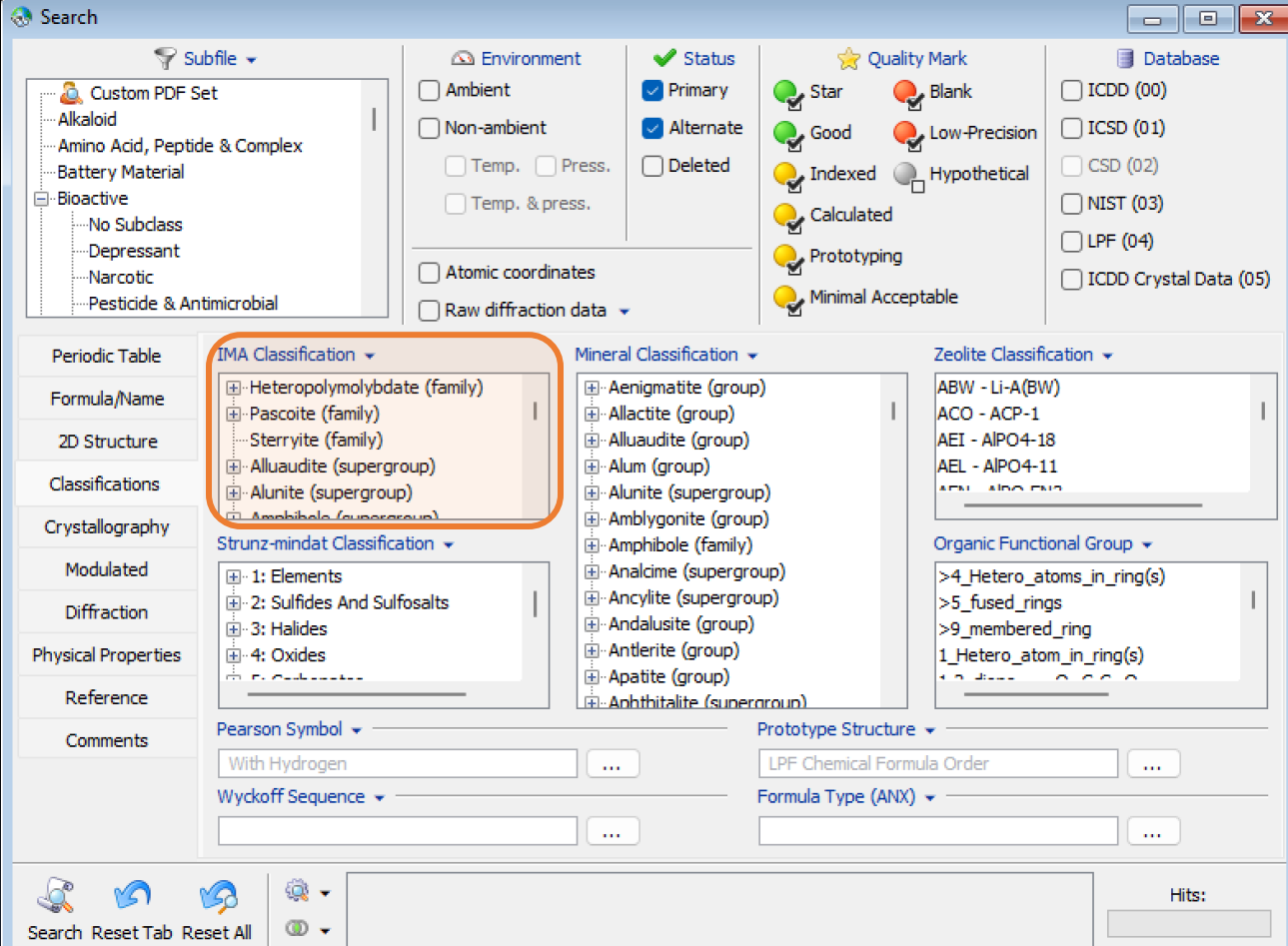




New Features for Release 2027

IMA Classification Search

Enables users to efficiently filter and explore entries by standardized mineral classification categories defined by the IMA (International Mineralogical Association)



