

MedeA InfoMaticA: Rapid Access to Comprehensive Experimental Structure Data

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1 Overview

MedeA InfoMaticA provides a graphical user interface to the experimental databases COD, ICSD, NCD, and Pearson's. Together these databases contain over 1.2 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 queries 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 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 People registered to COD can add published and unpublished structures of small molecules and small to medium-sized unit cell crystals.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 November 2022, the database has more than 495,000 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 Pearson Crystal Structure Database [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 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 [5]

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 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] http://www.materialsdesign.com/datasheet-pearson

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

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

^[3] https://www.asminternational.org/materials-resources/online-databases/pearson

^[5] https://www.materialsdesign.com/datasheet-ncd



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, and Options.
- · A configurable table for displaying search results in the upper region
- An adjustable separator
- Several panels in the lower region to formulate search phrases/criteria and to visualize structure specific results and properties

ID (completeness	space	group name H-I	M	sum		structural	
COD.220764: C	omplete	P-1		C20 H16	N4 05	C20 H16 N	14 05	(E)-1-[3-(Benzylo
COD.2207644 C	omplete	P-1		C23 H21	N5 06	C23 H21 N	15 06	(E)-1-[3-(Benzylo
COD.220764! C	omplete	P121/c1		C27 H27	N3 03	C27 H27 N	13 03	(E)-4-[4-(Benzylo
COD.220764(C	omplete	Pna21		C19 H22	Cu N4 07 S	C19 H22 C	u N4 07 S	thiophene-2,5-die
COD.220764. D	isordered	P121/c1		C22 H29	N3 05	C22 H29 N	13 05	(Z)-4-((E)-(4-buty
COD.220764{ C	omplete	P-1		C35 H32	N4 Ni O3	C35 H32 N	4 Ni O3	[2-phenyl-3,10,18
COD.220764! C	omplete	P121/n1		C17 H19	N3 04	C17 H19 N	13 04	(E)-1-(4-Methoxy
COD.220765(C	omplete	P121/n1		C14 H24	Ni 015	C14 H24 N	li 015	Tetraaquabis(3,5
COD.220765' C	omplete	P-1		C35 H41	N7 05	C35 H41 N	17 05	2,6-Bis(4-aminop
COD.2207652 C	omplete	P121/c1		C19 H22	N2 03	C19 H22 N	12 03	(E)-N'-(4-Butoxy-3
COD.220765: Complete P212121			1	C26 H36	05	C26 H36 C	05	Maleopimaric an
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COD.220765! C	omplete	P-1		C63 H63	Cu2 12 P3	C63 H63 C	Cu2 12 P3	Di-\m-iodo-1\kl:2
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Advanced	~
Empirical properties	×
	Run search Clear

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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 more than atoms of : I lower boundary for number of particular elements
- contains from to atoms of center 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 are 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 Bl₃. 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). Afterward 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)

ID	completeness	space group name	H-M	sum		
ICSD.1	Complete	P121/C1	Cr2 011 Te4			Cr2 011 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 03 P1			H2 Li1 03 P1
ICSD.8	Complete	PNMA	Ba1 S3 Te1			Ba1 S3 Te1
ICSD.9	Complete	P121/C1	H2 Cu1 K1 05 P1			H2 Cu1 K1 O5 P1
ICSD.10	Missing Atoms	PNMA	H14 025 P6 Sr3			H14 025 P6 Sr3
ICSD.11	Missing Atoms	P121/N1	H6 Ca1 N2 O9			H6 Ca1 N2 O9
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Search Cri	teria Detailed Info	ormation Coordinate	es Geometry Coordination	Pair Correlation	Powder pattern	
ICSD.1						Cr ₂ Te ₄ O ₁₁
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		o	xotetratellurium dichromate(I	1)		
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	SpGrp Num	ber:	Volum	e: 507.61		
	Pearson sym	bol: mP34	Calculated densi	ty:		
			Cell			
		a: 7.016±0.	Cell	a: 90.±0.		
		a: 7.016±0. b: 7.545±0.	Cell alph bet	ia: 90.±0. :a: 99.69±0.		
		a: 7.016±0. b: 7.545±0. c: 9.728±0.	Cell alph bei gamm	ia: 90.±0. ia: 99.69±0. ia: 90.±0.		
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Coordinates tab: Display positions of atoms, Wyckoff sites and their occupancies of structure records that have atomic coordinates

