

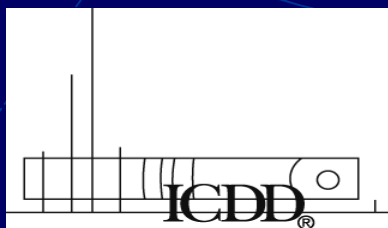
*Release by the International
Centre for Diffraction Data (ICDD)
of New Powder Data Mining Tools:
the PDF-4/Full File and
PDF-4/Organics Databases*

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Newtown Square, PA, USA.

* Curtin University of Technology, Perth

Oak Ridge National Laboratory, Tennessee



Topics to be Covered in Talk

- ICDD organisation
- The Powder Diffraction File
- The 'new' PDF-4 databases
- Materials identification with the PDF
- Database structure, and use in data mining
- Data mining examples
- PDF-4 demonstration

What is the ICDD?

The ICDD comprises a volunteer scientific membership of 350 diffractionists from 41 countries, plus a headquarters staff of 38.

Dedicated to -

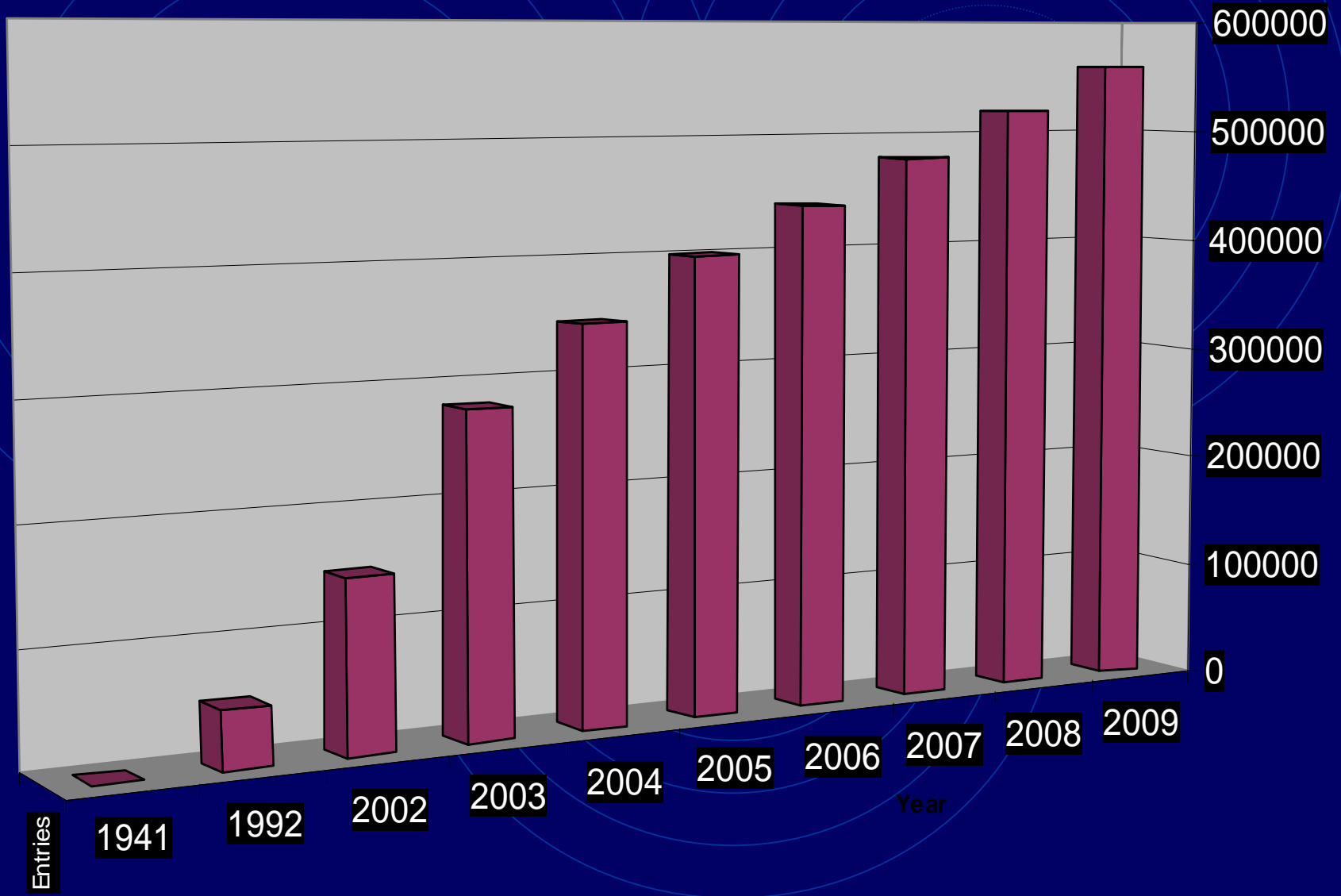
- On-going development of the PDF, including its Grant-in-Aid program
- Advancement of x-ray instrumental science
- X-ray analytical science education – workshops, Denver X-ray Conference, etc
- International networking – conference and workshop support, etc
- Supporting PhD students through its scholarship program

The PDF Data Base in 2003

- PDF is designed to identify crystalline material.
- Currently contains 279,854 unique data sets characterised by x-ray diffraction
- Physical properties, experimental preparation and literature citations included.

For the next several years ~ 30,000 materials will be added to the PDF per year.

Growth of the PDF



Searchable PDF Descriptors

In addition to 280,000 data sets, you will find:

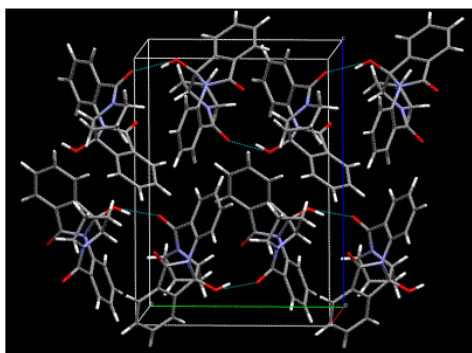
- 200,000 densities
- 100,000 colour classifications
- 50,000 melting points
- 173,000 distinct empirical formulae
- Over 500,000 reference citations
- 1,602 different searchable journal codens

Database Partners with the ICDD

92,011 entries – ICDD Sources

Cambridge Crystallographic Data Centre

- a Registered Charity



56,614 entries - PDF-4/Full File



122,816 entries - PDF-4/Organics

**National Institute of
Standards and Technology**

...working with industry to develop and apply technology, measurements and standards

NIST

8,423 entries - PDF-4/Full File

ICDD-MPDS Collaboration on Inorganic Materials – *New!*

- Inorganic structures and properties abstracted by the Materials Phases Data System and MPDS-JST (Japan Science & Technology Corporation)
- Access to future abstracts from Linus Pauling File project by MPDS
- S-entry structural data, including atomic coordinates added to the PDF
- Data sets are added to the database after carrying out the duplicate review to exclude overlap with all other sources.
- PDF entries will be updated with synthesis and reference citations
- ~ 100,000 atomic coordinate sets to be added in 2005

