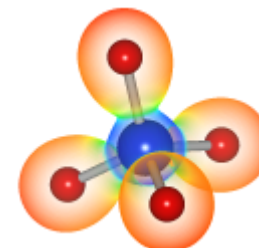
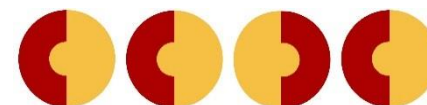
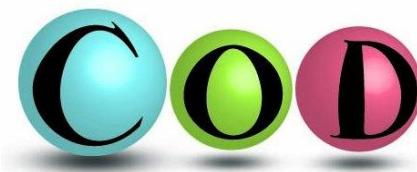


Lecture 2:

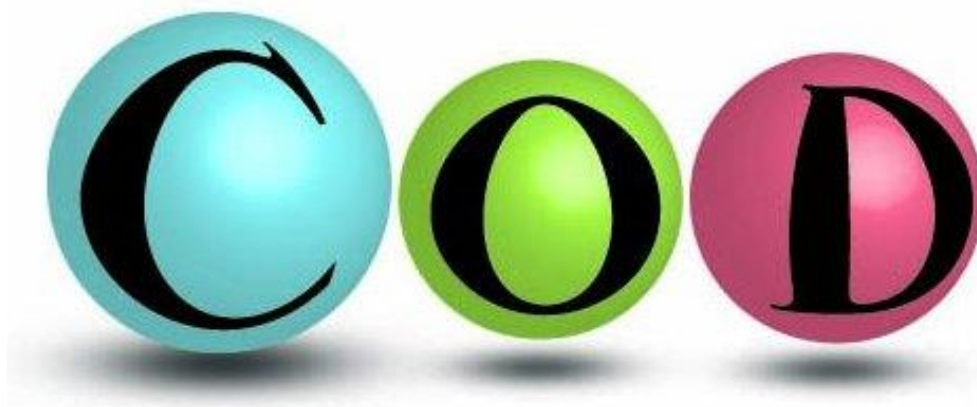
Structural databases, visualization

- Key structural databases
 - Crystallography Open Database (COD)
 - Inorganic Crystal Structure Database (ICSD)
 - Cambridge Structural Database (CSD). More relevant for small-molecule organic and organometallic species
 - ***Please use Firefox or Chrome browser for the database exercises! Internet Explorer will not work.***
- Jmol
 - Quick visualization and investigation of some properties
 - Retrieving data directly from databases
- VESTA
 - 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](https://www.rcsb.org/) (Protein Data Bank)
 - Over 400 000 structures (2019)
 - **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 200 000 structures (2019)
 - <http://icsd.fiz-karlsruhe.de/> (only from campus or with [Aalto VPN](#))