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	ID	completen	ess spac	e group na	ime H-M				sum	1			stri
IC	SD.1	Complete	P121/0	21		Cr2 011	Te4					Cr2 011 Te4	
IC	SD.2	Disordered	PNMA			Co0.93 M	/In1.07 O4	Si1				Co0.93 Mn1.07 04 Si1	
IC	SD.3	Complete	P3-C1			F3 La1						F3 La1	
IC	SD.4	Complete	P3-C1			Ce1 F3						Ce1 F3	
IC	SD.5	Complete	PNA21			H4 Na1	05 P1					H4 Na1 O5 P1	
IC	SD.6	Missing Ato	ms P121/M	/ 1S		H2 Al2 O	9 S1 Te1					H2 Al2 O9 S1 Te1	
IC	SD.7	Complete	P21NB			H2 Li1 0	3 P1					H2 Li1 03 P1	
IC	SD.8	Complete	PNMA			Ba1 S3 1	le1					Ba1 S3 Te1	
IC	SD.9	Complete	P121/0	01		H2 Cu1 I	K1 05 P1					H2 Cu1 K1 O5 P1	
IC	SD.10	Missing Ato	ms PNMA			H14 025	P6 Sr3					H14 025 P6 Sr3	
IC	SD.11	Missing Ato	ms P121/M	V1		H6 Ca1 I	N2 O9					H6 Ca1 N2 O9	-
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C	9.72800	gamma: 90.0)										
Si	te Wyck	off Position	Symmetry	Element	X	Y	Z	Occu	ipancy				F
	Te 4e		?	Те	0.13970	0.85990	0.17620	1.0					
	Te: 4e		?	Те	0.67230	0.86180	0.41580	1.0					
	Cr 4e		?	Cr	0.31920	0.50190	0.38420	1.0					
	01 4e		?	0	0.15800	0.64900	0.48660	1.0					
	02 4e		?	0	0.56300	0.64100	0.45170	1.0					
	03 4e		?	0	0.46800	0.37500	0.26230	1.0					
	04 4e		?	0	0.12700	0.31400	0.34290	1.0					
	05 4e		?	0	0.20500	0.64400	0.21210	1.0					
	06 2d		?	0	0.50000	0.00000	0.50000	1.0					
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Geometry tab: Display bond lengths and angles of structure records with atomic coordinates; define for which constituting Atom: and the corresponding Distance cutoff (A): in Å and confirm with Refresh

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	ICSD.1	Com	plete	P121/C1		Cr2 011	Te4					Cr2 011 Te4	
	ICSD.2	Diso	ordered	PNMA		Co0.93 N	/In1.07 O4 Si1					Co0.93 Mn1.07 04	Si1
	ICSD.3	Com	plete	P3-C1		F3 La1						F3 La1	
	ICSD.4	Com	plete	P3-C1		Ce1 F3						Ce1 F3	
	ICSD.5	Com	plete	PNA21		H4 Na1 (05 P1					H4 Na1 O5 P1	
	ICSD.6	Miss	sing Atoms	P121/M1	S	H2 Al2 0	9 S1 Te1					H2 Al2 O9 S1 Te1	
	ICSD.7	Com	plete	P21NB		H2 Li1 0	3 P1					H2 Li1 03 P1	
	ICSD.8	Com	plete	PNMA		Ba1 S3 T	ſe1					Ba1 S3 Te1	
	ICSD.9	Com	plete	P121/C1		H2 Cu1 k	(1 05 P1					H2 Cu1 K1 05 P1	
	ICSD.10	Miss	sing Atoms	PNMA		H14 025	P6 Sr3					H14 025 P6 Sr3	
	ICSD.11	Miss	sing Atoms	P121/N1		H6 Ca1 N	N2 09					H6 Ca1 N2 O9	
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	1	Te1-0	3 2.7	189 1									
	-	1e1-0	n 3.2 r 3.2	427 I 500 1									
	-	Te1-0	2 3.3	572 1									
	-	Te1-0	1 3.3	964 1									
	1	Te1-C	r 3.4	564 1									
		Fe1-C	r 3.48	812 1									
		[e1-0	5 3.5	368 1									
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	-	Te1-0	2 3.9	715 1									
L													-
								Atom:	All	• [Distance cutoff (A)	: 4.0	Refresh

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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



<u>F</u> ile	<u>E</u> dit	<u>O</u> pti	ons	<u>M</u> PM												
	ID		com	npleteness	space	group name H	-M			sum						stru
IC	SD.1		Com	plete	P121/C1		Cr2 O	11 Te4						Cr2 011	Te4	
IC	SD.2		Diso	rdered	PNMA		Co0.9	3 Mn1.07 O	4 Si1					Co0.93 N	/In1.07 C	04 Si1
IC	SD.3		Com	plete	P3-C1		F3 La	1						F3 La1		
IC	SD.4		Com	plete	P3-C1		Ce1 F	3						Ce1 F3		
IC	SD.5		Com	plete	PNA21		H4 Na	a1 05 P1						H4 Na1 (05 P1	
IC	SD.6		Miss	sing Atoms	P121/M1	S	H2 A	2 09 S1 Te1						H2 Al2 0	9 S1 Te	1
IC	SD.7		Com	plete	P21NB		H2 Li	I 03 P1						H2 Li1 0	3 P1	
IC	SD.8		Com	plete	PNMA		Ba1 S	3 Te1						Ba1 S3 1	îe1	
IC	SD.9		Com	plete	P121/C1		H2 Cu	1 K1 05 P1						H2 Cu1 H	(1 05 P1	1
IC	SD.10)	Miss	sing Atoms	PNMA		H14 (25 P6 Sr3						H14 025	P6 Sr3	
	SD.11		Miss	sing Atoms	P121/N1		H6 Ca	1 N2 O9						H6 Ca1 I	12 09	
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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 (A): in Å and confirm with Refresh