PDF-4 Master Database

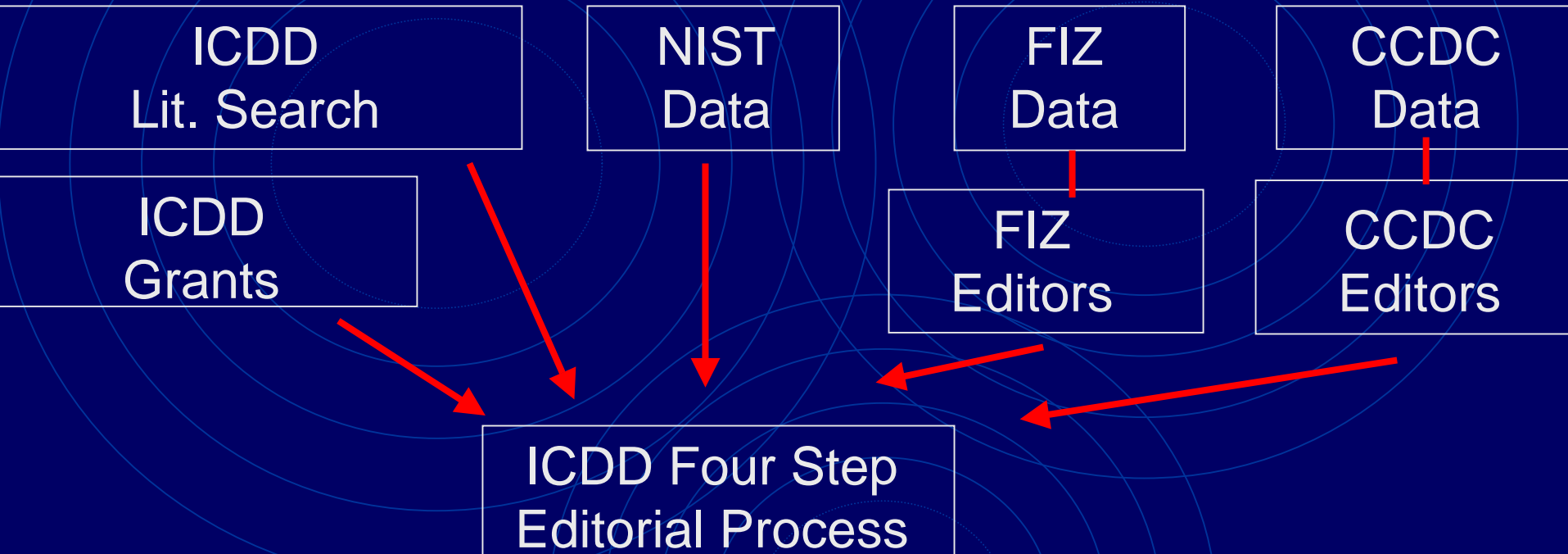
280,000 entries released in three PDF-4 products

PDF-4/Full File
157,048 entries

PDF-4/Minerals
17,535 entries

PDF-4/Organics
147,201 entries

ISO-9001 PDF Review Processes



All data put in a common format, statistically analyzed, and classified in numerous ways

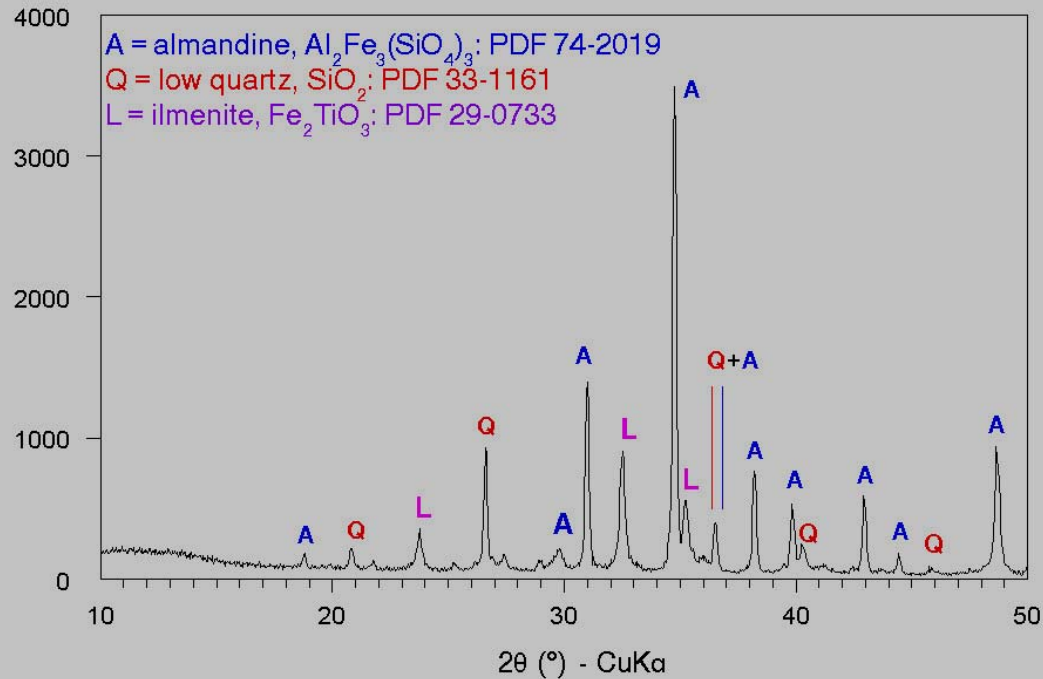
XRD Identification with the PDF

Example

Red coloured material covering beach at the mouth of the Chapman River, Geraldton, Western Australia.

Residents expressed concern that the material might be polluting residue from mineral sands Industry.

Powder data analysed with the MDI search/match identification program and the PDF-4 database



Result:

- The pattern is dominated by the phases almandine, quartz and ilmenite. Almandine and ilmenite are present as minor phases in 'normal' beach sand.
- Erosion of the beach by water outflow from the river, plus wave action, has preferentially removed the less-dense quartz. There is no evidence of mineral processing residues.
- The garnet almandine accounts for the red coloration.

PDF-4 Format

The PDF-4 format is a new relational database container for the PDF

- The data are arranged in a series of database tables.
- The format allows searchable access to all physical property data fields.
- The PDF-4 offers 30+ separate searchable diffraction and physical property fields.
- Integrated display, search and indexing software is standard with the PDF-4 format. (Contact your software distributor for automatic search/match software.)