The screenshot displays the 'Search' window of the ICDD database. The interface is organized into several sections for filtering and searching:

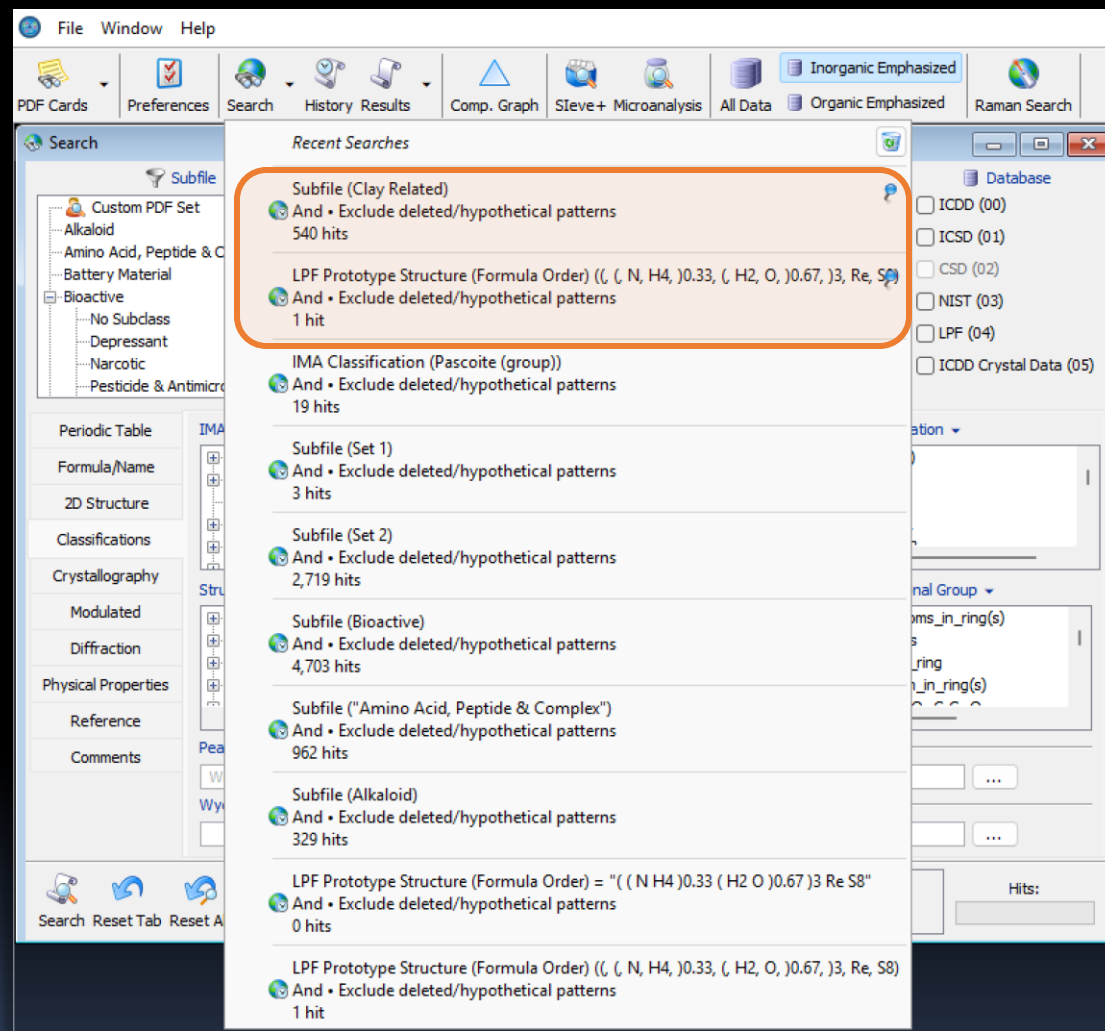
- Subfile:** A tree view on the left showing categories like 'Custom PDF Set', 'Alkaloid', 'Amino Acid, Peptide & Complex', 'Battery Material', 'Bioactive', 'No Subclass', 'Depressant', 'Narcotic', and 'Pesticide & Antimicrobial'.
- Environment:** Checkboxes for 'Ambient', 'Non-ambient', 'Temp.', 'Press.', and 'Temp. & press.'.
- Status:** Checkboxes for 'Primary', 'Alternate', and 'Deleted'.
- Quality Mark:** Radio buttons for 'Star', 'Good', 'Indexed', 'Calculated', 'Prototyping', 'Minimal Acceptable', 'Blank', 'Low-Precision', and 'Hypothetical'.
- Database:** Checkboxes for 'ICDD (00)', 'ICSD (01)', 'CSD (02)', 'NIST (03)', 'LPF (04)', and 'ICDD Crystal Data (05)'.
- IMA Classification:** A list of mineral families and supergroups, including 'Heteropolymolybdate (family)', 'Pascoite (family)', 'Sterryite (family)', 'Alluaudite (supergroup)', 'Alunite (supergroup)', and 'Amphibole (supergroup)'. This section is highlighted with an orange border.
