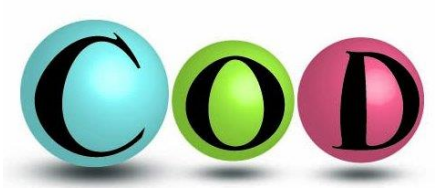
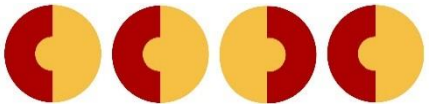
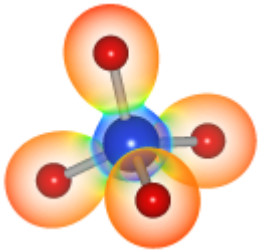
Lecture 2:
Structural databases, visualization

- 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

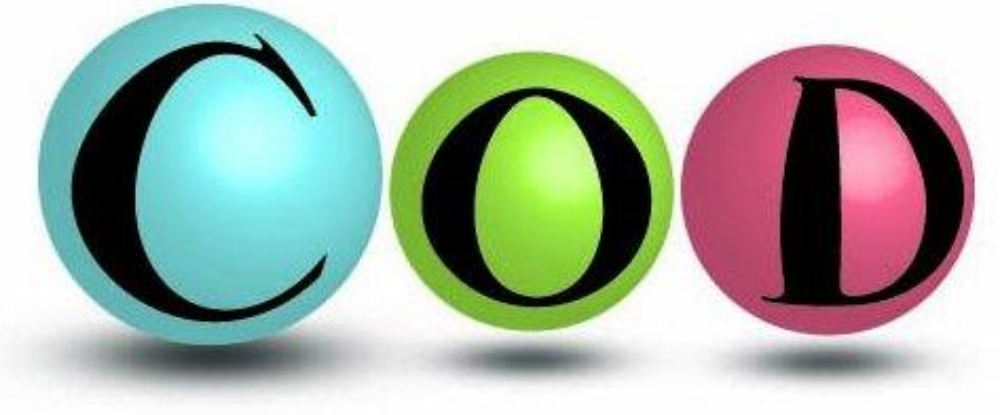






Structural databases: COD

- COD (Crystallography Open Database)
  - Inorganic, organic, metal-organic compounds, and minerals
  - Excludes biopolymers, which are covered by RCSB PDB (Protein Data Bank)
  - Over 460 000 structures (2021-01-10)
  - ***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 230 000 structures (2021-01-10)
  - http://icsd.fiz-karlsruhe.de/ (only from campus or with Aalto VPN)