PDF # Cu Kα(Ave) 1.54184A variable slit intensities linear intensity Print Card Print Graph Help

2θ d (Å) Int-v h k l

9.64	9.176	12	1	0	0
16.73	5.300	7	1	1	0
17.92	4.950	10	1	0	1
19.35	4.587	57	2	0	0
22.58	3.938	4	1	1	1
24.59	3.621	8	2	0	1
25.67	3.470	3	2	1	0
29.20	3.058	16	3	0	0
29.89	2.989	45	2	1	1
31.95	2.801	4	1	0	2
33.02	2.713	30	3	0	1
33.84	2.649	83	2	2	0
35.25	2.546	20	1	1	0
36.27	2.477	100	2	0	2
37.23	2.415	9	2	2	1
38.52	2.337	31	3	1	1
39.26	2.295	9	4	0	0
40.19	2.244	27	2	1	2
42.25	2.139	14	4	0	1
42.63	2.121	13	3	0	2
42.95	2.106	25	3	2	0
45.23	2.005	3	4	1	0
45.76	1.983	11	3	2	1

Calcium Manganese Oxide Borate Carbonate Hydroxide

Variable Slit Intensity

PDF Exper. Physical Crystal Data Optical Misc. Cmts. User's

Card 47-1836 Status Published Quality S

Formula Ca₄Mn_{2.74}(B₂O₃)₃(CO₃)(OH)₃

Name Calcium Manganese Oxide Borate Carbonate Hydroxide

Mineral Name Gaudefroyite

Also Called

Experimental Pattern Calculated Pattern

Still have "card" option

PDF Card

New format – data rearranged in tabular sections with point and click interfaces

46-1045 ★

SiO ₂	dÅ	Int	hkl	dÅ	Int	hkl
Silicon Oxide	4.2550	16	100	1.1530	<1	311
	3.3435	100	101	1.1407	<1	204
	2.4569	9	110	1.1145	<1	303
	2.2815	8	102	1.0816	2	312
	2.0361	4	111	1.0638	<1	400
	2.1277	4	200	1.0477	1	105
	1.9799	4	201	1.0438	<1	401
	1.8180	13	112	1.0346	1	214
	1.8017	<1	003	1.0149	1	223
	1.6717	4	202	0.9896	<1	115
	1.6592	2	103	0.9872	<1	313
	1.6083	<1	210	0.9783	<1	304
	1.5415	9	211	0.9762	<1	320
	1.4529	2	113	0.9608	<1	321
	1.4184	<1	300	0.9285	<1	410
	1.3821	6	212	0.9182	<1	322
	1.3750	7	203	0.9161	2	403
	1.3719	5	301	0.9152	2	411
	1.2879	2	104	0.9089	<1	224
	1.2559	3	302	0.9009	<1	006
	1.2283	1	220	0.8972	<1	215
	1.1998	2	213	0.8889	1	314
	1.1978	<1	221	0.8814	<1	106
	1.1840	2	114	0.8782	<1	412
	1.1802	2	310	0.8598	<1	305

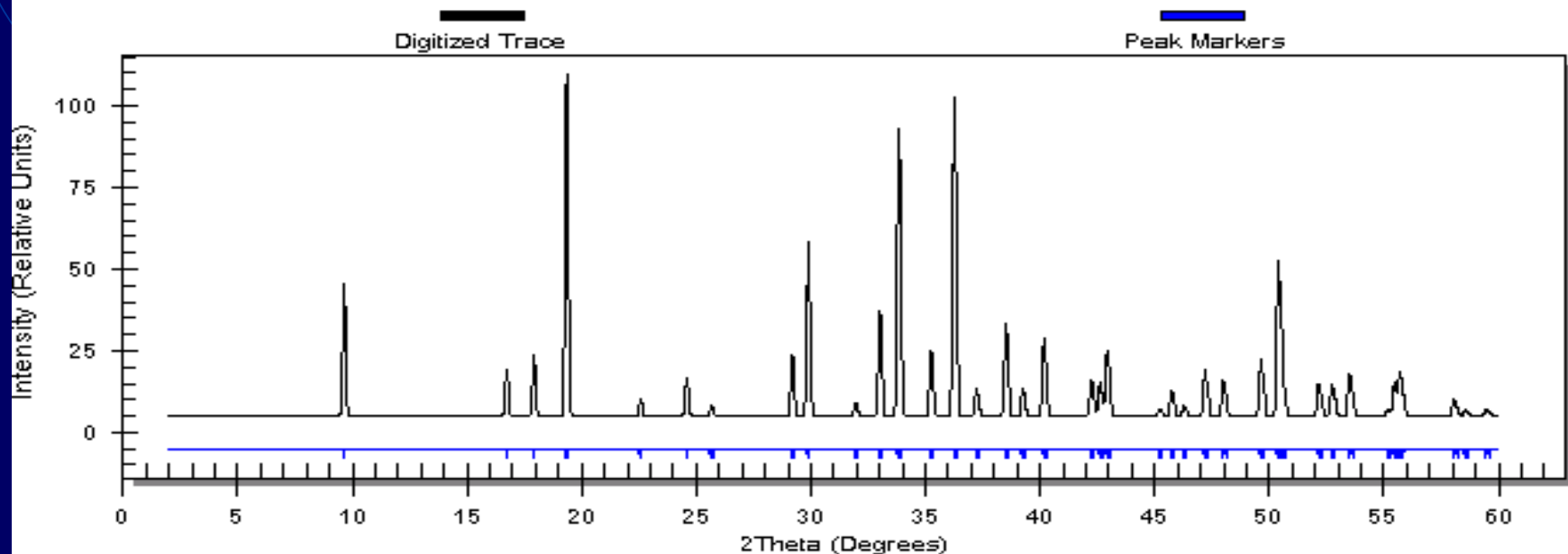
See following card.

On-the-Fly Pattern Calculation

- Generate both “stick patterns” and digital patterns
- Digital patterns can be user modified to simulate the users instrumental conditions
- Sophisticated data mining ability (upcoming slides)
- Visualization software included and integrated

Approximate Digitized Diffraction Pattern

PDF# 47-1836, Calcium Manganese Oxide Borate Carbonate Hydroxide, $\text{Ca}_4\text{Mn}_{2.74}(\text{B O}_3)_3(\text{C O}_3)(\text{O}, \text{OH})_3$



