

InfoMaticA

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1 Overview

MedeA InfoMaticA provides a graphical user interface to the experimental databases COD, ICSD, NCD, Pauling and Pearson's. Together these databases contain over 1.1 million structure entries, thus representing one of the largest integrated sources of solid state structure data accessible today.

InfoMaticA

Structure data from powder diffraction and scattering experiments

Lattice parameter and atomic positions

Bibliographic references

Experimental setup

Symmetry, stoichiometry, partial disorder

Phase diagrams

InfoMaticA provides an easy-to-use keyword search language to formulate complex requests on the full set of experimental and computed data available.

MedeA offers a simple interface to store computed structure data in *InfoMaticA*. You can build up your own database of computed structures along with comments and references and search this database in combination with the experimental ones.

2 *InfoMaticA's* Structure Databases

2.1 COD (Crystallography Open Database, University of Cambridge, UK)

COD is an open-access collection of crystal structures of organic, inorganic, metal-organic compounds and minerals, excluding biopolymers. People registered to COD can add published and unpublished structures of small molecules and small to medium sized unit cell crystals. As of Dec 2017, the database has more than 380,000 entries. COD is an academic project, and its development has been published in several peer-reviewed papers. More information: [MedeA COD](#) [1]

2.2 ICSD (Inorganic Crystal Structure Database, FIZ Karlsruhe, Germany)

ICSD contains crystal structure information for non-organic compounds mainly including ceramics and minerals and since recently also metallic systems. ICSD entries go back to 1915; currently the database has around 185,000 structure entries. More information: [MedeA ICSD](#) [2]

2.3 Pearson's File (ASM International, USA)

The Pearson's data file is a crystallographic database published by ASM International and originates from the well-known [LINUS PAULING FILE \(LPF\) project](#) [3]. The database contains crystal structures of the full range of inorganic compounds. The present *MedeA* release contains close to 303,000 structural data sets (including atom coordinates and displacement parameters, when determined) for more than 95,000 different phases. More information: [MedeA Pearson](#) [4]

2.4 The Linus Pauling file (LPF), binary edition (MPDS, Switzerland)

The binary edition of the Pauling file (LPF) within *MedeA* provides structural data and physical properties for approximately 28,000 binary inter-metallic and oxide systems. For a smaller subset of structures, phase diagram information is available. The Editor-in-chief of the Pauling file is Prof. Pierre Villars, Switzerland. More information: [MedeA Pauling](#) [5]

2.5 NCD (NIST Crystal Data, National Institute of Standards and Technology, USA)

NCD contains chemical, physical, and crystallographic information on approximately 237,000 inorganic and organic crystalline materials. NCD includes reliable data across the entire range of solid state materials including minerals, inter-metallic phases, metals, alloys, drugs, antibiotics, and pesticides. Data included in NIST comprise standard cell parameters, cell volume, space group number and symbol, calculated density, chemical formula, chemical name, and classification by chemical type. The National Institute of Standards and Technology (NIST), USA, maintains NCD. More information: [MedeA NCD](#) [6]

3 *Materials Design Database* for Computed Data

Computed structures can be saved to the "computational database" aka *Materials Design Database*. To save a structure, bring up the structure window in *MedeA* (e.g. by loading a minimized structure from a previous calculation) and select **Save to database** from the *MedeA File* menu. When saving a structure, you should provide a name and comments to save along with the structure. Structures saved this way can

[1] <http://www.materialsdesign.com/datasheet-cod>

[2] <http://www.materialsdesign.com/datasheet-icsd>

[3] <http://paulingfile.com/>

[4] <http://www.materialsdesign.com/datasheet-prearson>

[5] <http://www.materialsdesign.com/datasheet-pauling>

[6] <https://www.materialsdesign.com/datasheet-ncd>

be retrieved through a standard search request in the *InfoMaticA* dialog along with experimental database entries. Structures saved to the *Materials Design Database* are tagged with *MD*.

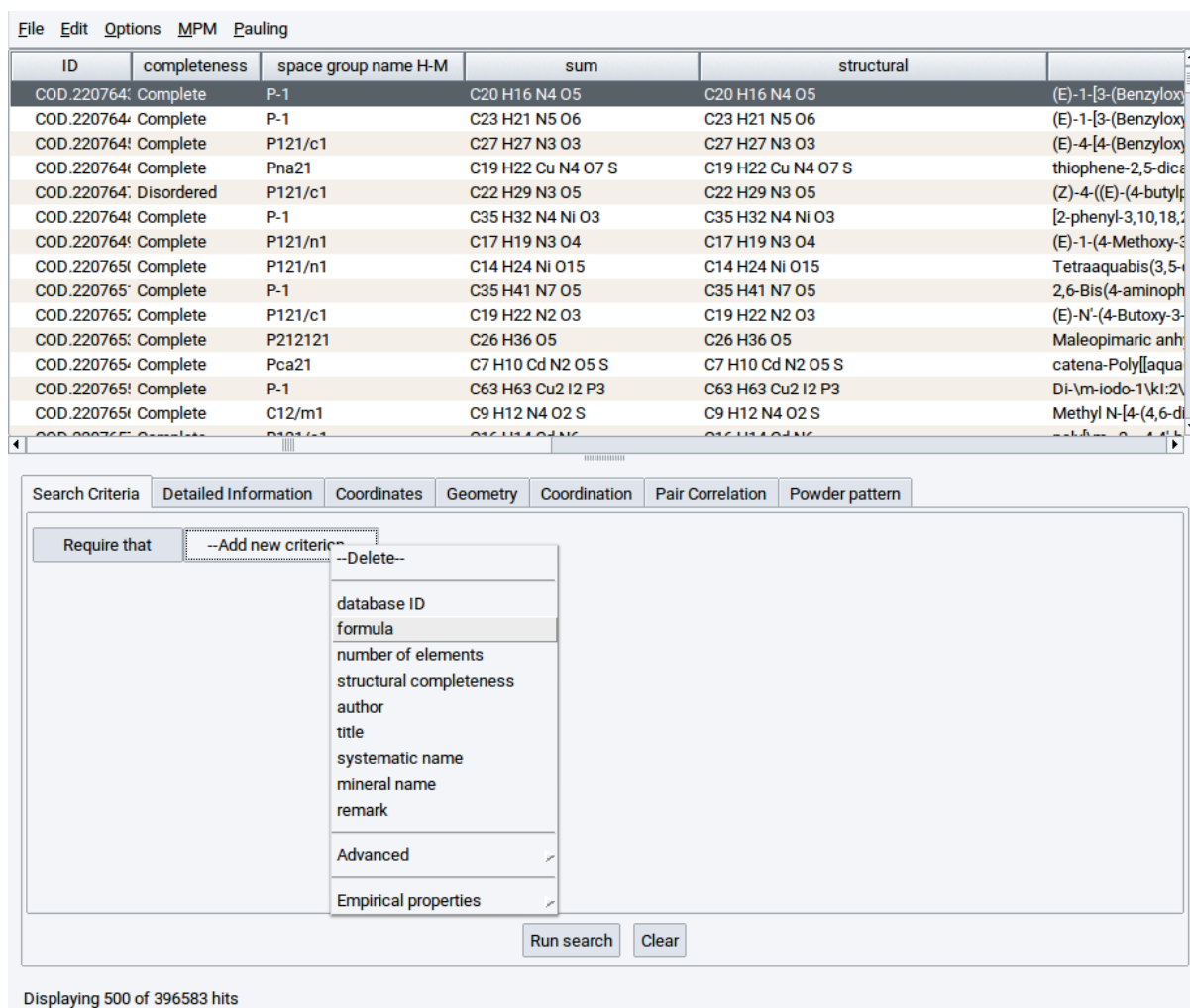
Hint: The *Materials Design Database* file is *MaterialsDesign.db* which is located in the *MedeA* installation directory, namely *MD/Databases*. This file can be easily overwritten upon updating *MedeA* or installing a newer version over an older *MedeA* version. The *MedeA* installer is prepared for such situations and asks to overwrite and replace existing *Materials Design Database* files.

4 Starting *InfoMaticA*

To bring up the *InfoMaticA* entry in the *MedeA* main menu bar, select the **InfoMaticA** item from the *MedeA* **Tools** menu. Next click **InfoMaticA >> Search** to bring up the *InfoMaticA* search window/dialog.