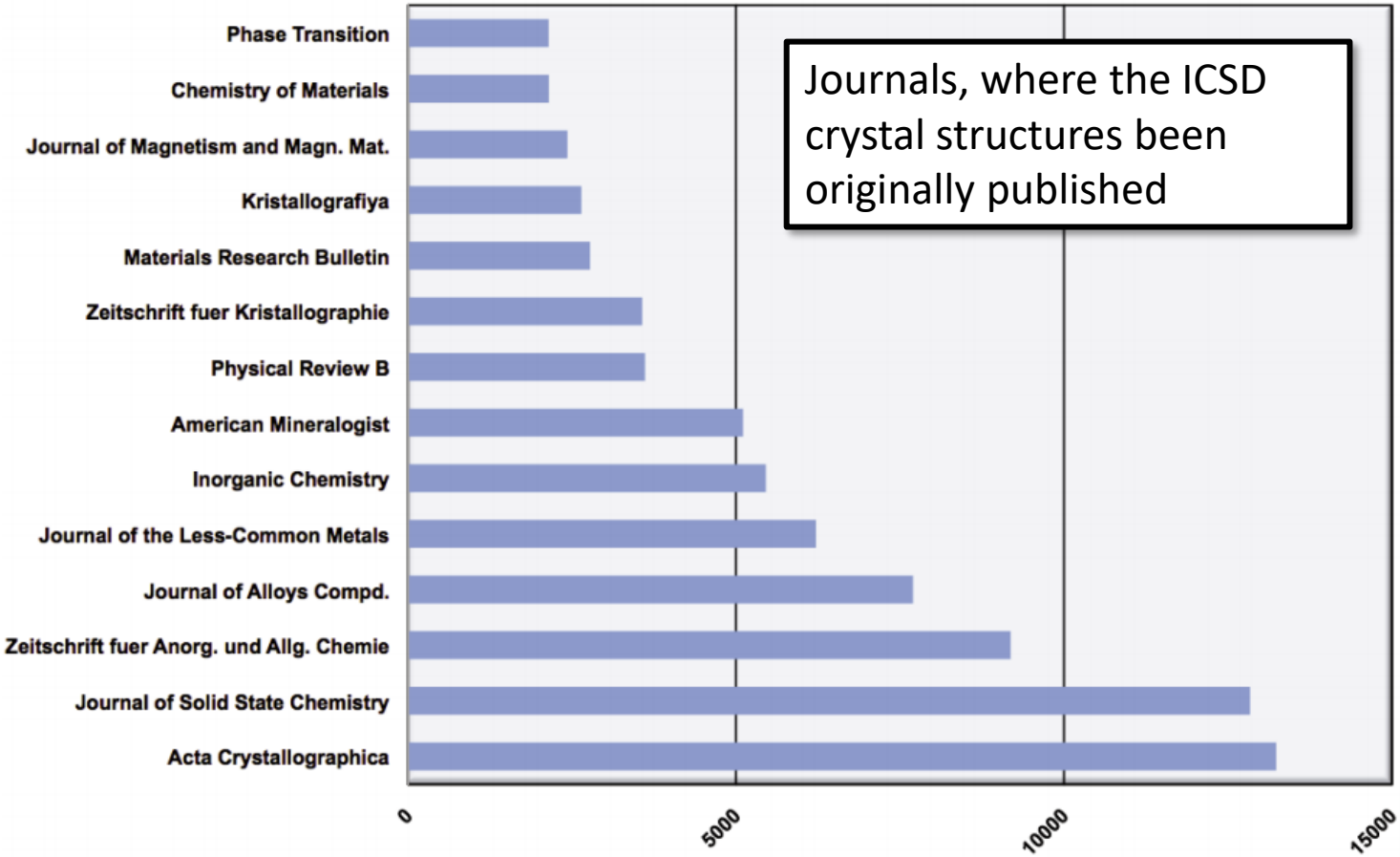


Figure: ICSD

Structural databases: CSD

- CSD (Cambridge Structural Database)
  - Small-molecule organic and metal-organic crystal structures
  - Over 1 097 000 structures (2021-01-10)
  - https://www.ccdc.cam.ac.uk/structures/ (only from campus or with Aalto VPN)

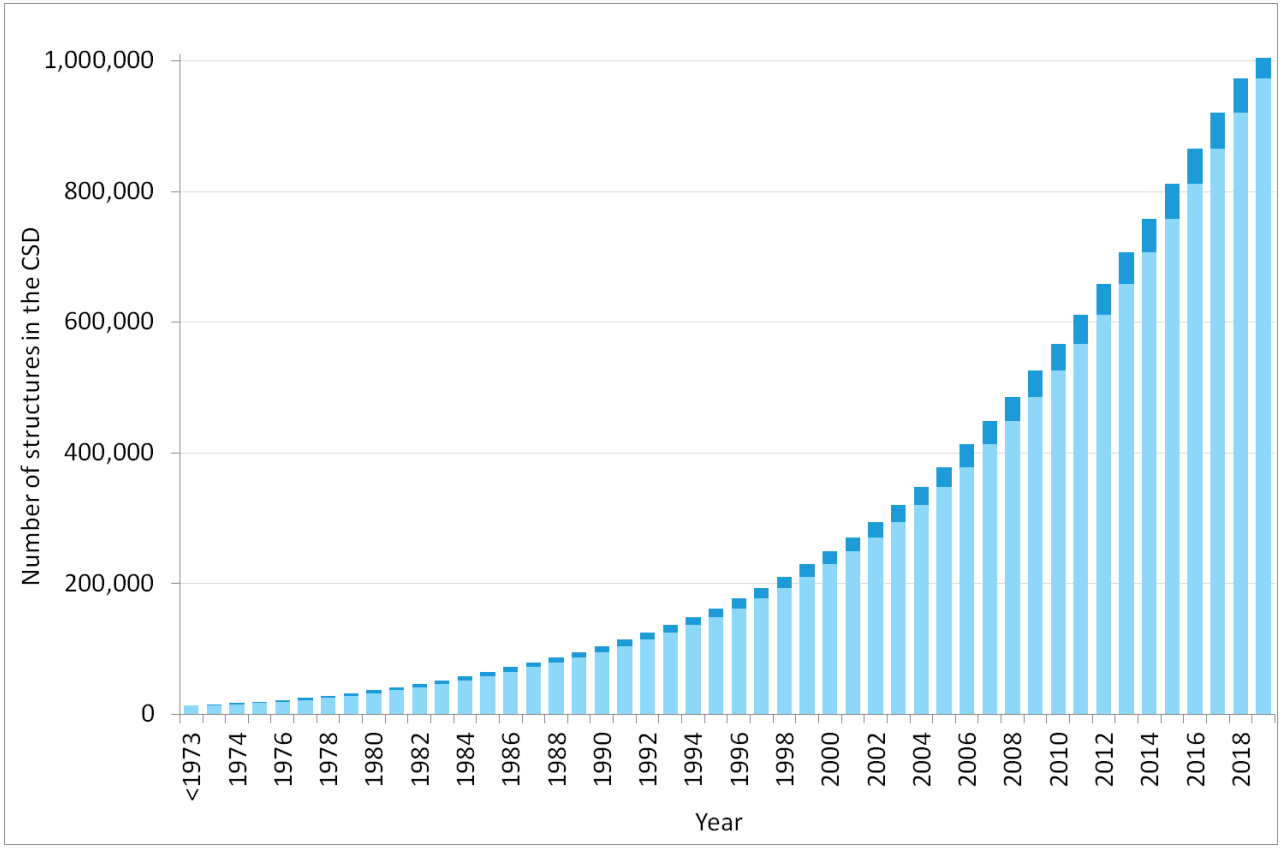


Figure: CCDC