- Strunz-mindat Classification:** A list of categories like '1: Elements', '2: Sulfides And Sulfosalts', '3: Halides', '4: Oxides', and '5: Carbonates'.
- Mineral Classification:** A list of mineral groups and supergroups, including 'Aenigmatite (group)', 'Allactite (group)', 'Alluaudite (group)', 'Alum (group)', 'Alunite (supergroup)', 'Amblygonite (group)', 'Amphibole (family)', 'Analcime (supergroup)', 'Ancylite (supergroup)', 'Andalusite (group)', 'Antlerite (group)', 'Apatite (group)', and 'Anorthite (supergroup)'.
- Zeolite Classification:** A list of zeolite types, including 'ABW - Li-A(BW)', 'ACO - ACP-1', 'AEI - AIPO4-18', 'AEL - AIPO4-11', and 'AFV - AIPO4-11'.
- Organic Functional Group:** A list of functional groups, including '>4_Hetero_atoms_in_ring(s)', '>5_fused_rings', '>9_membered_ring', '1_Hetero_atom_in_ring(s)', and '1_2_diazine_2,6,8,9-tetra'.
- Pearson Symbol:** A dropdown menu with 'With Hydrogen' selected.
- Wyckoff Sequence:** A dropdown menu.
- Prototype Structure:** A dropdown menu with 'LPF Chemical Formula Order' selected.
- Formula Type (ANX):** A dropdown menu.
- Search Bar:** A large text input field at the bottom with buttons for 'Search', 'Reset Tab', and 'Reset All'.
- Hits:** A text box on the right side of the bottom bar.