The main elements of the *InfoMaticA* interface are the following (top to bottom):

- A menu bar containing entries **Files**, **Edit**, **Options**, and **Pauling**.
- A configurable table for displaying search results in the upper region
- An adjustable separator
- A number of panels in the lower region to formulate search phrases/criteria and to visualize structure specific results and properties



The screenshot displays the *InfoMaticA* search window. At the top is a menu bar with **File**, **Edit**, **Options**, **MPM**, and **Pauling**. Below the menu is a table with columns: **ID**, **completeness**, **space group name H-M**, **sum**, **structural**, and a column for chemical structures. The table lists various COD entries with their respective properties and chemical formulas.

Below the table is a search criteria dialog box with tabs: **Search Criteria**, **Detailed Information**, **Coordinates**, **Geometry**, **Coordination**, **Pair Correlation**, and **Powder pattern**. The **Search Criteria** tab is active, showing a list of criteria to be searched for, including **database ID**, **formula**, **number of elements**, **structural completeness**, **author**, **title**, **systematic name**, **mineral name**, and **remark**. There are also sections for **Advanced** and **Empirical properties**. Buttons for **Run search** and **Clear** are at the bottom of the dialog.

At the bottom of the window, it says "Displaying 500 of 396583 hits".

5 Searching and Retrieving Data

Start your search in the tab labeled *Search Criteria* by formulating a search phrase. To do so, click on – Add new criterion – and select a search option. The following criteria are available:

- – Delete – : Remove search criterion
- Database ID : Provide identification numbers (IDs) under which structures are registered in the *MedeA* databases
- formula : Provide an entire chemical formula or parts of the formula
- number of elements : Allow a certain number or range of elements in the formula
- structural completeness : Display only structures with with particular structure type (select one option of the options complete , missing atoms , disordered , none available)
- author : Search for names of people who published relevant structure data in the literature
- title : Search in the titles of publications with structure data
- systematic name : Search by the systematic name of compounds (IUPAC nomenclature)
- mineral name : Search by mineral name of compounds (trivial/non-systematic name)
- remark : Search for keywords in the content of *Remark section* of structure records
- Advanced : Define additional search criteria (can be database specific)

Note that, as you select a search criterion from the selection, additional *sub-options* may appear on the right. Click these options to create a complete search phrase.

For example, the formula criterion has the following sub-options:

- is : Exact chemical formula, e.g. Cr₂O₃ , Be, TiC, etc.
- contains exactly atoms of : Number and type of atoms, e.g. contains exactly 3 atoms of Fe
- contains any number of atoms of : elements of a particular group or period of the periodic system of the elements, e.g. contains any number of atoms from group 3 (Sc..La Ac)
- contains less than atoms of : upper boundary for the number of particular elements
- contains more than atoms of : lower boundary for number of particular elements
- contains from to atoms of : define a range of number of particular elements
- does not contain atoms of : Exclude elements
- has a ratio of atoms of to atoms of : The exact ratio of two elements

Hint: Recognition of element symbols is case sensitive! For instance, the search algorithm has to decide whether structures with cobalt is requested (element symbol Co) or the structures that contain CO (carbon monoxide) molecules. Another example: Should the compound contain three units of bismuth (Bi₃) or BI₃. The latter is a binary compound that is formed by boron and iodine.

Some criteria like **author** , **remarks** , and **title** let you search for text strings of the data files. These options have the following sub-options:

- **Is** : Search for an exact text string
- **Is Not** : Search for anything but this exact string
- **Is like** : Search for a fraction of a text string defined in the field that is part of another text strings as names, terms, etc.. Use wildcards ? for a single character and % or * for multiple characters.
- **Is Not Like** : Search for text strings that do not have the fraction of the text string defined in the field
- **Contains** : Search for a substring

Furthermore, a given search statement can be made active, non-active or conditional by clicking on **Require that** on the left-hand side of each search phrase and selecting either of the options given below:

- **Require that** : Require that the search criterion in the present line is fulfilled
- **If present** : Require criterion in present line to be fulfilled if present or possible
- **Ignore** : Criterion is ignored

Once you have built a search phrase, click **Run search** to perform the search and display results. If needed, add additional criteria using a second line and so forth, until you are satisfied with the results. With **Clear** all search criteria can be erased.

Note: There is **no Undo** function to bring back search criteria that were cleared!

6 Displaying Detailed Information

To get more information on a structure entry, highlight the corresponding row in the table of results with the pointer (simple click onto the record). Afterwards switch to one of the following tabs:

- **Search criteria** tab: Formulate search phrase and run searches on all databases
- **Detailed information** tab: Display main structural data, symmetry data and bibliographic references, and remarks (if present)

File Edit Options MPM Pauling

ID	completeness	space group name H-M	sum	str
ICSD.1	Complete	P121/C1	Cr2 O11 Te4	Cr2 O11 Te4
ICSD.2	Disordered	PNMA	Co0.93 Mn1.07 O4 Si1	Co0.93 Mn1.07 O4 Si1
ICSD.3	Complete	P3-C1	F3 La1	F3 La1
ICSD.4	Complete	P3-C1	Ce1 F3	Ce1 F3
ICSD.5	Complete	PNA21	H4 Na1 O5 P1	H4 Na1 O5 P1
ICSD.6	Missing Atoms	P121/M1S	H2 Al2 O9 S1 Te1	H2 Al2 O9 S1 Te1
ICSD.7	Complete	P21NB	H2 Li1 O3 P1	H2 Li1 O3 P1
ICSD.8	Complete	PNMA	Ba1 S3 Te1	Ba1 S3 Te1
ICSD.9	Complete	P121/C1	H2 Cu1 K1 O5 P1	H2 Cu1 K1 O5 P1
ICSD.10	Missing Atoms	PNMA	H14 O25 P6 Sr3	H14 O25 P6 Sr3
ICSD.11	Missing Atoms	P121/N1	H6 Ca1 N2 O9	H6 Ca1 N2 O9

Search Criteria Detailed Information Coordinates Geometry Coordination Pair Correlation Powder pattern

ICSD.1 Cr₂Te₄O₁₁

Cr₂O₁₁Te₄
Oxotetratellurium dichromate(III)

Symmetry

Spacegroup: **P121/C1** Z: **2**
SpGrp Number: Volume: **507.61**
Pearson symbol: **mP34** Calculated density:

Cell

a: **7.016±0.** alpha: **90.±0.**
b: **7.545±0.** beta: **99.69±0.**
c: **9.728±0.** gamma: **90.±0.**

Reference

(1) Meunier, G., Frit, B. and Galy, J., Cr₂Te₄O₁₁: une structure a anions complexes (Cr₂O₁₀)(14-), *Acta Crystallographica B* (24,1968-38,1982) (*)

Displaying 500 of 1163824 hits

- **Coordinates** tab: Display positions of atoms, Wyckoff sites and their occupancies of structure records that have atomic coordinates

File Edit Options MPM Pauling

ID	completeness	space group name H-M	sum	str
ICSD.1	Complete	P121/C1	Cr2 O11 Te4	Cr2 O11 Te4
ICSD.2	Disordered	PNMA	Co0.93 Mn1.07 O4 Si1	Co0.93 Mn1.07 O4 Si1
ICSD.3	Complete	P3-C1	F3 La1	F3 La1
ICSD.4	Complete	P3-C1	Ce1 F3	Ce1 F3
ICSD.5	Complete	PNA21	H4 Na1 O5 P1	H4 Na1 O5 P1
ICSD.6	Missing Atoms	P121/M1S	H2 Al2 O9 S1 Te1	H2 Al2 O9 S1 Te1
ICSD.7	Complete	P21NB	H2 Li1 O3 P1	H2 Li1 O3 P1
ICSD.8	Complete	PNMA	Ba1 S3 Te1	Ba1 S3 Te1
ICSD.9	Complete	P121/C1	H2 Cu1 K1 O5 P1	H2 Cu1 K1 O5 P1
ICSD.10	Missing Atoms	PNMA	H14 O25 P6 Sr3	H14 O25 P6 Sr3
ICSD.11	Missing Atoms	P121/N1	H6 Ca1 N2 O9	H6 Ca1 N2 O9

