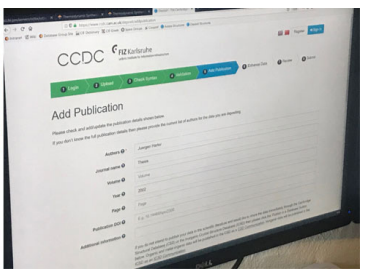
Throughout the year we have been highlighting each element in the periodic table with a crystal structure either including or related to that element - here's an example of one we made earlier.

We are looking for contributors to send us facts and figures about their favourite element which will be added to our interactive periodic table and promoted through our social media channels and @IYPTCrystals. You'll also be featured on our contributors webpage, see who's already involved! If you'd like to contribute to this project, contact us at hello@ccdc.cam.ac.uk.

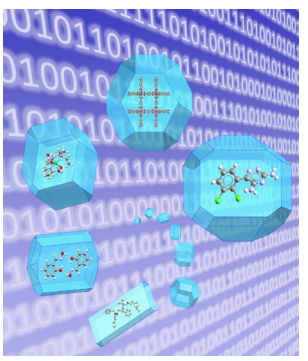
Thesis data summer project

We've been running a summer initiative this year to help you get your thesis data shared and acknowledged. Here's our summer student Jake Bowden helping CEO Jürgen Harter add structures from his PhD thesis. Discover how to publish structures from your thesis here.





CCDC Research



This year CCDC scientists have continued their collaboration with industry and academia to publish extensively in the open literature.

Some of the most recent research highlights include work published by Robin Taylor and Peter Wood in ACS Chemical Reviews - 'A million crystal structures: the whole is greater than the sum of its parts' (DOI: 10.1021/acs.chemrev.9b00155) highlighting applications of the CSD across the structural sciences to mark the recent one million milestone.

More recently in a collaboration with the University of Leeds, Britest Limited, Pfizer and GSK, our research on 'Particle Informatics: Advancing Our Understanding of Particle Properties through Digital Design' was published, introducing a new workflow that brings together novel approaches in the assessment and prediction of particle properties. The knowledge generated provides resolutions at key decision points in the pharmaceutical formulation and manufacturing process (DOI: 10.1021/acs.cgd.9b00654).

Want to be kept up to date with the latest news, resources and events from the home of structural science? Sign up to our newsletter to receive monthly updates. And make sure to follow us on social media!