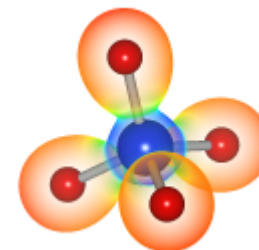
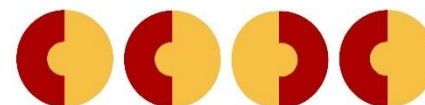
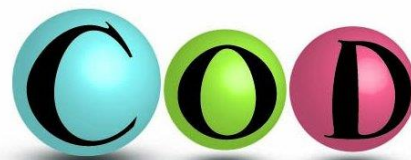


Lecture 2:

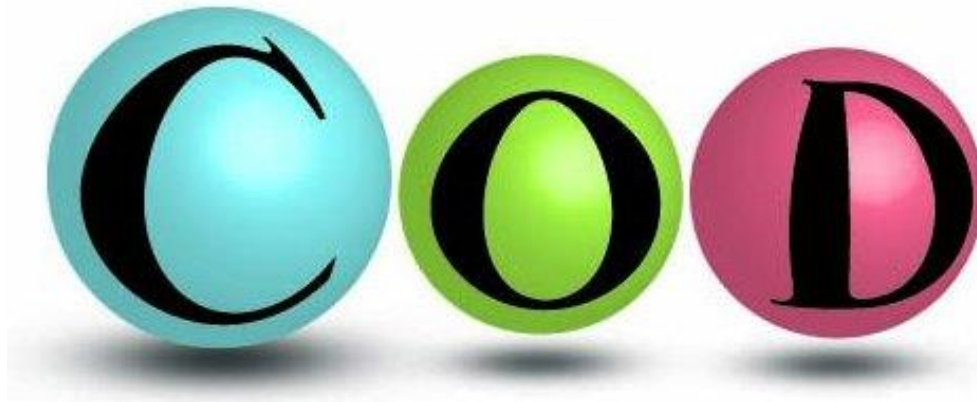
Structural databases, visualization

- Documentation for the databases and software
 - MyCourses -> Databases
 - MyCourses -> Software
- Key structural databases used on this course
 - Crystallography Open Database (COD)
 - Inorganic Crystal Structure Database (ICSD)
 - Cambridge Structural Database (CSD). More relevant for small-molecule organic and organometallic species
- Jmol visualization software
 - Quick visualization and investigation of some properties
 - Retrieving data directly from databases
- VESTA visualization software
 - Publication-quality visualization
 - Crystallographic tools



Structural databases: COD

- COD (Crystallography Open Database)
 - Inorganic, organic, metal-organic compounds, and minerals
 - Excludes biopolymers, which are covered by [RCSB PDB](#) (Protein Data Bank)
 - Over 480 000 structures (2022-01-12)
 - **Open access** database, available at <http://www.crystallography.net/>
 - COD Petition: *“The principle defended here is that the atomic positions in natural or synthetic crystal samples of our Universe are not copyrightable”*



Structural databases: ICSD

- ICSD (Inorganic Crystal Structure Database)
 - Crystal structures of inorganic compounds (No C-C **and** C-H bonds)
 - Over 210 000 structures (2022-01-12)
 - <http://libproxy.aalto.fi/login?url=https://icsd.fiz-karlsruhe.de/>
 - (or <http://icsd.fiz-karlsruhe.de/> when in the campus or with Aalto VPN)