Search Criteria Detailed Information Coordinates Geometry Coordination Pair Correlation Powder pattern

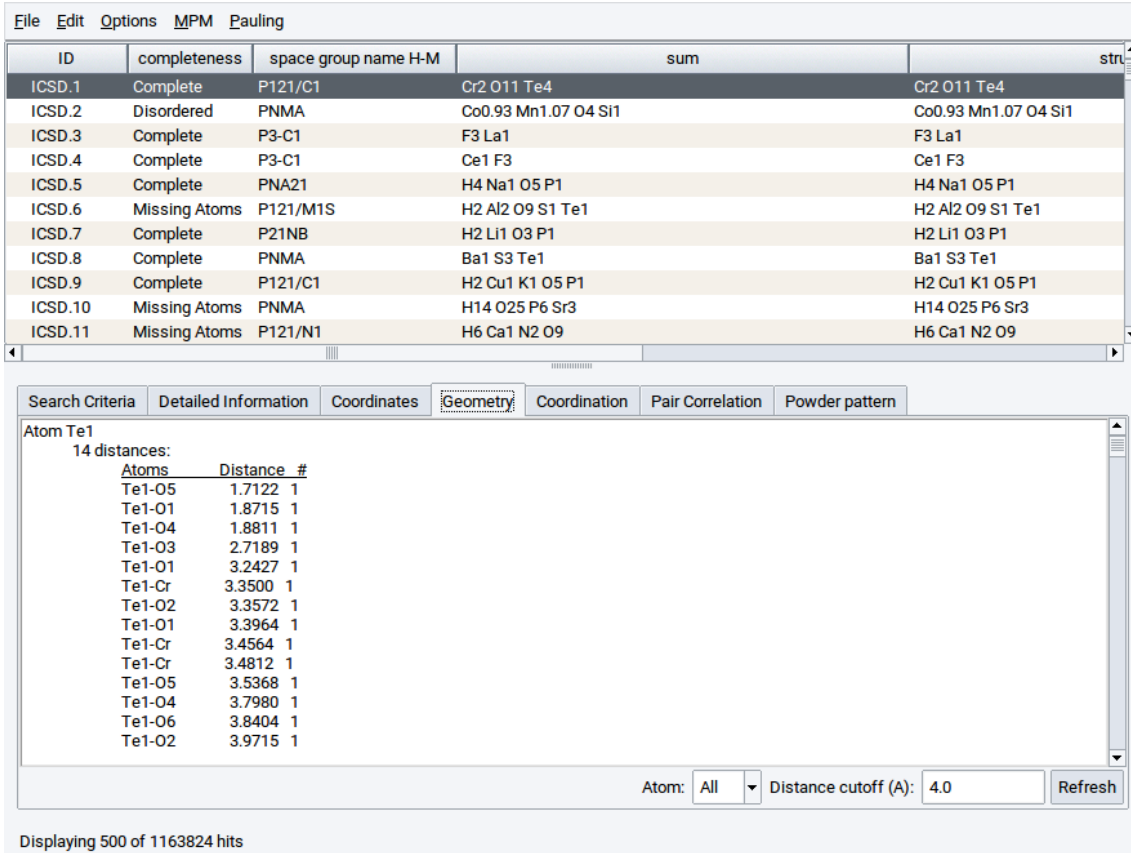
a: 7.01600 alpha: 90.0
b: 7.54500 beta: 99.7
c: 9.72800 gamma: 90.0

Site	Wyckoff Position	Symmetry	Element	X	Y	Z	Occupancy
Te: 4e	?		Te	0.13970	0.85990	0.17620	1.0
Te: 4e	?		Te	0.67230	0.86180	0.41580	1.0
Cr 4e	?		Cr	0.31920	0.50190	0.38420	1.0
O1 4e	?		O	0.15800	0.64900	0.48660	1.0
O2 4e	?		O	0.56300	0.64100	0.45170	1.0
O3 4e	?		O	0.46800	0.37500	0.26230	1.0
O4 4e	?		O	0.12700	0.31400	0.34290	1.0
O5 4e	?		O	0.20500	0.64400	0.21210	1.0
O6 2d	?		O	0.50000	0.00000	0.50000	1.0

Displaying 500 of 1163824 hits

- **Geometry** tab: Display bond lengths and angles of structure records with atomic coordinates; de-

fine for which constituting **Atom:** and the corresponding **Distance cutoff (A):** in Å and confirm with **Refresh**



The screenshot shows the MedeA software interface. At the top is a menu bar with 'File', 'Edit', 'Options', 'MPM', and 'Pauling'. Below it is a table of ICSD records with columns: ID, completeness, space group name H-M, sum, and str. The table contains 11 rows of data. Below the table is a tabbed interface with 'Search Criteria', 'Detailed Information', 'Coordinates', 'Geometry', 'Coordination', 'Pair Correlation', and 'Powder pattern'. The 'Coordination' tab is active, showing a list of 14 distances for Atom Te1. At the bottom of the window, there are controls for 'Atom:' (set to 'All'), 'Distance cutoff (A):' (set to '4.0'), and a 'Refresh' button. Below the controls, it says 'Displaying 500 of 1163824 hits'.

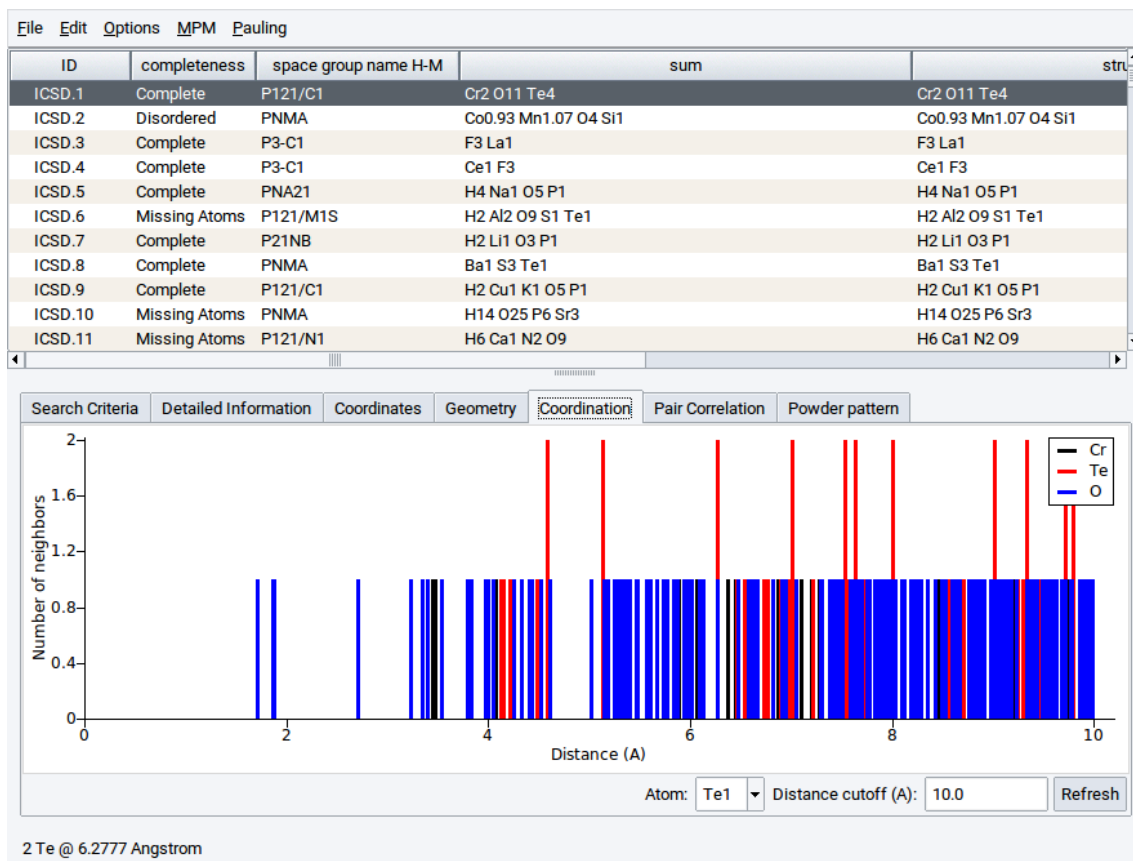
ID	completeness	space group name H-M	sum	str
ICSD.1	Complete	P121/C1	Cr2 O11 Te4	Cr2 O11 Te4
ICSD.2	Disordered	PNMA	Co0.93 Mn1.07 O4 Si1	Co0.93 Mn1.07 O4 Si1
ICSD.3	Complete	P3-C1	F3 La1	F3 La1
ICSD.4	Complete	P3-C1	Ce1 F3	Ce1 F3
ICSD.5	Complete	PNA21	H4 Na1 O5 P1	H4 Na1 O5 P1
ICSD.6	Missing Atoms	P121/M1S	H2 Al2 O9 S1 Te1	H2 Al2 O9 S1 Te1
ICSD.7	Complete	P21NB	H2 Li1 O3 P1	H2 Li1 O3 P1
ICSD.8	Complete	PNMA	Ba1 S3 Te1	Ba1 S3 Te1
ICSD.9	Complete	P121/C1	H2 Cu1 K1 O5 P1	H2 Cu1 K1 O5 P1
ICSD.10	Missing Atoms	PNMA	H14 O25 P6 Sr3	H14 O25 P6 Sr3
ICSD.11	Missing Atoms	P121/N1	H6 Ca1 N2 O9	H6 Ca1 N2 O9