<u>F</u> ile <u>E</u> dit <u>O</u> p	tions <u>M</u> PM				
ID	completeness	space group name H-M	sum		stri
ICSD.1	Complete	P121/C1	Cr2 011 Te4	Cr2 011 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 05 P1	H4 Na1 O5 P1	
ICSD.6	Missing Atoms	P121/M1S	H2 Al2 09 S1 Te1	H2 Al2 O9 S1 Te1	
ICSD.7	Complete	P21NB	H2 Li1 03 P1	H2 Li1 03 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 025 P6 Sr3	H14 025 P6 Sr3	
ICSD.11	Missing Atoms	P121/N1	H6 Ca1 N2 O9	H6 Ca1 N2 O9	-



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

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ID		completeness	space	group name H-N	1		sum			stri
ICSD.	1 C	omplete	P121/C1		Cr2 011	Te4			Cr2 011 Te4	
ICSD.	2 D	isordered	PNMA		Co0.93 N	/In1.07 O4 Si1			Co0.93 Mn1.07 O4 Si1	
ICSD.	з с	omplete	P3-C1		F3 La1				F3 La1	
ICSD.4	4 C	omplete	P3-C1		Ce1 F3				Ce1 F3	
ICSD.	5 C	omplete	PNA21		H4 Na1 (05 P1			H4 Na1 O5 P1	
ICSD.	6 N	lissing Atoms	P121/M	1S	H2 Al2 0	9 S1 Te1			H2 Al2 O9 S1 Te1	
ICSD.	7 C	omplete	P21NB		H2 Li1 0	3 P1			H2 Li1 03 P1	
ICSD.	8 C	omplete	PNMA		Ba1 S3 T	Гe1			Ba1 S3 Te1	
ICSD.	9 C	omplete	P121/C1		H2 Cu1 k	K1 05 P1			H2 Cu1 K1 O5 P1	
ICSD.	10 N	lissing Atoms	PNMA		H14 025	P6 Sr3			H14 025 P6 Sr3	
ICSD.	11 N	lissing Atoms	P121/N1		H6 Ca1 N	N2 09			H6 Ca1 N2 O9	-
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Search	h Criteria	Detailed Inf	ormation	Coordinates	Geometry	Coordination	Pair Correlation	Powder pattern		
100- 80-									 lines smooth 	ed
60- 40-										



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.

	ematic	name syste	tural	n struc	sun	name H-M	e group r	ness space	ompletene	ID c
		ioxide	Silicon di	02 Si1	02 Si1		S	C12/C1S	omplete	CSD.193155 C
		xide	Silicon o	02 Si1	02 Si1		6	P3121S	omplete	CSD.79637 C
		ioxide	Silicon di	02 Si1	02 Si1		S	C12/C1S	omplete	CSD.193156 C
		xide	Silicon o	02 Si1	02 Si1			F1	omplete	CSD.1440 C
		ioxide	Silicon di	02 Si1	02 Si1		S	C12/C1S	omplete	CSD.193157 C
		xide	Silicon o	02 Si1	02 Si1			CMC21	omplete	CSD.201689 C
		ioxide	Silicon di	02 Si1	02 Si1		S	C12/C1S	omplete	CSD.193158 C
		ioxide	Silicon di	02 Si1	02 Si1		S	C12/C1S	omplete	CSD.193160 C
		ioxide	Silicon di	02 Si1	02 Si1		S	C12/C1S	omplete	CSD.193159 C
		xide - HT	Silicon o	02 Si1	02 Si1		мс	P63/MM	omplete	CSD.38126 C
-		xide	Silicon o	02 Si1	02 Si1		NM	P42/MN	omplete	CSD.68158 C
► I										
	1									
		Powder pattern	Pair Correlation	Coordination	Geometry	dinates	Coord	d Information	Detailed	earch Criteria
				SiO2	is			formula		Require that
						1	erion	-Add new criter	/	Require that
										nequire that

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).