PDF-4 Master Database

272,000 entries released in three PDF-4 products

PDF-4/Full File
157,048 entries

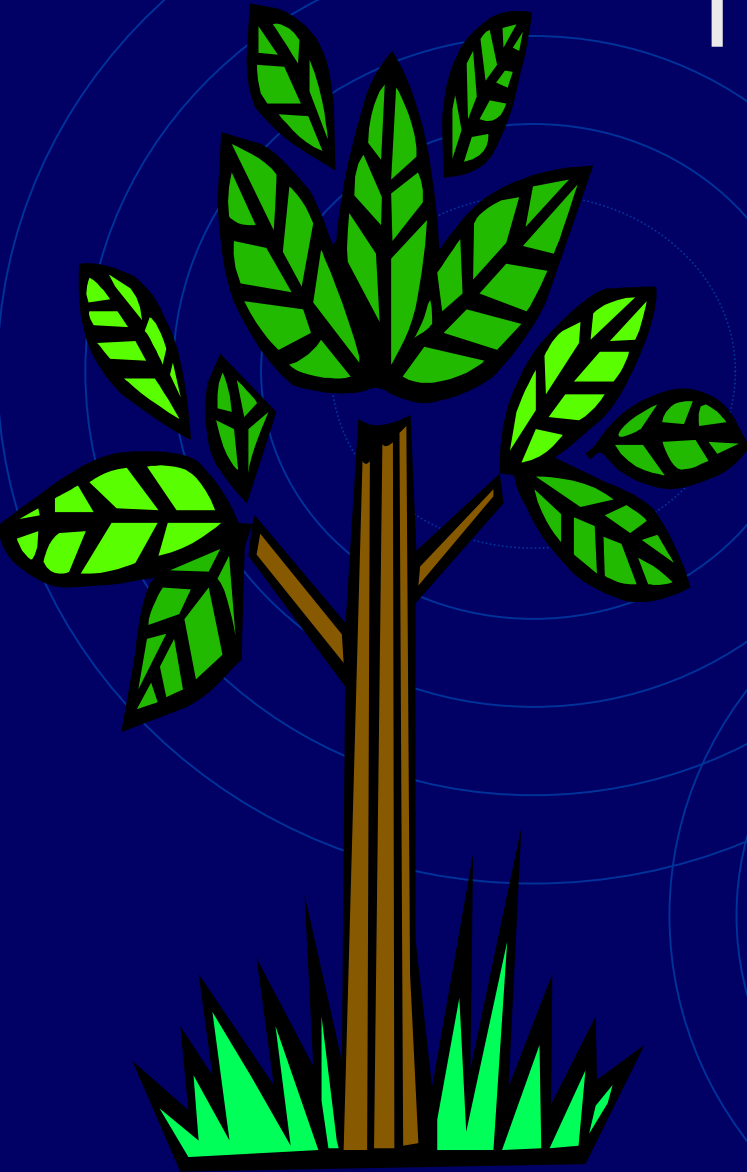


PDF-4/Organics
147,201 entries



PDF-4/Minerals
17,535 entries

The PDF Tree



Trunk = PDF Entry Number

Branches = 30+ Searchable Property Fields

Twigs = Classification Systems of the Property Fields

Leaves = Individual Material Property Values

Branches & Twigs

Searchable Property Fields



14 Colors
26 Subfiles
458 Mineral Classifications
230 Space Groups
206 Organic Functional Groups
1620 Journals Codes
> 500,000 Reference Citations

*Continuous ranges of melting points,
densities, I/lc , unit cell parameters, temperature
and pressure*

Leaves

Types of Searches

- Type of Element
- Number of Elements
- Empirical Formula
- Common Name
- Compound Name
- Mineral Name
- Mineral Classification
- d-Spacing
- PDF Quality Mark
- Reference Intensity Ratio, I/I_c
- PDF-4 Sub-files
- Space Group
- Pearson Symbol Code
- Prototype Structure
- Reduced Cell Parameters
- Temperature and Pressure
- Density
- Melting Point
- Color
- Author Name
- Journal

Additional Searches for PDF-4 Organics

- Organic Functional Group (206)
- Pharmaceutical
- Drug Activity
- Polymers
- Pigments
- Forensics

The Main Branches

PDF-4/Full File 2002 Version 2.01

File PDF Card Subfiles/Database Filters Elements Names References Structures Misc. Searches Global Searches Global Operators Tools PCSIWIN Window Help

PDF-4/Full File 2002 Version 2.01

File PDF Card Subfiles/Database Filters Elements Names References Structures Misc. Searches Global Searches Global Operators Tools PCSIWIN Window Help

Get PDF Numbers

Enter PDF Set Number, Card Number

31-1234 -

CAS Number:
Molecular We
Volume[CD]:
Dx: 2.649

View Cards In Set
 No Yes

Search Print Preview Clear Help

PDF #	QM	Chemical Formula	Compound Name	D1	D2	D3	SYS
01-0001	B	C10 H7 Bi O2	β -Naphthylbismuth dioxi	20.000	9.900	2.670	X
01-0002	B	C9 H8 N Na O3	Sodium hippurate	19.000	4.200	10.800	X
01-0003	B	C10 H8 N Na O3 S *4 H	Sodium- α -naphthylamine	18.500	5.500	3.850	X
01-0004	B	C12 H9 Ba O7 S2	Barium phenolsulfonate	18.000	11.500	4.250	X
01-0005	B	C6 H5 K O	Potassium phenoxide	17.000	4.290	5.300	X
01-0006	O	C21 H15 Bi2 O9	Bismuth salicylate	16.000	6.200	3.980	X
01-0007	B	C14 H10 Cd O6 * H2 O	Cadmium salicylate hydr	16.000	3.820	6.600	X
01-0008	B	C12 H10 Ca3 O14 *4 H2	Calcium citrate hydrate	15.300	3.950	3.090	X
01-0009	B	C12 H10 Ba3 O14 *7 H2	Barium citrate heptahydr	15.100	9.000	3.320	X
01-0010	B	C6 H6 K O3 S	Potassium benzenesulfic	15.000	5.100	3.910	X
01-0011	B	C14 H10 Hg O4	Mercury benzoate	15.000	3.720	4.300	X

Record: 1 of 136895

Set Number NUM

More Branches

PDF-4/Full File 2002 Version 2.01

File PDF Card Subfiles/Database Filters Elements Names References Structures Misc. Searches Global Searches Global Operators Tools PC^SIWIN Window Help

Ambient/Nonambient Search
Quality Mark Search
Subfile Search

PDF-4/Full File 2002 Version 2.01

File PDF Card Subfiles/Database Filters Elements Names References Structures Misc. Searches Global Searches Global Operators Tools PC^SIWIN Window Help

