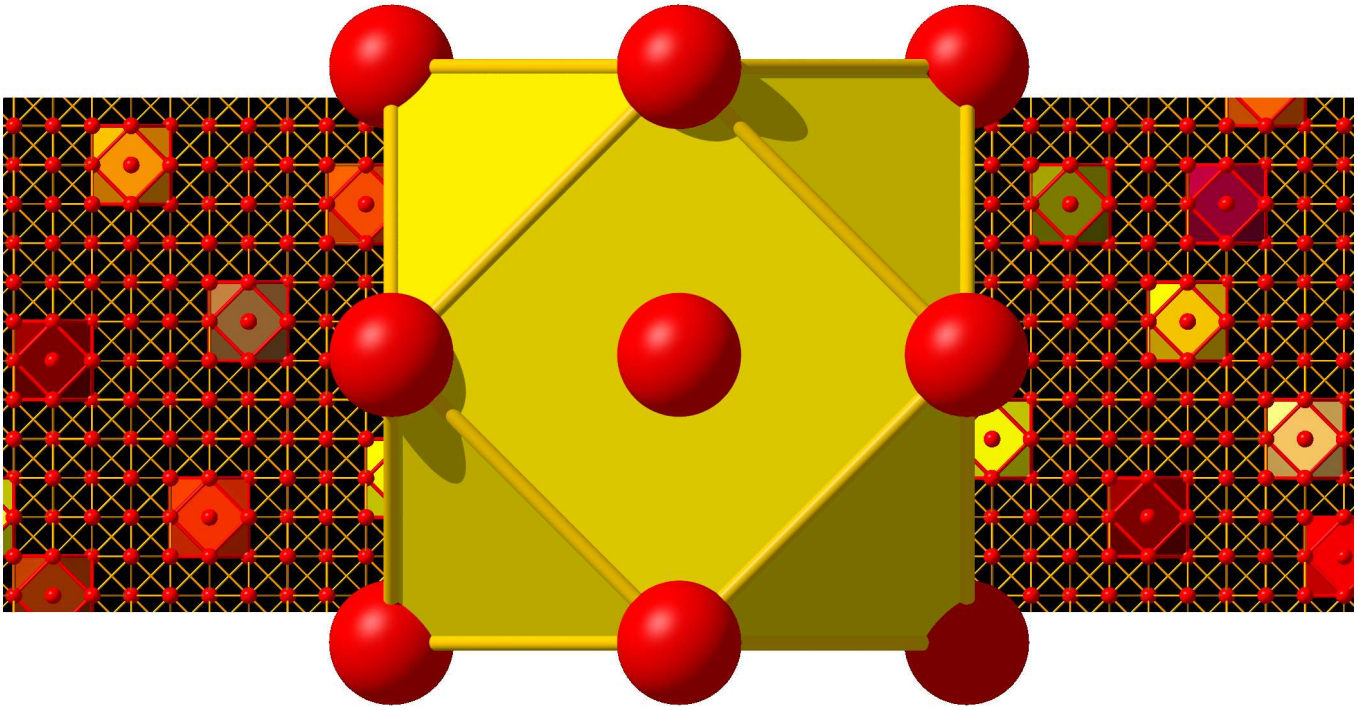
Pearson's Crystal Data

Crystal Structure Database for Inorganic Compounds

RELEASE 2022/23 · 380,000 ENTRIES

Pierre Villars and Karin Cenzual (editors)



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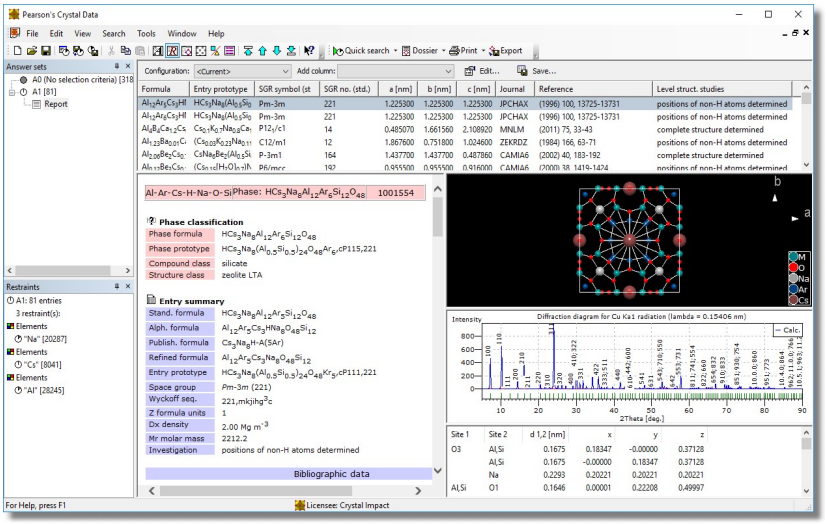
CRYSTAL IMPACT