New Subfiles

- Rock-forming Minerals
 - Represent the most abundant and geologically significant minerals in the Earth's crust and constitute the principal components of igneous, sedimentary, and metamorphic rocks.
 - The rock-forming minerals subset enables users to work with a targeted dataset consisting of the primary mineral constituents of rocks, minimizing interference from accessory and minor minerals.
- Clay Related
 - Brindley & Brown
 - Interstratified
 - Oriented
 - Random
 - Related Phyllosilicates

Pin Searches to Top

You can now pin a favorite search to the top of the recent searches drop-down menu for quick and easy access



Faster Periodic Table Searches

The performance of periodic table searches has been significantly improved through implementation of bitmask fields

	2026	2027
Contains H	6s	1s
Just 8 elements	5s	1s
Just 16 elements	17s	1s

The screenshot displays the ICDD Search application window. On the left, a 'Subfile' tree lists categories like 'Metal & Alloy', 'Metal-Organic Phase', 'Micro & Mesoporous', 'Clathrate', 'Metal-Organic Framework', 'Zeolite', 'Mineral Related', and 'No Subclass'. To the right of the tree are filter sections for 'Environment' (Ambient, Non-ambient, Temp., Press., Temp. & press.), 'Status' (Primary, Alternate, Deleted), 'Quality Mark' (Star, Good, Indexed, Calculated, Prototyping, Minimal Acceptable, Blank, Low-Precision, Hypothetical), and 'Database' (ICDD (00), ICSD (01), CSD (02), NIST (03), LPF (04), ICDD Crystal Data (05)). Below these is a 'Periodic Table' section with tabs for Formula/Name, 2D Structure, Classifications, Crystallography, Modulated, Diffraction, Physical Properties, Reference, and Comments. The periodic table itself is shown with elements color-coded by group. A search bar at the bottom right contains the text 'And' and a dropdown menu. The bottom of the window features a 'Search' button, 'Reset Tab', 'Reset All', and a 'Hits:' counter.

Links to WebCSD

PDF entries from the CSD (02) database now have an active link to the WebCSD online platform

The image shows two overlapping windows. The background window is a PDF entry from the ICDD database, titled 'C19 H30 O3 - 02-087-3314'. It contains a table of diffraction data and a sidebar with various tabs. An orange arrow points from the 'WebCSD' link in the sidebar to the foreground window. The foreground window is a web browser displaying the 'CCDC FIZ Karlsruhe CSD Entry: MAGWOH' page. The browser address bar shows the URL 'www.ccdc.cam.ac.uk/structures/search?pid=csd-MAGWOH&sid=k...'. The page includes search filters, a search result table, and a 3D molecular viewer.

ICDD Entry Data:

2 θ (°)	d (Å)	I (%)	h	k	l	*
8.968	9.85296	17.2	0	0	1	
9.162	9.64434	51.6	1	0	0	
11.651	7.58912	0.2	-1	0	1	
13.246	6.67868	70.8	0	1	1	
13.379	6.61258	53.9	1	1	0	
13.918	6.35758	0.8	1	0	1	
15.200	5.82409	100.0	-1	1	1	
17.009	5.20866	32.1	1	1	1	

PDF Entry Details:

- Status: Primary
- Environment: Non-ambient temperature
- Temperature: 14
- Phase: -
- Chemical Formula: $C_{19}H_{30}O_3$
- Empirical Formula: $C_{19}H_{30}O_3$
- Weight %: C 74.47 H 9.87 O 15.66
- Atomic %: C 36.54 H 57.69 O 5.77
- Compound Name: (-)-(1R,2R,3R,4R,5R,6R)-1-Ethyl-2,4,6-trimethyl-5-phenylethoxycyclohexane-1,3-diol
- CAS Number: -
- Entry Date: 09/01/2007
- Modification Date: 09/01/2010
- Modifications: Update

WebCSD Search Results:

Search Results - Access Structure: X

www.ccdc.cam.ac.uk/structures/search?pid=csd-MAGWOH&sid=k...

Sign in

ICDD Powder Diffraction Databases XRF M-22-18 Postmark

CCDC FIZ Karlsruhe CSD Entry: MAGWOH

Sign in

Simple Search Structure Search Unit Cell Search Formula Search

Your query was: Identifier(s): MAGWOH and the search returned 1 record. [Modify Search](#) [New Search](#)

Database Identifier	Deposition Number
☒ MAGWOH	245522

[Download](#)

MAGWOH : (-)-(1R,2R,3R,4R,5R,6R)-1-Ethyl-2,4,6-trimethyl-5-((1"S)-1"-phenylethoxy)cyclohexane-1,3-diol
Space Group: P 2₁ (4), Cell: a 9.796(2)Å b 9.084(2)Å c 10.0079(16)Å, α 90° β 100.095(17)° γ 90°