Atom Te1		
14 distances:		
Atoms	Distance	#
Te1-O5	1.7122	1
Te1-O1	1.8715	1
Te1-O4	1.8811	1
Te1-O3	2.7189	1
Te1-O1	3.2427	1
Te1-Cr	3.3500	1
Te1-O2	3.3572	1
Te1-O1	3.3964	1
Te1-Cr	3.4564	1
Te1-Cr	3.4812	1
Te1-O5	3.5368	1
Te1-O4	3.7980	1
Te1-O6	3.8404	1
Te1-O2	3.9715	1

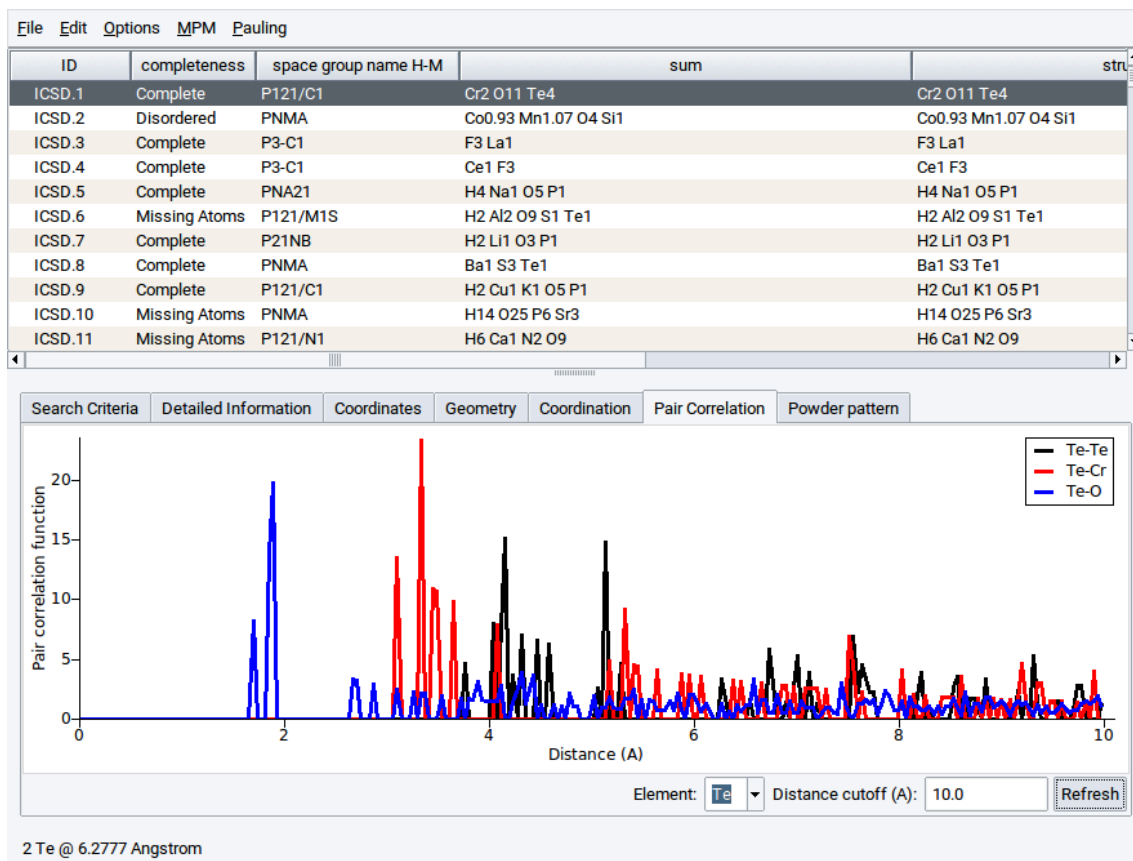
Atom: All Distance cutoff (A): 4.0 Refresh

Displaying 500 of 1163824 hits

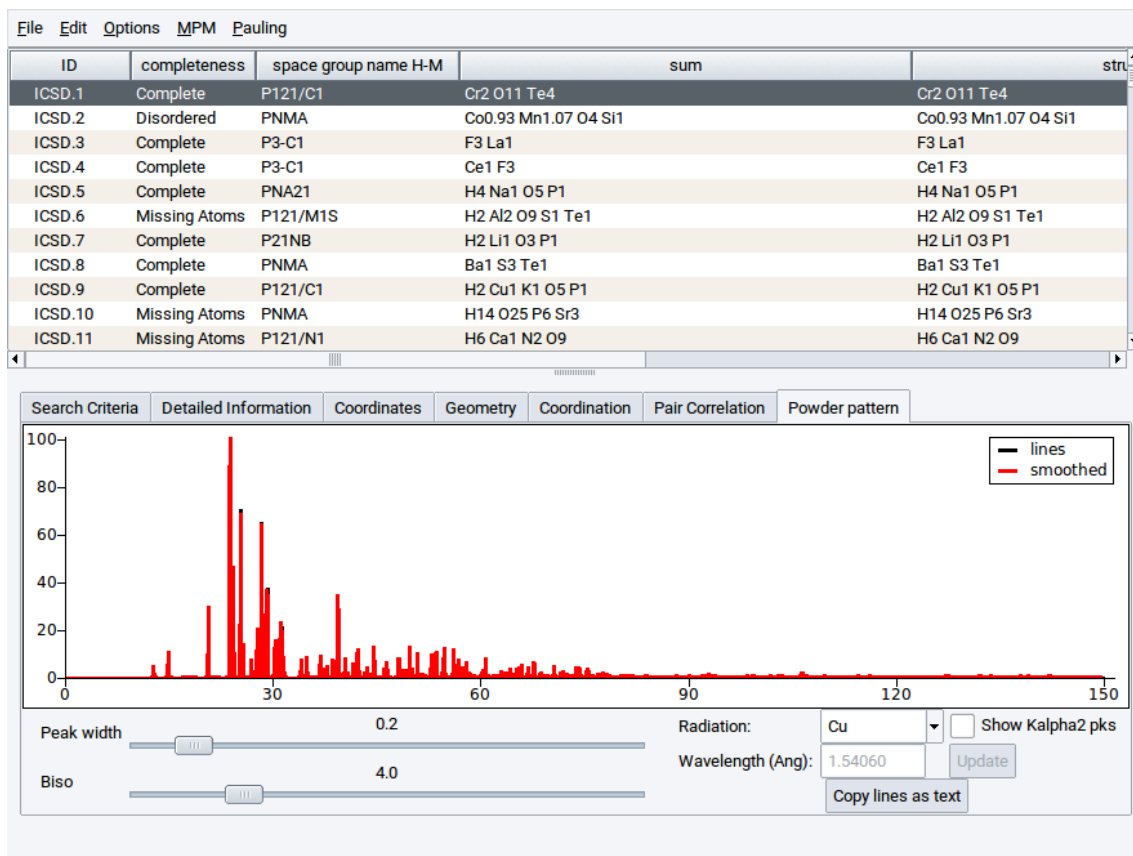
- **Coordination** tab: Select a lattice site (atom position) and display a chart with the nearest neighbors, next-nearest neighbors, etc. (requires that structure records have atomic coordinates) Define for which constituting **Atom:** the coordination shell should be calculated, the corresponding **Distance cutoff (A):** in Å and confirm with **Refresh**