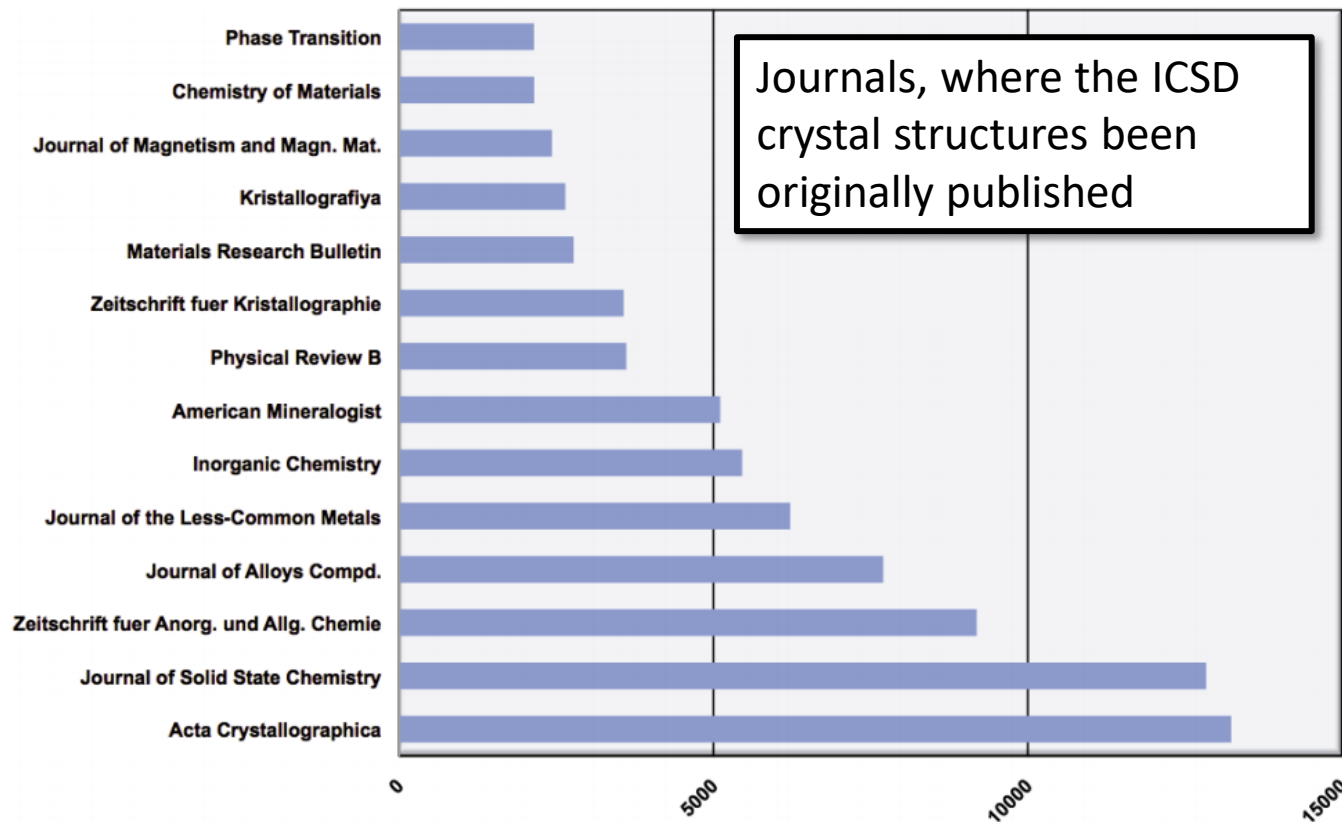


Figure: ICSD

Structural databases: CSD

- CSD (Cambridge Structural Database)
 - Small-molecule organic and metal-organic crystal structures
 - Over 1 170 000 structures (2022-01-12)
 - <https://www.ccdc.cam.ac.uk/structures/> (only from campus or with Aalto VPN)

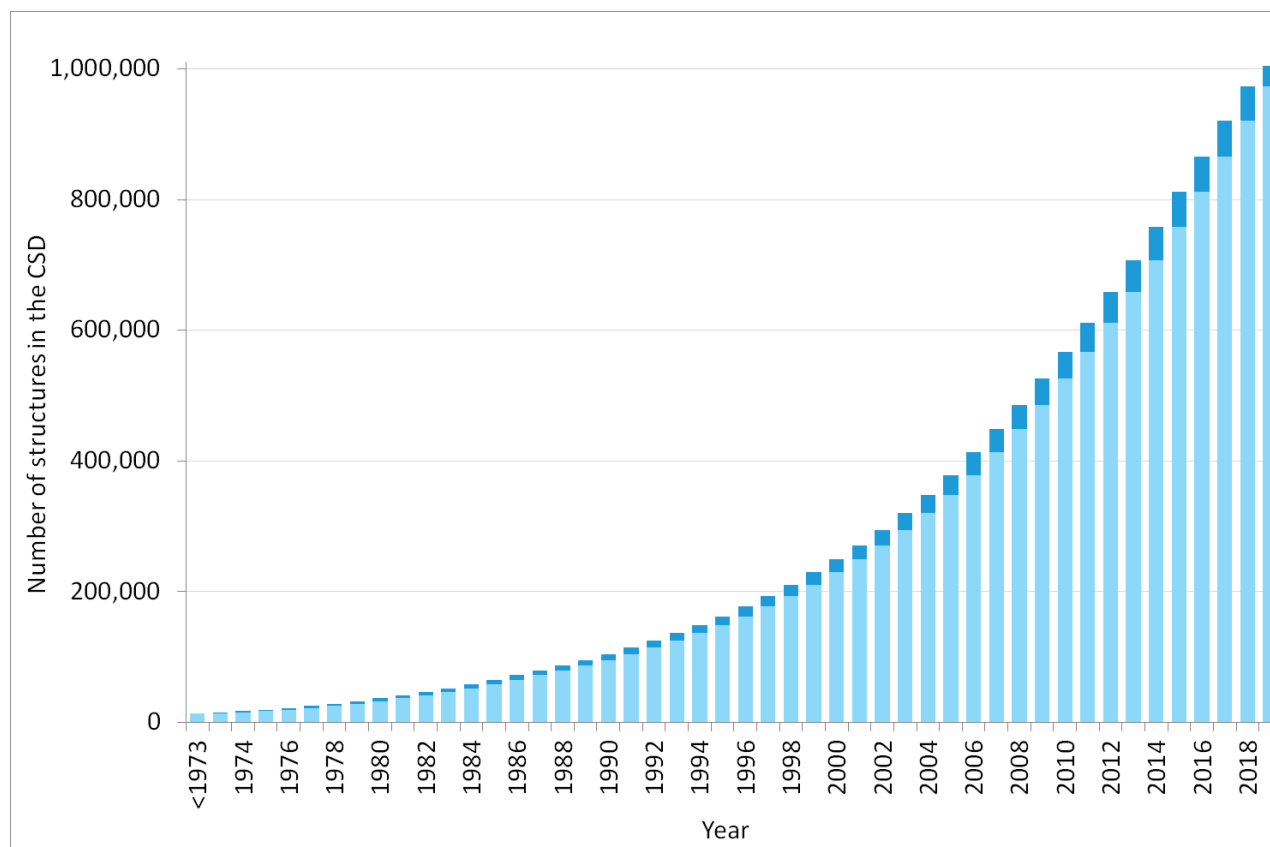


Figure: CCDC