Pearson's Crystal Data is a crystallographic database published by ASM International. It contains crystal structures of a large variety of inorganic materials and compounds, edited by P. Villars and K. Cenzual.

The current release 2022/23 contains about 380,000 structural data sets (including atom coordinates and displacement parameters, when determined) for about 210,000 different chemical formulas, roughly 21,400 experimental powder diffraction patterns and about 355,000 calculated patterns (interplanar spacings, intensities, Miller indices).

The database comes with an innovative retrieval software developed by Crystal Impact. It offers a large variety of elaborate new features which makes retrieval of the desired information extremely easy.

More information and a free demo is available at https://www.crystalimpact.de/pcd

Database

- Comprehensive world literature coverage, data from over 118,000 original publications
- Data were checked using an elaborate software package
- Phase information available due to distinct phases concept; the prototype entry is selected by editors for each individual entry
  - ✓ Phase defined by crystal structure (prototype) and chemical system
  - ✓ Each phase has a unique formula ("phase formula")
- Fully standardized and comparable crystal structure data
- Both published and standardized crystallographic data are present, with assigned atomic coordinates if a prototype could be assigned but atom coordinates were not determined
- Pearson Symbol, Prototype, Wyckoff Sequence-classifications
- Inclusion of derived data: interatomic distance, coordination number, atomic environment
- Atomic environment type (coordination polyhedron) specified for each atom of the parameter list of each prototype structure
- More than twice as many fields per entry than ICSD entries
- Includes published powder patterns as well as on the fly computed powder patterns
- About 56,000 figure descriptions for cell parameters as a function of temperature, pressure or concentration
- General and editor's remarks, information about preparation and experimental details
- 10,000 corrections of chemical formulas, cell parameters, symmetry or atom coordinates, applied and reported in errata
- Each entry contains links to external data sources
  - ✓ Phase diagram (through Phase Diagrams Online)
  - ✓ Original publication (through crossref.org)
- Excellent coverage of alloys and intermetallics as a consequence of its origin (Pearson's Handbook of Crystallographic Data for Intermetallic Phases)

Software

- Perpetual restraining: Always see your entered restraints and the number of matching entries for each single criterion
- List selection boxes: View and select all available values for a database field (selection criterion) using the mouse
- Two alternative dialogs for the input of the selection criteria (quick and exhaustive)
- Visualization (3D-pictures) of crystal structures
- Elaborate data views at different "levels"
  - ✓ Entry report (answer set level)
  - ✓ System matrix (chemical system level)
  - ✓ Phases list (phase level)
  - ✓ Entry data (entry level)
    - Data sheet
    - 3D structure picture
    - powder diffraction pattern (published and calculated)
    - Distances/angles table with 3D-view of coordination polyhedral
    - Dynamic plots of cell parameters against p or T
    - Figure plots prepared by editors
- Radii/volumes diagram for comparison of similar crystal structures
- Elaborate data selection beyond normal selection criteria dialogs
  - ✓ Search for entries with same prototype
  - ✓ Logical combination of arbitrary answer sets
  - ✓ Create answer set from sel. entries, phases or chemical syst.
  - ✓ Cut/copy/paste of selected entries
- Compilation of phase data sheet from user-selected entries
- Printing and exporting of all kinds of information and views
- Export of crystal structure data to CIF or Diamond directly
- Links to external data sources from the database entries

System requirements

- Microsoft Windows XP, Vista, Windows 7, 8, 10 or 11
- Microsoft Internet Explorer 5.01 (or higher)
- 1 GB of RAM (2 GB or more recommended)
- 4 GB of free disk space
- Min. graphics resolution 1024x768 with 32,767 colors (“high color”)

Licensing/Pricing

The PCD database can either be purchased with unlimited usage time or as 1-year licenses, starting at **530 EUR**.

Details about the large variety of different licenses and their prices can be obtained from

https://www.crystalimpact.de/pcd/sales.htm

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