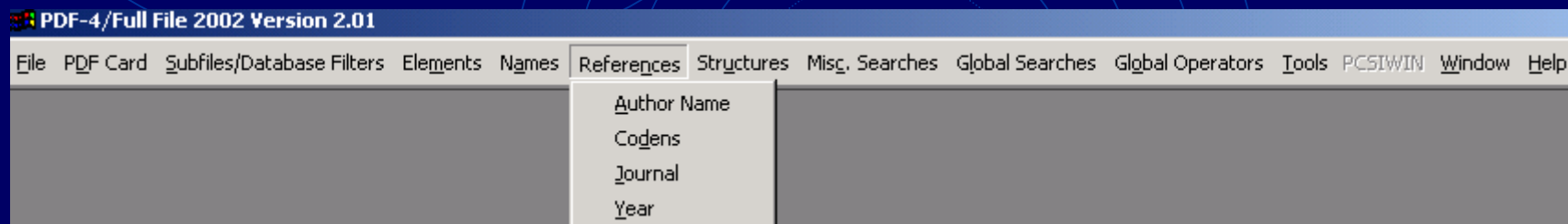
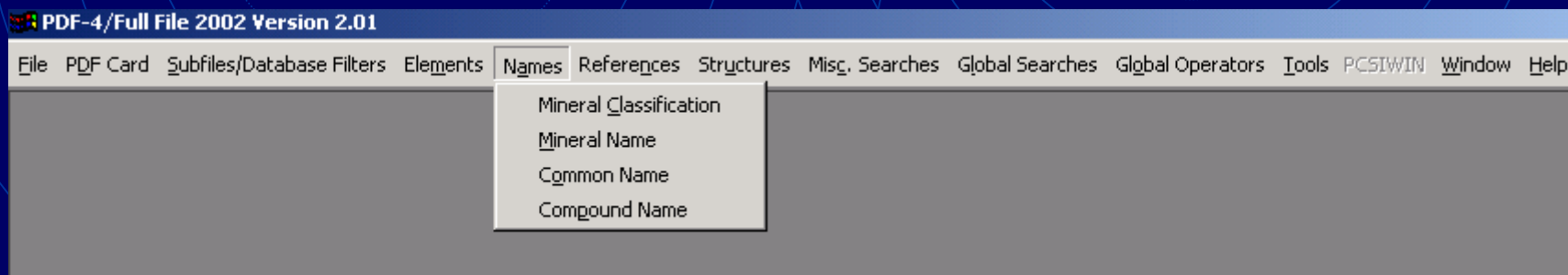
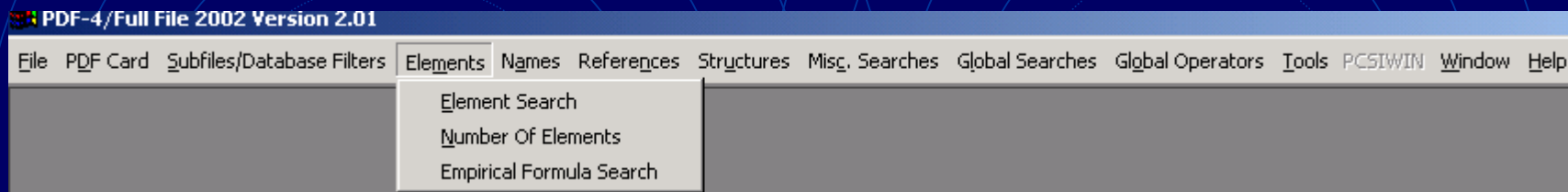
Lines
Colors
Density(Measured&Calculated)
I/IC Search
Melting Points
Organic Functional Group

PDF-4/Full File 2002 Version 2.01

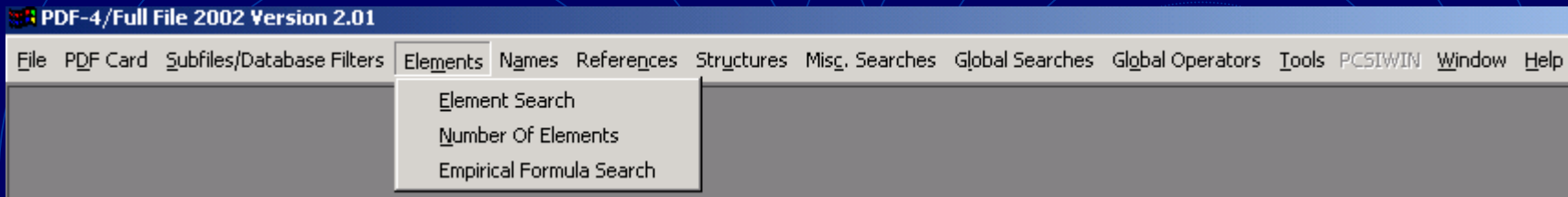
File PDF Card Subfiles/Database Filters Elements Names References Structures Misc. Searches Global Searches Global Operators Tools PC^SIWIN Window Help

Pearson Symbol Code
Prototype Structure
Reduced Cell
Space Groups
Int'l Table SPG Search
Author-Defined SPG Search

And Even More Branches



Example: Mining the Database Start with an Element Search



Point and Click for Elements

Period 1: H (1.008), He (4.003)

Period 2: Li (6.941), Be (9.012), B (10.811), C (12.011), N (14.007), O (15.999), F (18.998), Ne (20.180)

Period 3: Na (22.990), Mg (24.305), Al (26.982), Si (28.086), P (30.974), S (32.064), Cl (35.453), Ar (39.948)

Period 4: K (39.098), Ca (40.08), Sc (44.956), Ti (47.88), V (50.942), Cr (51.996), Mn (54.938), Fe (55.847), Co (58.933), Ni (58.69), Cu (63.546), Zn (65.38), Ga (69.72), Ge (72.61), As (74.922), Se (78.96), Br (79.904), Kr (83.80)

Period 5: Rb (85.47), Sr (87.62), Y (88.906), Zr (91.22), Nb (92.906), Mo (95.94), Tc (98), Ru (101.07), Rh (102.91), Pd (106.4), Ag (107.87), Cd (112.41), In (114.82), Sn (118.69), Sb (121.75), Te (127.60), I (126.90), Xe (131.29)

Period 6: Cs (132.91), Ba (137.33), Hf (178.49), Ta (180.95), W (183.85), Re (186.21), Os (190.2), Ir (192.22), Pt (195.08), Au (196.97), Hg (200.59), Tl (204.38), Pb (207.19), Bi (208.98), Po (209), At (210), Rn (222)

Period 7: Fr (223), Ra (226.03)

Ln: Ln

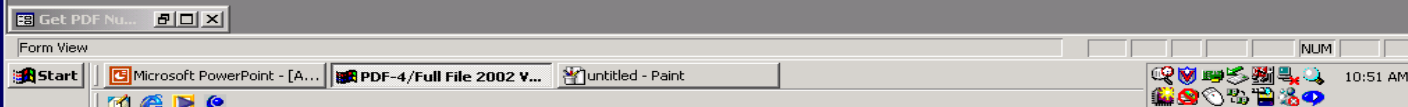
AC: La (138.91), Ce (140.12), Pr (140.91), Nd (144.24), Pm (145), Sm (150.36), Eu (151.97), Gd (157.25), Tb (158.93), Dy (162.5), Ho (164.93), Er (167.26), Tm (168.93), Yb (173.04), Lu (174.97)

87 Ac (227.03), 89 Th (232.04), 90 Pa (231.04), 91 U (238.03), 92 Np (237.05), 93 Pu (244), 94 Am (243), 95 Cm (247), 96 Bk (247), 97 Cf (251), 98 Es (252), 99 Fm (257), 100 Md (258), 101 No (259), 102 Lr (260)

And Not Or Only Just

Search Save Clear Help Legend

Operators – And/Or/Not/Only/Just



Mining the Database for Aluminium

Search Just Aluminium

7 Aluminium Entries

PDF-4/Full File 2002 Version 2.01

File PDF Card Subfiles/Database Filters Elements Names References Structures Misc_ Searches Global Searches Global

Periodic Table Search

Periodic Table Search Results

PDF #	QM	Chemical Formula	Compound Name	D1	D2	D3	SYS
01-1176	B	Al	Aluminum	2.34	1.22	2.02	C
01-1179	B	Al	Aluminum	2.33	2.03	1.21	C
01-1180	B	Al	Aluminum	2.33	2.02	1.43	C
02-1109	B	Al	Aluminum				
03-0932	O	Al	Aluminum				
04-0787	S	Al	Aluminum				
85-1327	C	Al	Aluminum				

Global Search Results

PDF Card Chemistry Unit Cell Lines Misc.

