MedeA ICSD

Reliable Crystal Structure Data of High Quality

MedeA ®[1] *ICSD* offers experimental crystal structure information for non-organic compounds, including ceramics, minerals, and metallic systems. With *MedeA ICSD* (Inorganic Crystal Structure Database), you have access to the structure database most frequently cited in literature.[2]

At-a-Glance

MedeA ICSD is an indispensable resource for any solid-state materials research and engineering project.

Key Benefits

- Speeds up your modeling projects by providing validated experimental crystal structures
- Seamless integration with all *MedeA* modules

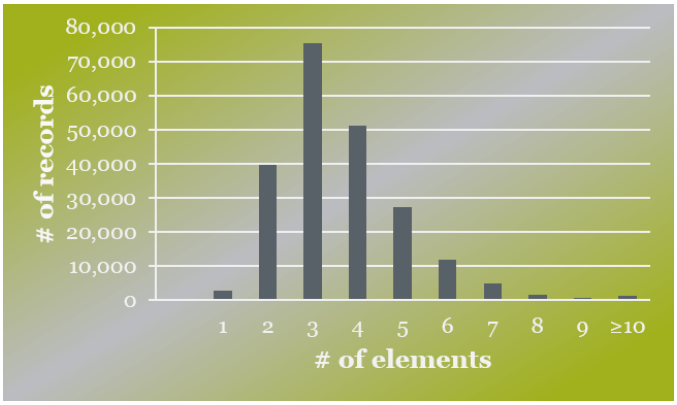

Figure 1: MedeA ICSD - *Number of records by constituent count*

Together with *MedeA InfoMaticA*, *ICSD* is the ideal starting point for any materials modeling project. With a few mouse clicks, search *ICSD* along with other *MedeA* databases, view search results in tables, sort by any type of available data, and visualize one or more chemical unit cells. Use as direct input for simulations, or as a building block for further editing and model construction.

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

[2] According to search in Google Scholar with the keywords "FIZ" and "ICSD".

Specifications

- Extensive coverage for inorganic crystal structures. Total Number of Records: 217,000
- All entries include lattice parameters and atomic coordinates
- 9,093 structure prototypes
- Comprehensive data sets dating back to 1913

MedeA ICSD provides many essential properties for experimentally determined crystal structures, as well as meta data on experimental conditions such as temperature, pressure, etc.

Key Features

- Integration with *MedeA InfoMaticA* provides fast, on-disk, cross-database search
- Quick, efficient structure retrieval using an intuitive, menu-based query language
- Regular database updates, along with *MedeA* updates
- Compatible with all *MedeA* compute engines and *MedeA* property modules

'ICSD is an indispensable source of information for chemists, physicists, crystallographers, mineralogists, and geologists teaching or doing research in the field of crystallography.'

-FIZ Karlsruhe, Germany

Properties

- Atomic coordinates, interatomic distances, and angles
- Lattice parameters, symmetry (space group), and site occupancy

- Bibliographic references and detailed information on experimental conditions and setup
- Experimental conditions
- Structural descriptors, such as Pearson symbol, ANX formula, Wyckoff sequences, and temperature factors
- Atomic coordination
- Pair correlation function
- X-ray diffraction (XRD) powder pattern (radiation source dependent)

Required Modules

- *MedeA Environment* (includes *MedeA InfoMaticA*)

Recommended Modules

- *MedeA COD*
- *MedeA Pearson*
- *MedeA NCD*
- *MedeA VASP GUI*
- *MedeA VASP 5*
- *MedeA HT-Launchpad*

Find Out More

Learn more about *MedeA InfoMaticA* in the video tutorial: How to Calculate Elastic Constants with MedeA VASP 5 on the Materials Design Youtube Channel.

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