- **Pair Correlation** tab: Chart to show which pairs of atoms of which distance; by default pair distances of all atoms are shown; select an element of the relevant system to display specific distributions of pair distances (requires that structure records have atomic coordinates) Define for which constituting **Atom**: the pair correlation should be calculated, the corresponding **Distance cutoff (Å)**: in Å and confirm with **Refresh**



- Powder pattern tab: Show the powder diffraction pattern of the selected structure; can be calculated for different radiation sources and manually defined radiation wave lengths (requires that structure records have atomic coordinates)

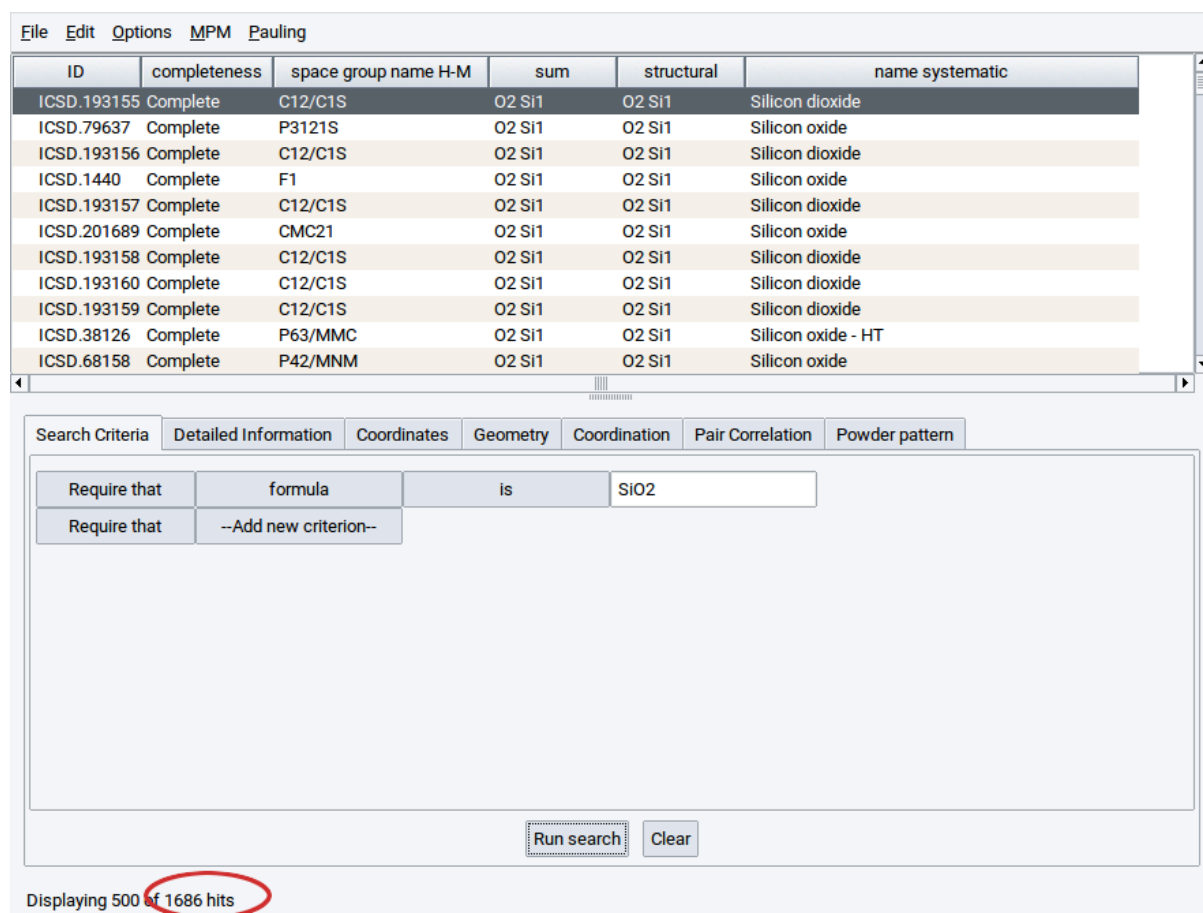


7 Assessing Structures and Overview

Often the number of structures matching your search criteria is rather large. For single compounds there are multiple entries (measured at different temperatures and pressures, hence structures represent different phases), the assignment of space groups changed with higher resolution or improved sample preparation techniques in the measurements, etc. *InfoMaticA* has features to efficiently select an appropriate set of structures from the search results.

One possibility to create an essence of relevant structures is to reduce the list of found structures to a list of the median structures. The latter are representatives for each class of structures found in the search.

For instance: A search for structures with the search criterion **formula** is SiO2 yields more than 1000 hits if all *MedeA* databases are considered.



ID	completeness	space group name H-M	sum	structural	name systematic
ICSD.193155	Complete	C12/C1S	O2 Si1	O2 Si1	Silicon dioxide
ICSD.79637	Complete	P3121S	O2 Si1	O2 Si1	Silicon oxide
ICSD.193156	Complete	C12/C1S	O2 Si1	O2 Si1	Silicon dioxide
ICSD.1440	Complete	F1	O2 Si1	O2 Si1	Silicon oxide
ICSD.193157	Complete	C12/C1S	O2 Si1	O2 Si1	Silicon dioxide
ICSD.201689	Complete	CMC21	O2 Si1	O2 Si1	Silicon oxide
ICSD.193158	Complete	C12/C1S	O2 Si1	O2 Si1	Silicon dioxide
ICSD.193160	Complete	C12/C1S	O2 Si1	O2 Si1	Silicon dioxide
ICSD.193159	Complete	C12/C1S	O2 Si1	O2 Si1	Silicon dioxide
ICSD.38126	Complete	P63/MMC	O2 Si1	O2 Si1	Silicon oxide - HT
ICSD.68158	Complete	P42/MNM	O2 Si1	O2 Si1	Silicon oxide

Search Criteria: Detailed Information | Coordinates | Geometry | Coordination | Pair Correlation | Powder pattern

