# MS20- Rating and improving data quality: instrumentation, analysis and postprocessing

**Chairs: Dr. Karine Röwer, Dr. Loes Kroon-Batenburg**

## MS20-P01

### Structurefinder

Daniel Kratzert[1]

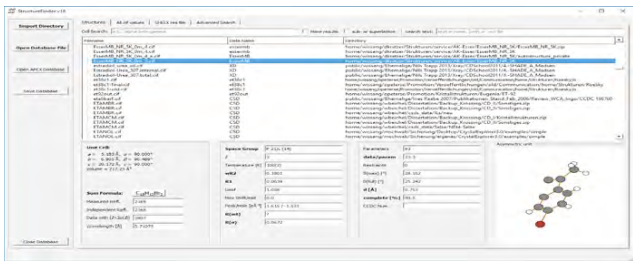
1. Albert-Ludwigs-Universität Freiburg, Inorganic Chemistry, Freiburg im Breisgau, Germany

**email: daniel.kratzert@ac.uni-freiburg.de**

Databases like the Cambridge Structural Database or the Crystallographic Open Database are good at collecting information from crystallographic experiments and making it searchable. But to my knowledge, there is no easy-to-use software to find and present the results of crystallographic experiments for a single workgroup.

Presented is a new computer program called StructureFinder. It creates a database of crystallographic structures on a computer and makes them searchable. The program can search for various properties: Unit cell, free text, creation date, included atom types and space group. To build the database, StructureFinder collects all computer information files (cif file format) below certain directorys on a hard disk. The containing information is stored into a SQLite database. The database can be accessed by two different interfaces. A stand-alone Qt program (figure 1) to install on a single computer or a web interface (figure 2) to be accesses by a whole work group.

StructureFinder greatly enhances the ability to find old structures in huge collections of crystallographic datasets. The program can easily handle more than 10.000 structures. It can be downloaded at https://www.xs3.uni-freiburg.de/research/structurefinder.



References:

[1] https://www.xs3.uni-freiburg.de/research/structurefinder

**Keywords: structure search, unit cell, cif files**

## MS20-P02

### Low-cost portable devices for inert low-temperature sample manipulation

Nils Trapp[1], Michael Solar[1], Michael Wörle[1]

1. Small Molecule Crystallography Center, ETH Zürich, Zürich, Switzerland

**email: nils.trapp@org.chem.ethz.ch**

Sample cooling has become widely implemented in crystal structure determination, due to the broad array of advantages it offers (Goeta & Howard, 2004). In particular, measurement at reduced temperatures can severely improve data accuracy and resolution for small molecule crystals, due to reduced and more isotropic atomic vibration (Brock & Dunitz, 1990). In addition, it can reduce radiation damage in protein crystals, enable variable temperature or phase transition studies and allow measurements of samples that are not stable or solid under ambient conditions. Low temperature can also prevent crystal damage due to the escape of co-crystallized solvent, which often retains a relatively high vapor pressure. Because the cooling medium used in open-flow sample cryostats is either nitrogen or helium gas, air-sensitive and even pyrophoric crystals can be measured using standard equipment. However, transferring sensitive samples from storage vessel to diffractometer, without compromising crystal and data quality, remains a challenge in many cases.

A straightforward procedure for preparing and mounting crystals under inert conditions is demonstrated, using a specialized apparatus (μCHILL). The technique is extremely flexible, requiring only a single operator, little practice and almost no preparation time. The device enables a wide temperature range (at least –60 °C to room temperature), providing temperature control and very stable conditions with no ice formation over extended time periods. The flexible, modular and low-cost design is based on 3D printed parts and readily available standard components, potentially making the device available to a wide range of users and applications not limited to single crystal studies.

References:

Trapp, N, & Solar, M. (2018). Journal of Applied Crystallography, accepted.

Goeta, A. E. & Howard, J. A. K. (2004). Chemical Society Reviews 33, 490–500.

Brock, C. P. & Dunitz, J. D. (1990). Acta Cryst. B. 46, 795–806.

**Keywords: crystal mounting, instrumentation, cryocrystallography**