PDF #	QM	Chemical Formula	Compound Name	D1	D2	D3	SYS
03-0932	O	Al	Aluminum	2.320	2.030	1.430	C
02-1109	B	Al	Aluminum	2.330	1.220	2.020	C
01-1180	B	Al	Aluminum	2.330	2.020	1.430	C
01-1179	B	Al	Aluminum	2.330	2.030	1.210	C
85-1327	C	Al	Aluminum	2.338	2.025	1.432	C
04-0787	S	Al	Aluminum	2.338	2.024	1.221	C
01-1176	B	Al	Aluminum	2.340	1.220	2.020	C

Al
Aluminum
Record: 1 of 7

Al
Aluminum
Record: 6 of 7

Form View

Start Microsoft PowerPoint - [A...] PDF-4/Full File 2002 V... untitled - Paint 10:58 AM

Mining the Database for Aluminium

PDF-4/Full File 2002 Version 2.01

File PDF Card Subfiles/Database Filters Elements Names References Structures Misc. Searches Global Searches Global Operators Tools PCSIWIN Window Help

PDF #04-0787

PDF # Cu K α (Ave) 1.54184A variable slit intensities: linear intensity Print Card Print Graph Help

2 θ	d (Å)	Int-v	h	k	l
38.51	2.338	100	1	1	1
44.78	2.024	55	2	0	0
65.19	1.431	36	2	2	0
78.30	1.221	46	3	1	1
82.52	1.169	14	2	2	2
99.24	1.012	5	4	0	0
112.18	0.928	21	3	3	1
116.72	0.905	21	4	2	0
137.70	0.826	23	4	2	2

Aluminum

Variable Slit Intensity

PDF Exper. Physical Crystal Data Optical Misc. Cmts. User's

Author's Reported Data:

Rad CuK α 1 I 1.54056 Filter Ni d-sp

Cut off Int. Diffractometer I/cor. 3.62

Ref: Swanson, Tatge. Natl. Bur. Stand. (U.S.), Circ. 539 I, 11 (1953)

Camera Diameter

Experimental Pattern Calculated Pattern PDF-3 Pattern Display 2D Structure

Diffraction Pattern

Aluminum, Al

Peak Markers

Intensity (Relative Unit)

2Theta (Degrees)

NUM

11:04 AM

Select Best Phase –
Based on Quality Mark

Generated digital XRD Pattern

Mining the Database for Aluminium

PDF-4/Full File 2002 Version 2.01

File PDF Card Subfiles/Database Filters Elements Names References Structures Misc. Searches Global Searches Global Operators Tools PC5IWIN Window Help

PDF #02-0004

PDF #	Cu K α (Ave) 1.54184Å	variable slit intensit	2 θ	d (Å)	Int-v	h	k	l	Int
5.67	15.60	10							
19.51	4.550	34							
28.70	3.110	10							
29.99	2.980	11							
34.22	2.620	47							
35.05	2.560	48							
53.26	1.720	36							
54.98	1.670	37							
60.95	1.520	100							
71.47	1.320	47							
72.74	1.300	47							
74.75	1.270	48							
76.16	1.250	49							

Full Trace Settings

Radiation Profile Range

Anode: Cu Components: 66.7% 1.54056, 33.3% 1.54439

Type: K-alpha-1+2

Beta fraction: 0.00

Wavelength: 1.54184

Average wavelength: 1.54184

PDF# 02-0004

File Settings Help

2.722, 38.863

Approximate Digitized Diffraction Pattern

PDF# 02-0004, Iron Aluminum Silicate Hydrate, (Fe, Al) Si₂O₅(OH) · H₂O

Digitized Trace Peak Markers

Intensity (Relative Units)

2Theta (Degrees)

Ready...

Get PDF Nu...

Form View NUM

Start Microsoft PowerPoint - [A... PDF-4/Full File 2002 V... untitled - Paint

11:12 AM

Change the XRD Pattern

Range
Wavelength
Peak Profile

PDF-4/Organic Functional Group Search

206 Functional Group Classifications

Fused Rings

PDF-4/Full File 2002 Version 2.01

File PDF Card Subfiles/Database Filters Elements Names References Structures Misc. Searches Global Searches Global Operators Tools PC\$WIN Window Help

Organic Functional Group Search

Local Operators
 Not (And Or)

Search Save Print Preview Clear Help

Example

PDF #	QM	Chemical Formula	Compound Name	D1	D2	D3	SYS
08-0641	B	C19 H23 N3 O2 • C4 H4 N-(α -(Hydroxymethyl)ethyl		9.96	4.69	11.60	X
08-0676	I	C15 H24 N2 O2 • 2 H2 C-d-Hydroxylupanine dihydro		6.03	5.48	6.42	O
08-0699	B	C13 H14 N2 O4 S2	Gliotoxin	6.92	9.63	9.04	M
08-0702	I	C30 H46 O2	Ergosterol acetate	5.49	4.53	6.06	M
08-0743	B	C24 H40 O5	Cholic acid	7.59	6.90	5.96	X
08-0759	B	C24 H40 O4	Deoxycholic acid	6.34	4.88	4.03	X
08-0764	I	C15 H24 N2 O	dl-Lupanine	5.81	6.79	5.13	M
08-0765	I	C15 H20 N2 O	l-Thermopsine	4.03	6.19	4.98	T
08-0792	B	C24 H40 O3	Lithocholic acid	5.94	5.50	5.03	X
09-0571	B	C10 H6 Cl8	γ -Chlordane	6.80	4.03	6.50	X
09-0653	B	C29 H44 O12	Strophanthin-G	6.57	8.93	4.84	X

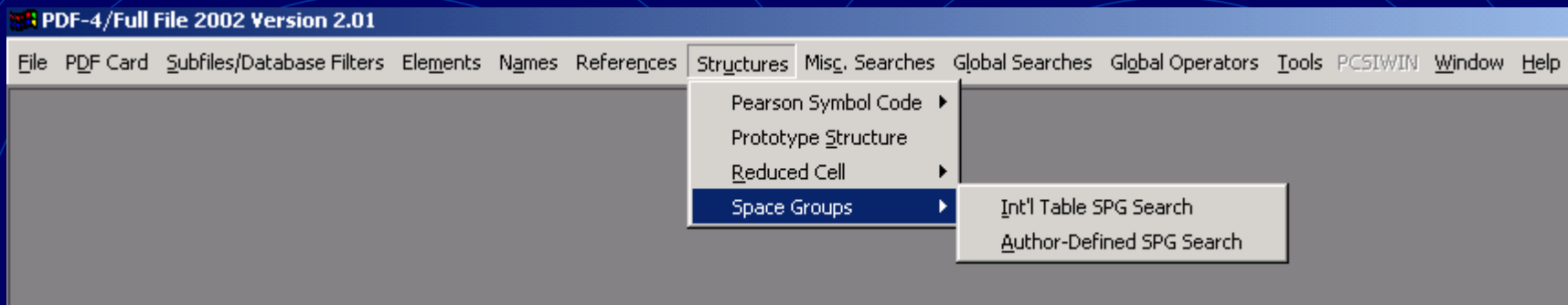
Record: 1 of 1055

Perform Search Now

Start Microsoft PowerPoint - [A...] Untitled - Paint PDF-4/Full File 2002 v... 11:30 AM

1055 entries for fused rings

Space Group Search – P2₁2₁2₁ (19)



PDF-4/Full File
841 Inorganics

PDF-4/Organics
13,271 Organics

PDF-4/Full File 2002 Version 2.01

File PDF Card Subfiles/Database Filters Elements Names References Structures Misc. Searches Global Searches Global Operators Tools PCSTWIN Window Help

Global Search Results

Display Print Preview Help

PDF Card Chemistry Unit Cell Lines Misc.