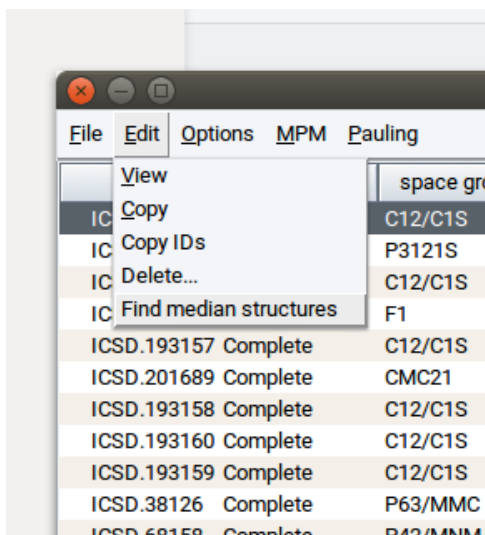
Require that: formula is SiO2

Require that: --Add new criterion--

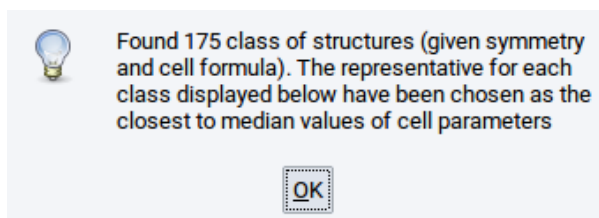
Run search | Clear

Displaying 500 of 1686 hits

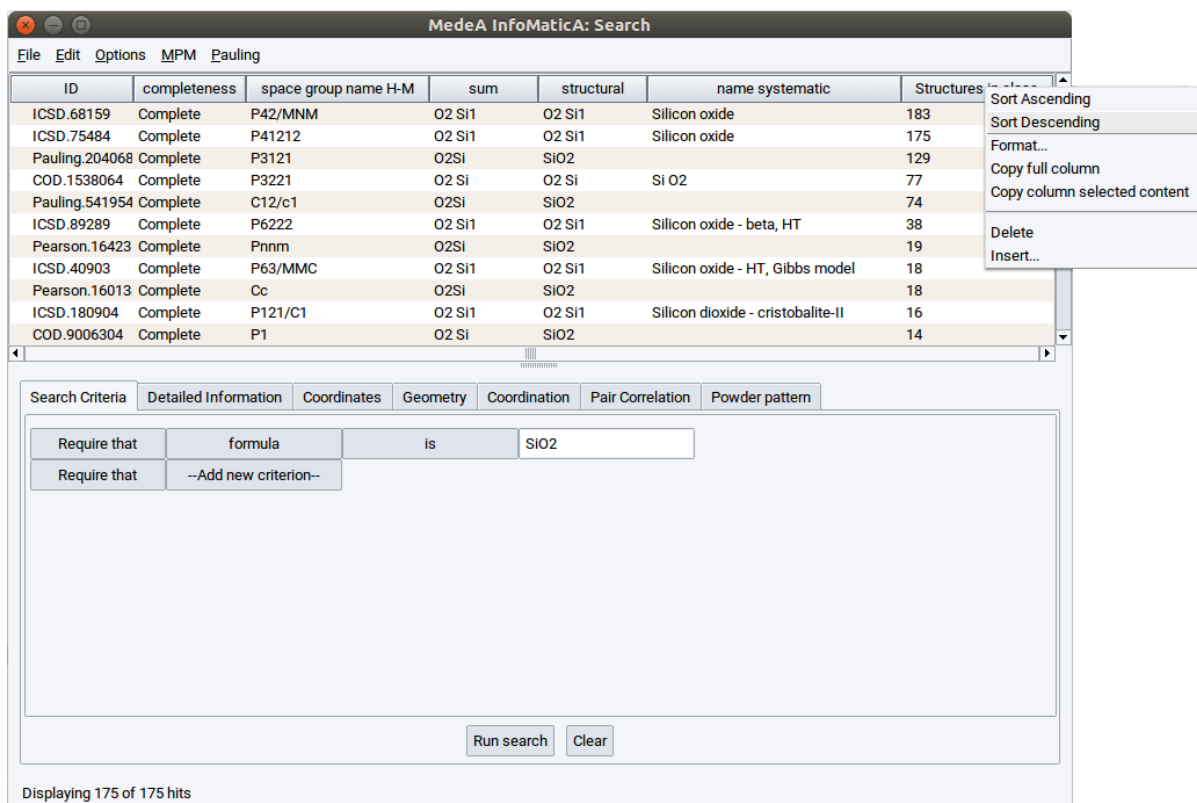
With the menu sequence **Edit** >> **Find median structures** *InfoMaticA* examines the structural properties of the complete structures that have been found (those with atomic coordinates).



InfoMaticA takes into account the space groups, lattice parameters, atomic positions, compositions, etc. In this example, *InfoMaticA* finds 175 classes of structures whereby each structure found is a representative of each class.



Upon confirming with OK the 175 structures are summarized in the main table of the *InfoMaticA* dialog. The largest class of structures found in the current example is that for alpha quartz which is thermodynamically the most stable SiO_2 phase.



The screenshot shows the 'MedeA InfoMaticA: Search' dialog with a table of structures. A context menu is open over the 'Structures' column header, showing options like 'Sort Ascending', 'Sort Descending', 'Format...', 'Copy full column', 'Copy column selected content', 'Delete', and 'Insert...'. Below the table, there are tabs for 'Search Criteria', 'Detailed Information', 'Coordinates', 'Geometry', 'Coordination', 'Pair Correlation', and 'Powder pattern'. The 'Search Criteria' tab is active, showing a search criterion: 'Require that formula is SiO2'. There are 'Run search' and 'Clear' buttons at the bottom of the search criteria section. The status bar at the bottom indicates 'Displaying 175 of 175 hits'.

ID	completeness	space group name H-M	sum	structural	name systematic	Structures
ICSD.68159	Complete	P42/MNM	O2 Si1	O2 Si1	Silicon oxide	183
ICSD.75484	Complete	P41212	O2 Si1	O2 Si1	Silicon oxide	175
Pauling.204068	Complete	P3121	O2Si	SiO2		129
COD.1538064	Complete	P3221	O2 Si	O2 Si	Si O2	77
Pauling.541954	Complete	C12/c1	O2Si	SiO2		74
ICSD.89289	Complete	P6222	O2 Si1	O2 Si1	Silicon oxide - beta, HT	38
Pearson.16423	Complete	Pnm	O2Si	SiO2		19
ICSD.40903	Complete	P63/MMC	O2 Si1	O2 Si1	Silicon oxide - HT, Gibbs model	18
Pearson.16013	Complete	Cc	O2Si	SiO2		18
ICSD.180904	Complete	P121/C1	O2 Si1	O2 Si1	Silicon dioxide - cristobalite-II	16
COD.9006304	Complete	P1	O2 Si	SiO2		14

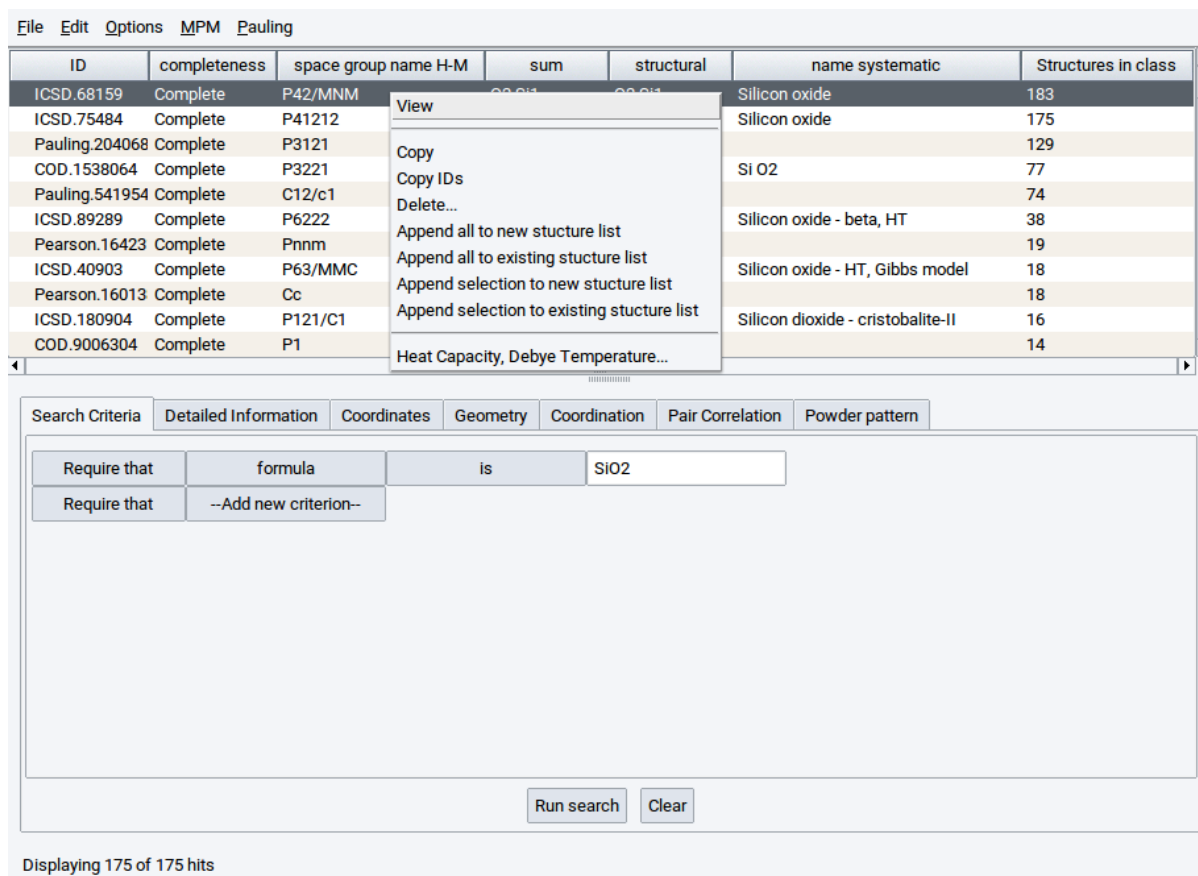
A right-click in the header cells of the table (the black row on top) opens a context menu to change what and

how information is displayed:

- **Sort Ascending** and **Sort Descending** : Allow to sort data in columns. *MedeA* keeps a memory of previous sorts, so you can sort first by volume to find the most likely candidates for the low temperature structure with smallest volume, then sort by space-group: The results are grouped by space group, then within each space group by volume.
- **Insert. . .** : Add any available property to the results table such as cell lengths and volume. Some other properties might not be reported for all structures from search results.
- **Delete** : Remove the selected column
- **Format** : Change how results are displayed: numbers are displayed with all digits as reported in the database. With the format option restrict the display of numbers to a required precision, cutting off digits and filling missing numbers as 0.