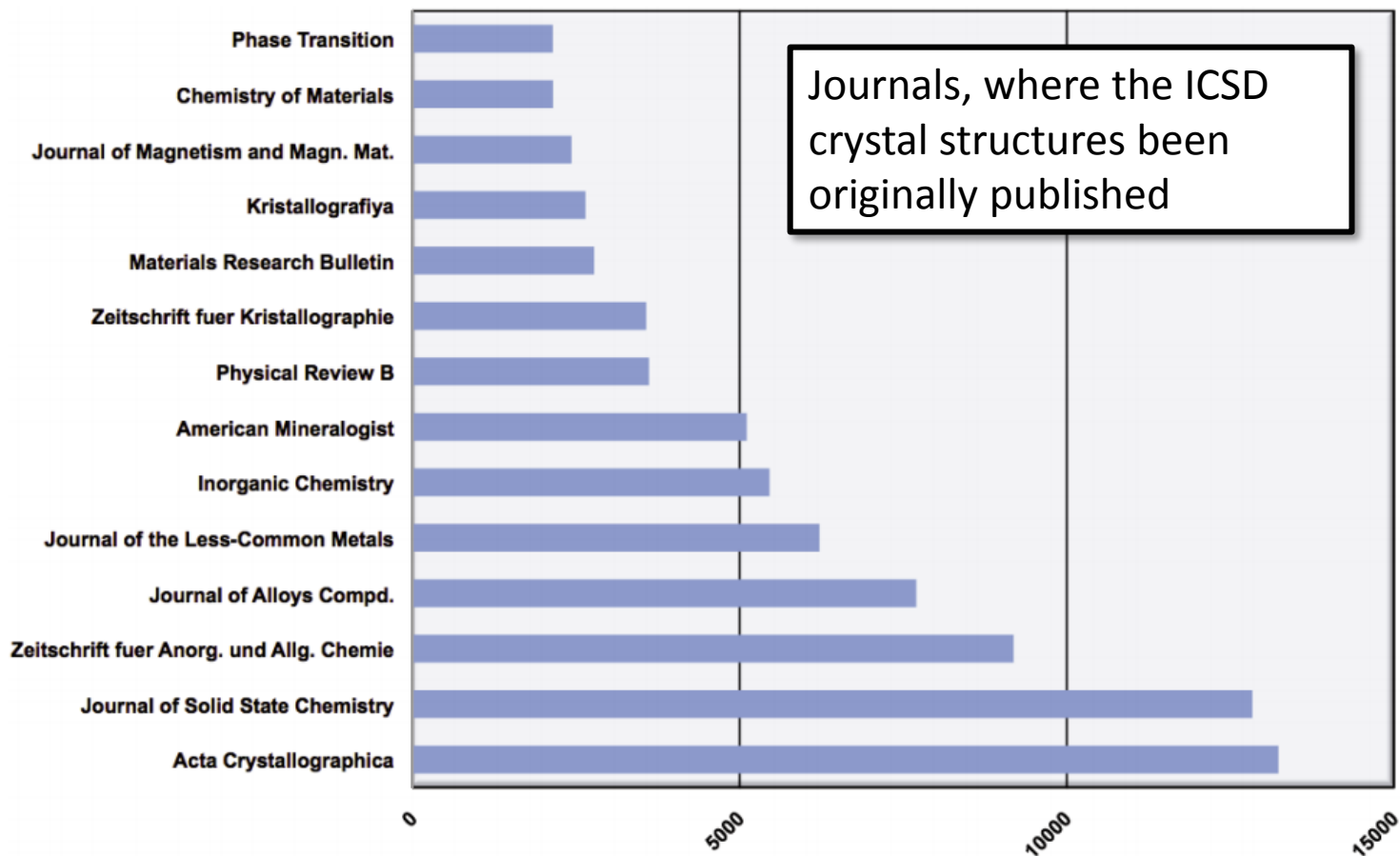


Figure: ICSD

Structural databases: CSD

- CSD (Cambridge Structural Database)
 - Small-molecule organic and metal-organic crystal structures
 - Over 900 000 structures (2019)
 - <https://www.ccdc.cam.ac.uk/structures/> (only from campus or with [Aalto VPN](#))

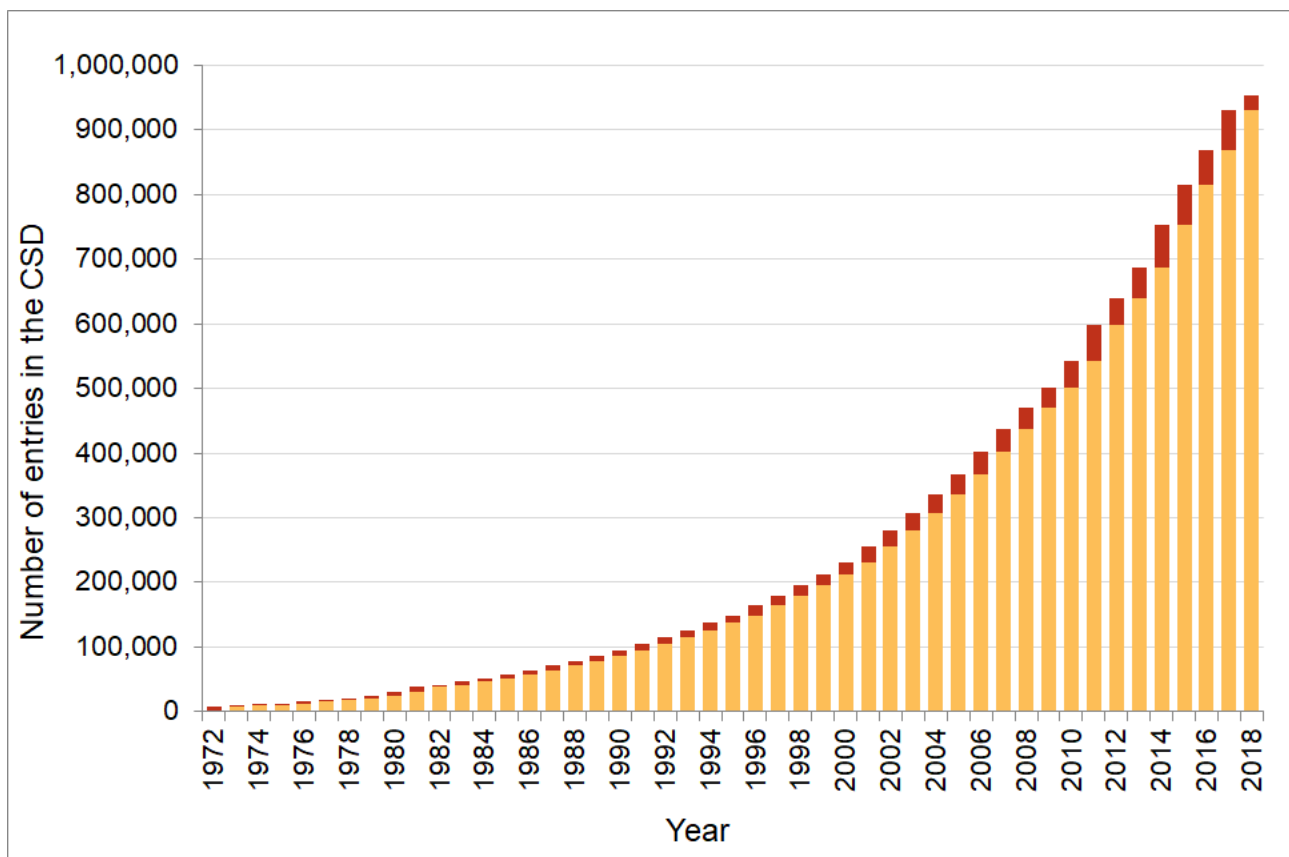


Figure: CCDC

Software and database documentation

- Documentation for installing and using Jmol and VESTA is in MyCourses
 - MyCourses -> Software ([link](#))
 - Only Jmol is needed for Lecture 2, we start using VESTA on Lecture 3
- Documentation for using the structural databases is in MyCourses
 - MyCourses -> Databases ([link](#))
 - On Lecture 2, we focus on using COD
- Please see the documentation slides and Exercise set 2 for more content.