PDF #	QM	Chemical Formula	Compound Name	D1	D2	D3	SYS
25-0644	I	C ₄ H ₅ KO ₆	Potassium Hydrogen Tartrate	3.658	3.808	2.879	O
25-0889	I	Na ₂ (Zr(SO ₄) ₃)·xH ₂ O	Sodium Zirconium Sulfate Hydrate	6.330	5.090	3.700	O
25-1067	C	K ₂ ZnBr ₃ ·2H ₂ O	Potassium Zinc Bromide Hydrate	3.184	3.411	2.882	O
25-1068	C	K ₂ ZnI ₃ ·2H ₂ O	Potassium Zinc Iodide Hydrate	3.584	3.331	3.368	O
25-1205	C	K ₂ ZnI ₃ ·2H ₂ O	Potassium Zinc Iodide Hydrate	5.764	6.287	3.584	O
25-1265	B	Tl ₂ U(C ₂ O ₄) ₂ ·O ₂ ·2H ₂ O	Thallium Uranium Oxalate Oxide	3.350	2.137	3.880	O
25-1323	I	Na ₂ Ba(P ₂ O ₇) ₂	Sodium Barium Phosphate	3.950	3.820	4.750	O
25-1423	B	Pb ₃ Cu ₂ S ₂ Bi ₆ Sb ₂ S ₂ O	Copper Lead Antimony Bismuth	2.027	3.438	3.484	O
26-0006	B	β-Al ₂ B ₃ H ₁₂	Aluminum Boron Hydride	3.480	5.020	4.470	O
26-0052	I	(NH ₄ BeF ₃) ₂	Ammonium Beryllium Fluoride	6.400	3.210	5.260	O
26-0192	S	C ₄ H ₄ BaO ₆ ·0.5H ₂ O	Barium Tartrate Hydrate	6.360	5.350	3.513	O
26-0240	S	C ₄ H ₆ CdO ₄ ·2H ₂ O	Cadmium Acetate Hydrate	7.020	4.050	6.890	O
26-0285	I	Cd(P ₂ O ₇) ₂	Cadmium Phosphate	4.290	3.710	5.610	O
Cd (P ₂ O ₇) ₂							
Cadmium Phosphate							
Record: 107 of 841							

Structure

Form View

PDF-4/Organics 2003 Version 2.50

File PDF Card Subfiles/Database Filters Elements Names References Structures Misc. Searches Global Searches Global Operators Tools Window Help

Int'l Table SPG Search

Int'l SG Number: 19

Local Operator Not

Search Save Print Preview Clear Help

Chemistry Unit Cell

PDF #	SPGR	QM	Chemical Formula	Prototype Structure
02-063-7430	P212121	C	C ₁₅ H ₂₈ N ₂ O	Br
02-063-7433	P212121	C	C ₂₆ H ₃₇ BrN ₂ O ₅ S	S
02-063-7436	P212121	C	C ₄ H ₉ O ₂ P	P
02-063-7439	P212121	C	C ₁₂ H ₂₄ K ₂ O ₅ S ₂ C ₂ N ₂ S	S
02-063-7444	P212121	C	C ₂₁ H ₂₆ N ₂ O ₄ C ₂ H ₄ O	O
02-063-7458	P212121	C	C ₁₄ H ₁₁ N ₃ O ₂ S	S
02-063-7488	P212121	C	C ₂₄ H ₂₀ P ₂ Cl ₁₁ Br ₄ O ₁₁	O
02-063-7522	P212121	C	C ₁₆ H ₁₂ Fe ₂ O ₈ Pr	Pr
02-063-7527	P212121	C	C ₁₇ H ₁₄ N ₄ S ₂	S
02-063-7554	P212121	C	C ₁₃ H ₂₇ N ₄ O ₂ Pr ₂ N ₂ O ₃	O
02-063-7570	P212121	C	C ₁₆ H ₁₈ N ₂	N

Record: 1 of 13271

Form View

PDF-4 Organics – File Search

PDF-4/Organics 2003 Version 2.50

File PDF Card Subfiles/Database Filters Elements Names References Structures Misc. Searches Global Searches Global Operators Tools Window Help

PDF #	Cu K α (Ave) 1.54184A	variable slit intensities	linear intensity	Print Card	Print Graph	Help
5.13	17.23	38	0	1	1	
7.12	12.42	2	0	0	2	
7.39	11.96	1	0	2	0	
8.02	11.02	2	0	1	2	
8.20	10.78	3	0	2	1	
10.27	8.616	4	0	2	2	
11.31	7.825	16	0	1	3	

5,6,9,9-Tetramethyl-10-oxa-tricyclo(6.2.2.01,6*)dodec-2-y

Variable Slit Intensity

PDF #02-066-1398 Two Dimensional Structure

PDF #: 02-066-1398 CSD Refcode: TALGES
Formula: C22 H29 Br O3
Name: 5,6,9,9-Tetramethyl-10-oxa-tricyclo(6.2.2.01,6*)dodec-2-yl p-bromo benzoate

02-066-1398 Status Published Quality C
a C22 H29 Br O3

02-066-1398 5,6,9,9-Tetramethyl-10-oxa-tricyclo(6.2.2.01,6*)dodec-2-yl p-bromo ben...

File Settings Display Help

Intensity

2 θ

Cu K α 1+ α 2 (< λ > = 1.54184 A); Bragg-Brentano geometry; pseudo-Voigt profile.

Ready.

Form View

Start Microsoft PowerPoint -... untitled - Paint PDF-4/Full File 2002 V... PDF-4/Organics 200... 12:52 PM

“Card” File

Small Crystallite XRD Simulation

Molecular Drawing

PDF-4 Organics – File Search

The screenshot displays the PDF-4 Organics 2003 Version 2.50 software interface. The main window has a menu bar with options: File, PDF Card, Subfiles/Database Filters, Elements, Names, References, Structures, Misc., Searches, Global Searches, Global Operators, Tools, Window, and Help. A dropdown menu is open under 'Subfiles/Database Filters', showing options: Ambient/Nonambient Search, Quality Mark Search, and Subfile Search.

A 'Subfile Search' dialog box is open, showing a list of subfiles on the left: Organics, Cambridge Database, Drug Activity Index (highlighted), Pharmaceutical, Excipient, and Polymer. The 'Local Operators' section includes a checkbox for 'Not' and radio buttons for 'And' and 'Or'. Buttons for Search, Save, Print, Preview, and Clear are visible.