8 Viewing and Editing Structures

Structures indicated by *MedeA* to be **complete** have all information on unit cell and atomic positions needed to display them in a 3D structure model. To view such a structure, left click on the corresponding row in the table of results to select it, then right-click >> select **View** from the pop-up menu (see below).



The screenshot shows the MedeA software interface. At the top, there is a menu bar with 'File', 'Edit', 'Options', 'MPM', and 'Pauling'. Below the menu bar is a table of search results. The table has columns for 'ID', 'completeness', 'space group name H-M', 'sum', 'structural', 'name systematic', and 'Structures in class'. A context menu is open over the first row (ICSD.68159), showing options like 'View', 'Copy', 'Copy IDs', 'Delete...', 'Append all to new structure list', 'Append all to existing structure list', 'Append selection to new structure list', 'Append selection to existing structure list', and 'Heat Capacity, Debye Temperature...'. Below the table is a search criteria dialog box with tabs for 'Search Criteria', 'Detailed Information', 'Coordinates', 'Geometry', 'Coordination', 'Pair Correlation', and 'Powder pattern'. The 'Search Criteria' tab is active, showing a search for 'SiO2' with the criteria 'Require that formula is SiO2'. There are 'Run search' and 'Clear' buttons at the bottom of the dialog. Below the dialog, it says 'Displaying 175 of 175 hits'.

ID	completeness	space group name H-M	sum	structural	name systematic	Structures in class
ICSD.68159	Complete	P42/MNM	00.011	00.011	Silicon oxide	183
ICSD.75484	Complete	P41212			Silicon oxide	175
Pauling.204068	Complete	P3121				129
COD.1538064	Complete	P3221			Si O2	77
Pauling.541954	Complete	C12/c1				74
ICSD.89289	Complete	P6222			Silicon oxide - beta, HT	38
Pearson.16423	Complete	Pnnm				19
ICSD.40903	Complete	P63/MMC			Silicon oxide - HT, Gibbs model	18
Pearson.16013	Complete	Cc				18
ICSD.180904	Complete	P121/C1			Silicon dioxide - cristobalite-II	16
COD.9006304	Complete	P1				14

Alternatively, you can use the menu items **Copy** and **Copy ID**, respectively, to copy structure information to *MedeA*'s internal clipboard for later use.

The **Delete. . .** option can be used to delete structure entries from the *Materials Design Database* but cannot be applied to the experimental databases such as, e.g. *ICSD*.

Hint: As known from spreadsheet programs as *Microsoft Excel* or *Libreoffice* it is possible to select (highlight) several table rows, i.e. structures at the same time. Multiple rows can be selected by holding the **Shift**

key (keyboard) or the **Ctrl** key (keyboard) while selecting rows with the pointer. With multiple table rows selected it is possible to view, copy, etc. several structures at the same time.

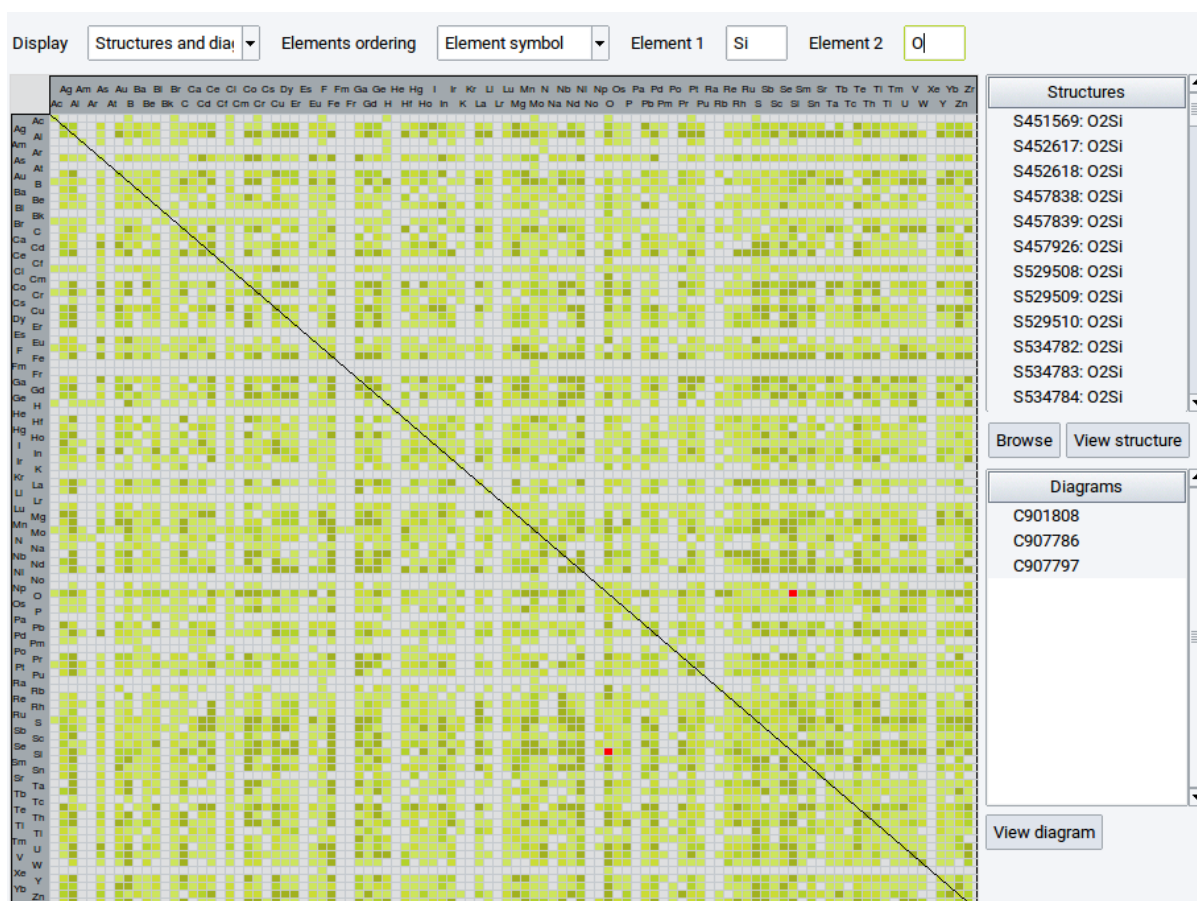
With a valid license for *Medea HT-Launchpad* it possible to add structures found in *InfoMaticA* to existing structures list and to create new structure lists. The relevant menu items are

- **Append all to new structure list** : Create a new structure list with all structures collected in the table
- **Append all to existing structure list** : Add all structures in the table to an existing structure list
- **Append selection to new structure list** : Create a new structure list with a selection of structures, i.e. records that are highlighted in the table - either select one structure or a multiple of structures
- **Append selection to existing structure list** : Add one highlighted or several selected structures in the table to an existing structure list

9 Phase Diagrams of Binary Compounds

The Pauling File Database includes phase diagrams for binary compounds and their structures.

To access this additional information, click on **Pauling** >> **Show binaries matrix** to open the Pauling binary compounds matrix:

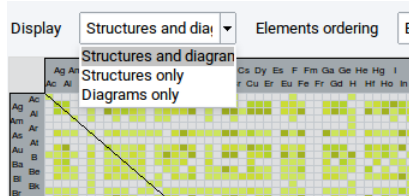


Above the matrix are tools for finding phase diagrams for a specific binary compound and related systems. Each green and gray field in the matrix represents one binary compound. On the right side is the detailed information about the selected system.

