



Datasheet MedeA *NCD*

Large Database with Physical, Chemical, and Crystallographic Information

*MedeA*¹ *NCD* is equivalent to the NIST Crystal Database, and provides chemical, physical, and crystallographic information for a broad range of solid state materials. These materials include minerals, inter-metallic phases, metals, alloys, drugs, antibiotics, and pesticides.

At-a-Glance

In combination with *MedeA InfoMaticA* and other *MedeA* databases, *MedeA NCD* provides a useful backbone of crystal structure data for both organic and inorganic compounds.

Key Benefits

- Seamless integration with *MedeA InfoMaticA*
- Quick and efficient search of compounds and their properties

Specifications

- Data for organic and inorganic structures
- More than 237,000 records
- About 50% of entries are experimentally refined structures
- Pertinent chemical, physical, and bibliographic Information

'NCD is useful in conjunction with other data for materials design and properties prediction.'

-Vicky Lynn Karen, NIST

Key Features

- *MedeA NCD* permits rapid on-disk (offline) search
- Integration with *MedeA InfoMaticA* offers many data management options

Properties

- Physical and chemical information of crystalline materials
- Chemical formula and name
- Classification by chemical type
- Standard lattice parameters
- Symmetry (space group numbers and symbols)
- Calculated density
- Bibliographic reference
- Remarks to experimental setup (where available)

Required Modules

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

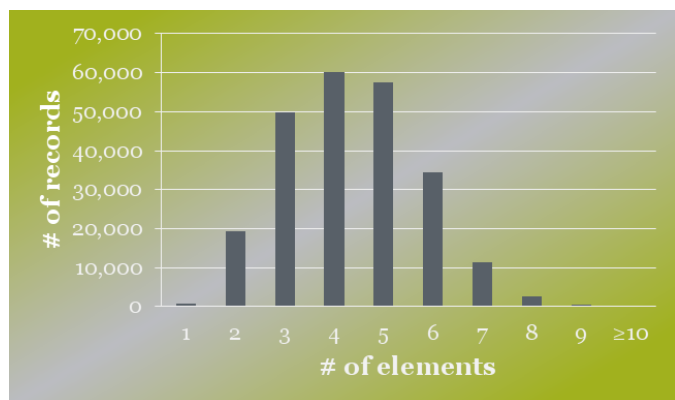


Fig. 1: MedeA NCD - number of records by constituent count

All NCD records have been evaluated by the National Research Council Canada and the National Institute of Standards and Technology (NIST). The data have been extracted from the literature published up to 1995 and were originally in ASCII format. Searching *NCD* through the *MedeA InfoMaticA* is straightforward, as multiple hits are displayed in tables easy to sort, export, and post-process.

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Recommended Modules

- *MedeA Pearson*
- *MedeA ICSD*
- *MedeA COD*

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](#).

NCD structure data was validated by the National Research Council Canada (NRCC) and the National Institute of Standards and Technology (NIST).