<u>F</u> ile	<u>E</u> dit	<u>O</u> pti	ons	<u>M</u> PM		
	<u>V</u> iew					space gr
IC	<u>C</u> opy				- 1	C12/C1S
IC	Сору	IDs			- [P3121S
IC	Delet	e				C12/C1S
IC	Find	media	in str	uctures	;	F1
IC	SD.19	3157	Com	plete	_	C12/C1S
IC	SD.20	1689	Com	plete		CMC21
IC	SD.19	3158	Com	plete		C12/C1S
IC	SD.19	3160	Com	plete		C12/C1S
IC	SD.19	3159	Com	plete		C12/C1S
IC	SD.38	126	Com	plete		P63/MMC
10	0 A 0	150	Com	ploto		D42/MANIM

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



Found 175 class of structures (given symmetry and cell formula). The representative for each class displayed below have been chosen as the closest to median values of cell parameters

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 SiO₂phase.

<u>0</u>K

😣 🖨 📵				Mede	A Infol	MaticA	: Search				
<u>F</u> ile <u>E</u> dit <u>O</u> ption	ns <u>M</u> PM										
ID	completeness	space g	proup name H-	Ms	um	stru	uctural		name systematic	Structure	Sort Ascending
ICSD.68159	Complete	P42/MN	N	02 Si1		02 Si1	l Sili	con	oxide	183	Sort Descending
ICSD.75484	Complete	P41212		02 Si1		02 Si1	l Sili	con	oxide	175	Format
Pauling.204068	Complete	P3121		02Si		SiO2				129	Conv full column
COD.1538064	Complete	P3221		02 Si		02 Si	Si)2		77	Copy rul column
Pauling.541954	Complete	C12/c1		O2Si		Si02				74	Copy column selected conte
ICSD.89289	Complete	P6222		02 Si1		02 Si1	I Sili	con	oxide - beta, HT	38	Delete
Pearson.16423	Complete	Pnnm		02Si		SiO2				19	Insert
ICSD.40903	Complete	P63/MM	C	02 Si1		02 Si1	l Sili	con	oxide - HT, Gibbs model	18	moert
Pearson.16013	Complete	Cc		02Si		SiO2				18	
ICSD.180904	Complete	P121/C1		02 Si1		02 Si1	I Sili	con	dioxide - cristobalite-II	16	
COD.9006304	Complete	P1		02 Si		SiO2				14	•
				-					-		
Search Criteria	Detailed Infor	mation C	coordinates	Geometry	Coordi	nation	Pair Correlati	on	Powder pattern		
Require tha	t fo	ormula		is	5	SiO2					
Require tha	tAdd ne	ew criterion	-								
								_			
				F	Run sear	rch C	lear				
Displaying 175 of	f 175 hits										
sisplaying 1700											

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).

<u>File Edit Option</u>	ns <u>M</u> PM										
ID	completeness	space group	name H-M	sum	struc	tural		name systematic	Structures in clas	ss	
ICSD.68159	Complete	P42/MNM	View	00.011	00.01	_	Silicon	oxide	183		
ICSD.75484	Complete	P41212	view				Silicon	oxide	175		
Pauling.204068	Complete	P3121	CODV						129		
COD.1538064	Complete	P3221	Copy IDs				Si 02		77		
Pauling.541954	Complete	C12/c1	Delete						74		
ICSD.89289	Complete	P6222	Append all t	to new stucture	liet		Silicon	oxide - beta, HT	38		
Pearson.16423	Complete	Pnnm	Append all t	to new stucture	uro liet				19		
ICSD.40903	Complete	P63/MMC	Append and	o existing stud	ure list		Silicon	oxide - HT, Gibbs model	18		
Pearson.16013	Complete	Cc	Append sei	ection to new s	lucture list	line a			18		
ICSD.180904	Complete	P121/C1	Append sei	ection to existin	g stucture	list	Silicon	dioxide - cristobalite-II	16		
COD.9006304	Complete	P1	Heat Capac	ity Debye Tem	noraturo				14	·	
			Ticut oupue	ity, Debye rem							
Require that	t fo	rmula w criterion		is	SiO2						
				Run sea	rchCle	ar					

Alternatively, you can use the menu items Copy and Copy ID 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 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

10 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, and Person.db. If not, you can download any of them from update.materialsdesign.com/db [6]. Please use your my.materialsdesign.com [7] 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:

- 1. In the MedeA GUI click on Tools >> InfoMaticA , followed by InfoMaticA >> Search
- 2. In *InfoMaticA* Options >> Databases
- 3. Make sure all available databases are tagged with a green mark:

[7] http://my.materialsdesign.com/

^[6] http://update.materialsdesign.com/db/



Databases	^
VCD_Organic	
✓ Pearson	
√MD	
√ NCD_Inorganic	
√ COD	
	-
OK Cancel	