You can select a compound with your mouse and while hovering over the gray and green, respectively, fields in the matrix. The number of structures and diagrams is displayed in the upper right corner. When selecting a system (click on a gray or green field or enter the symbols of two elements in fields for Element 1 and 2) the

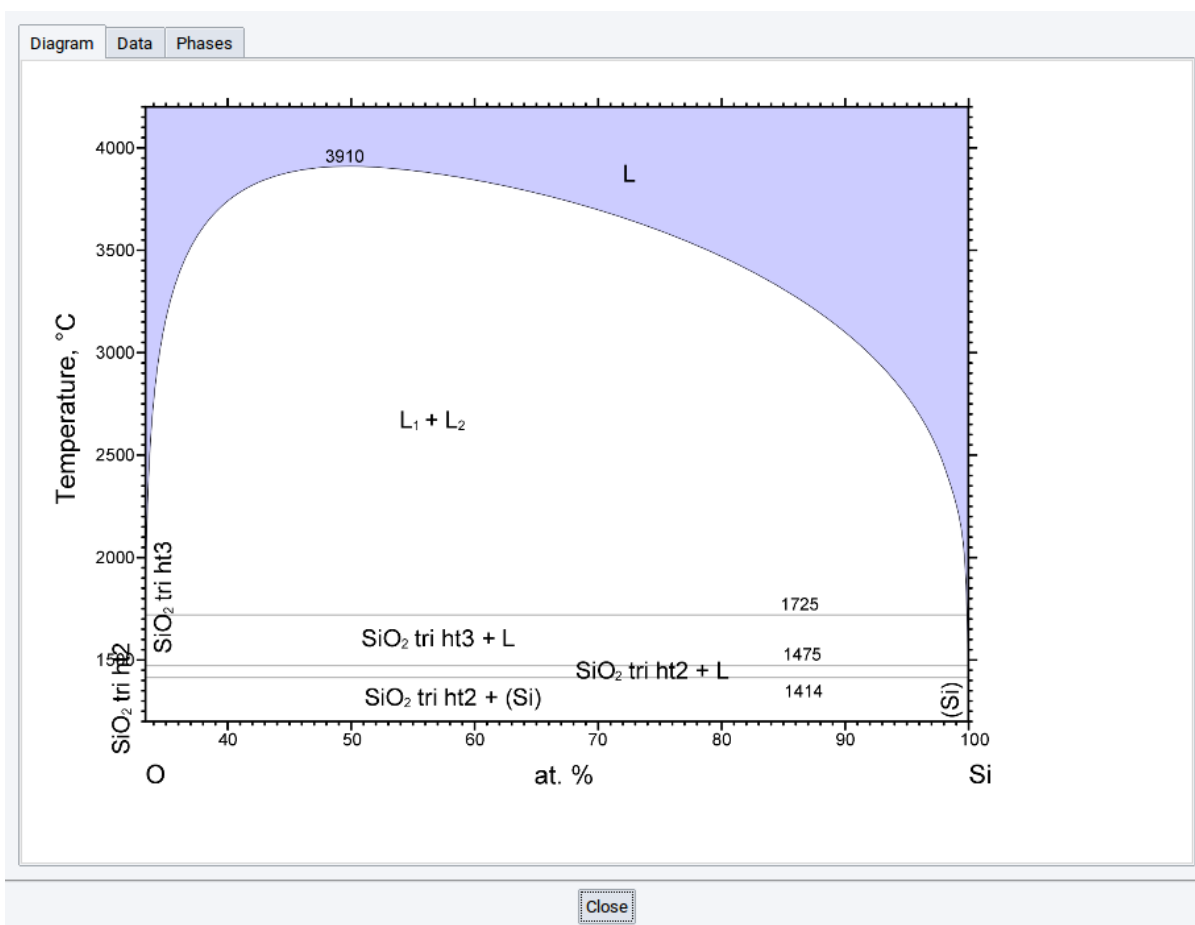
two tables on the right are filled with the structure information and an abbreviation of the phase diagram. In the above example structures and phase diagrams are selected for the binary compounds that contain Si and O. The fields that represent the binary compound are highlighted in red. The Pauling file has eight structures and 3 phase diagrams.

In the matrix gray fields indicate a combination of elements without known binary compounds or phase diagrams. The shade of green indicates the number of structures and diagrams present in the database, the darker the shade, the higher the number.



You can restrict the selection to binary compounds with known structures (**Structures only**) or diagrams (**Diagrams only**); the default shows compounds with known structures and diagrams. For example, there is only a phase diagram for Fe-Cd, but no distinct binary compound. On the other hand there are multiple entries for FeCl₂ and FeCl₃, but no complete phase diagram.

If you want to visualize a structure just click on **View Structure** and the structure is opened in the structure viewer of *MedeA*. With **Browse** you return to *InfoMaticA*'s search window to get the detailed list of binary structures that contain the two relevant elements. Use **View diagram** to display the selected phase diagram in a new window.



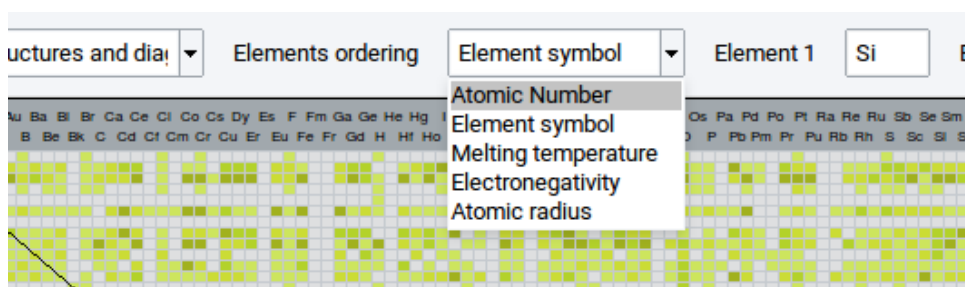
Information on the source of the diagram is found on the **Data** tab, and the list of all phases present, space group information, reaction and temperatures limits (as far as known) are found on the **Phases** tab.

Diagram Data Phases									
Formula	Modif.	Type	P. Symbol	Space-group	S.G. No.	Upper Limit (°C)	Reaction	Lower Limit (°C)	Reaction
(Si)		C	cF8	Fd-3m	227	1414	melting		
SiO2	tri ht3	SiO2	hP12	P6_3/mmc	194	1475	polymorphic		
SiO2	cri ht	SiO2	cF104	Fd-3m	227	1725	melting	1475	polymorphic

Close

In the case of Fe-Al, this lists the well-known 1:1 and 1:3 inter-metallic compounds next to the 2:3 high temperature phase and a (disordered) Fe₄Al₁₃ phase among others.

To discover relationships and similarities between different systems, you can change the order of elements, to sort them by **Atomic Number**, **Element symbol**, **Melting temperature**, **Electronegativity**, or **Atomic Radius**, respectively.



10 Configuration Options

Use the **Option** menu in *InfoMaticA*'s top menu bar to change *InfoMaticA*'s default settings:

- **Options** : Set the number of maximum hits to display in the results table
- **Properties** : Add/Remove properties to be displayed in the results table
- **Databases** : Select the databases to include in a search

11 Missing Databases

If you are missing a database in your *InfoMaticA* results, please check whether your *C:/MD/Databases* and *~/MD/Databases* directories include the following files: COD.db, ICSD.db, Pauling.db, and Person.db. If not, you can download any of them from update.materialsdesign.com/db [7]. Please use your my.materialsdesign.com [8] login to access this link. Please make sure the downloaded file has an extension name *.dbz*.

Once downloaded, please save them to *MD/Databases/* and restart MedeA. Upon restarting MedeA, the database is automatically extracted and installed. You only need these database files on the computer with the MedeA GUI installed - you do not need these databases on computers that serve as JS/TS only.

After MedeA restarted, please start the *InfoMaticA* tool: "MedeA GUI >> Tools >> InfoMaticA", then "MedeA GUI >> InfoMaticA >> Search". Then "InfoMaticA GUI >> Options >> Databases". Please make sure all available databases are on the right side titled "Current".

[7] <http://update.materialsdesign.com/db/>

[8] <http://my.materialsdesign.com/>