The search results are displayed in a table with the following columns: PDF #, QM, Chemical Formula, Compound Name, D1, D2, D3, and a final column with a partial label 's'. The table contains 12 rows of data.

PDF #	QM	Chemical Formula	Compound Name	D1	D2	D3	s
02-060-0006	C	C15 H23 N4 C2 H5 O3	2,4-Diamino-5-(1-adama	13.65	6.45	4.83	A
02-060-0149	C	C15 H22 N2 O7	N-Acetylactinobolin	8.20	3.90	3.89	C
02-060-0184	C	C12 H19 Cl2 N2 O Cl	1-(4-Amino-3,5-dichloro	11.78	3.41	4.09	A
02-060-0185	C	C18 H29 N2 O4 Cl	2-(2-Hydroxy-3-isoprop	14.36	13.59	5.40	M
02-060-0271	C	C7 H16 N O2 Cl	Acetylcholine chloride	5.09	3.83	4.60	C
02-060-0278	C	C30 H27 I O14	Tri-O-acetyl-O-iodoacet	8.98	4.65	4.27	C
02-060-0413	C	C10 H18 N O2 I	(R)-(-)-3-Acetoxy-quinu	5.53	6.76	4.09	A
02-060-0434	C	C9 H8 O4	Acetylsalicylic acid	5.67	3.93	11.39	M
02-060-0435	C	C9 H8 O4	2-(Acetyloxy)-benzoic ai	5.67	3.93	11.37	M
02-060-0447	C	C29 H44 O9	Actodigin	6.42	5.31	5.52	M
02-060-0483	C	C2 H5 N O2 *0.5 (H2 O	Acetohydroxamic acid he	3.48	3.11	3.64	C

At the bottom of the dialog box, it shows 'Record: 1 of 4508'.

On the right side of the screenshot, a blue box contains the following text: Drug Activity, Excipients, Pharmaceuticals, Polymers, and 26 Total Subfiles.

The Windows taskbar at the bottom shows the Start button, several open applications (Microsoft PowerPoint, Paint, PDF-4/Full File 2002 V..., PDF-4/Organics 200...), and the system tray with the time 12:59 PM.



Data Mining – Global Searches

Organic Crystal Identification (1)

Pink crystal

Density = 1.25 – 1.30 g/cc

Melting point = 75 – 80 °C

PDF-4 Organics – 147,201 Entries

Density Window – 13,269 Materials

The screenshot displays the PDF-4 Organics 2003 Version 2.50 software interface. A search window titled "Melting Point" is open, showing search criteria: Lower Limit: 75, Upper Limit: 80, and Temperature Parameter: °C. The search results are displayed in a table with columns: PDF #, QM, Chemical Formula, Compound Name, Melt Point, D1, D2, D3, and SYS. The table shows 142 records, with the first few rows visible. The bottom of the screen shows the Windows taskbar with the Start button and several open applications, including Microsoft PowerPoint and PDF-4 Organics 2003.

PDF #	QM	Chemical Formula	Compound Name	Melt Point	D1	D2	D3	SYS
00-001-0028	B	Pb (C2 H3 O2)2	Lead Acetate Hydrate	76.000	11.70	3.60	7.70 X	
00-002-0109	B	C14 H21 Cl O	2,6-Di-tert-butyl-4-chl	78.000	4.79	7.50	4.37 X	
00-004-0103	B	C18 H15 N	Triphenylamine	78.000	9.25	3.17	6.48 M	
00-004-0199	B	C14 H22	1,4-Di-tert-butylbenzene	77.200	7.10	5.80	4.92 X	
00-004-0371	B	C19 H31 N O	Tridocylamine	79.000	4.06	4.30	10.10 X	
00-004-0402	B	C18 H14	4-Ethylstyrene	76.000	3.82	8.80	7.70 X	
00-006-0001	B	C18 H34 O2	Vaccenic acid	511.250	49.10	4.13	3.72 X	
00-006-0088	B	C23 H29 N O2	6-(N-Morpholino)-4,4	75.500	6.20	4.50	7.62 X	
00-007-0988	B	C18 H22 O	2-Isobornylstereol	78.000	10.70	5.90	4.76 X	
00-007-0561	B	C14 H22 O	4-Cyclohexenol	60.000	6.40	15.10	5.00 X	
00-007-0564	B	C15 H24 O	4,8-Di-tert-butyl-3-methyl	80.000	4.74	5.80	8.20 X	

Organic Crystal Identification (2)

MP Window – reduces to 8 materials

Colour Window – reduces to 1 material
dibenzoxylmethane, C₁₅H₁₂O₂

The screenshot displays the PDF-4/Organics 2003 software interface. The main window shows a search results table with columns for PDF #, d [Å], h, k, and l. The search results are filtered to 8 materials. A 'Variable Slit Intensity' plot is visible in the background. A 'PDF #00-032-1641' window is open, showing the chemical structure of Dibenzoxylmethane (C₁₅H₁₂O₂) and its physical and crystal data. The chemical structure is shown as two benzene rings connected by a central carbon atom, which is also bonded to two oxygen atoms.

PDF #	d [Å]	h	k	l
7.29	12.12	5	0	2
12.48	7.050	3	0	2
13.80	6.560	2	1	1
14.87	6.080	2	0	0
14.91	5.940	2	1	2
16.36	5.410	5	1	2
16.99	6.220	8	1	3
17.70	5.010	2	0	4
19.64	4.520	26	2	1
20.27	4.380	5	0	2
20.61	4.210	11	2	1
21.62	4.110	17	0	2
21.89	4.060	2	1	0
22.41	3.967	12	1	5
23.11	3.840	12	1	2
24.14	3.696	5	0	4
24.64	3.620	100	2	5
25.83	3.550	9	0	4
26.29	3.390	10	1	4
26.95	3.269	11	3	1
27.19	3.280	3	2	2
27.70	3.221	3	3	1
28.29	3.144	22	2	2

PDF #00-032-1641
Name: Dibenzoxylmethane
Formula: C₁₅H₁₂O₂
Quality: 1

PDF #00-032-1641
Name: Dibenzoxylmethane

Search for Passive Solar Home Heating Materials

Step 1 – Melting point search (home comfort)

Step 2 – Eliminate photodegradable hydrocarbons: extended application life

Step 3 – Review search and eliminate potentially harmful materials

1. Element Search

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graph TD; A[1. Element Search] --> B[2. Melting Point Search]; B --> C[Produces a list of 17 candidates, 8 contain heavy metals, 1 is an explosive];
```

2. Melting Point Search

Produces a list of 17 candidates,
8 contain heavy metals,
1 is an explosive

All 8 candidate materials are referenced in the patent literature for passive solar heating applications

The background of the slide is a solid dark blue color. It features a decorative pattern of three sets of concentric circles. Each set consists of four circles of increasing size, centered around a common point. The circles are light blue and overlap each other, creating a subtle, geometric design. The word "Demonstration" is centered in the middle of the slide in a white, bold, sans-serif font.

Demonstration