3D viewer

Ball and Stick No Labels

PDF Entry Export Enhancements

- PDF entries can now be exported directly as Adobe PDF files
- The XML export format has been redesigned to provide a cleaner structure and improved browser-based presentation

PDF Card - 04-002-3600.xml

File C:/Users/jblanton/Downloads/PDF%20Card%20-%2004-002-3600.xml

PDF Card - 04-002-3600

Status	Alternate	Environment	Ambient
Quality Mark	Prototyping	Temperature	298.0 K

Chemical Formula	Si O2
Empirical Formula	O2 Si
Refined Formula	O2 Si
Weight %	O53.26 Si46.74
Atomic %	O66.67 Si33.33

Compound Name	Silicon Oxide
Mineral Name	Quartz
IMA Symbol	Qz
Alternate Name	quartz enfume

Entry Date	09/01/2005	Modification Date	09/01/2015
		Modifications	Add unit cell precision

Experimental Data

Radiation	CuKα1 (1.5406 Å)
d-spacing	Calculated
Intensity	Calculated - Peak

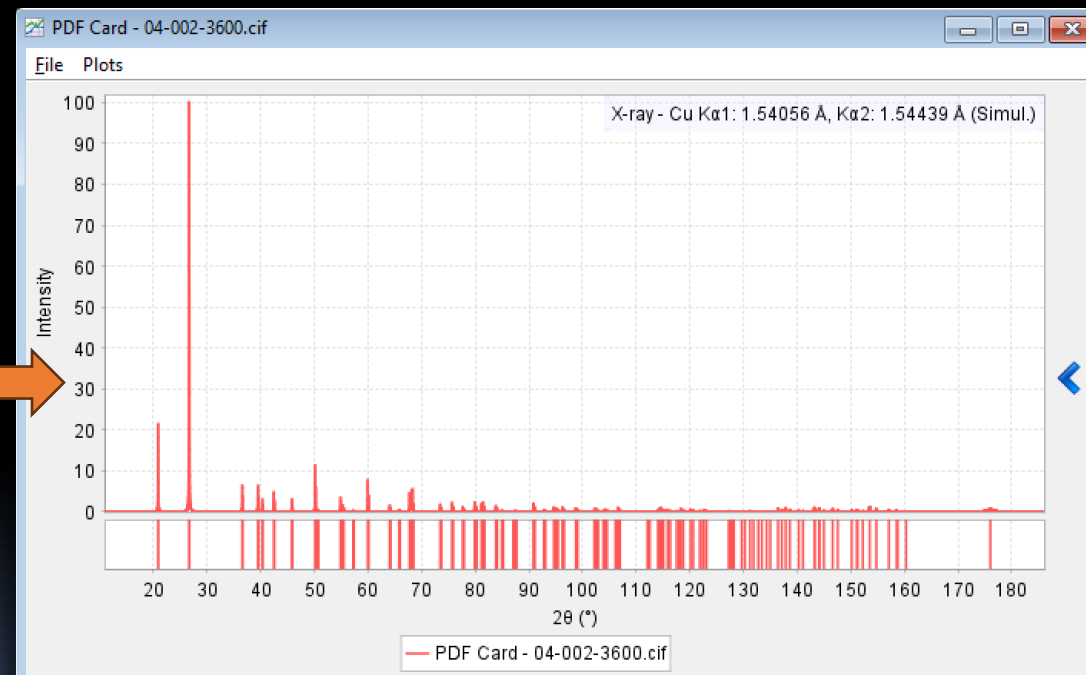
Simulate 1D Diffraction Patterns from CIF Files

```
data_04-002-3600
# Copyright 2026 International Centre for Diffraction Data. All rights reserved.

_audit_creation_date      2026-02-19
_audit_creation_method    'Generated by PDF-5+ 2027 null'

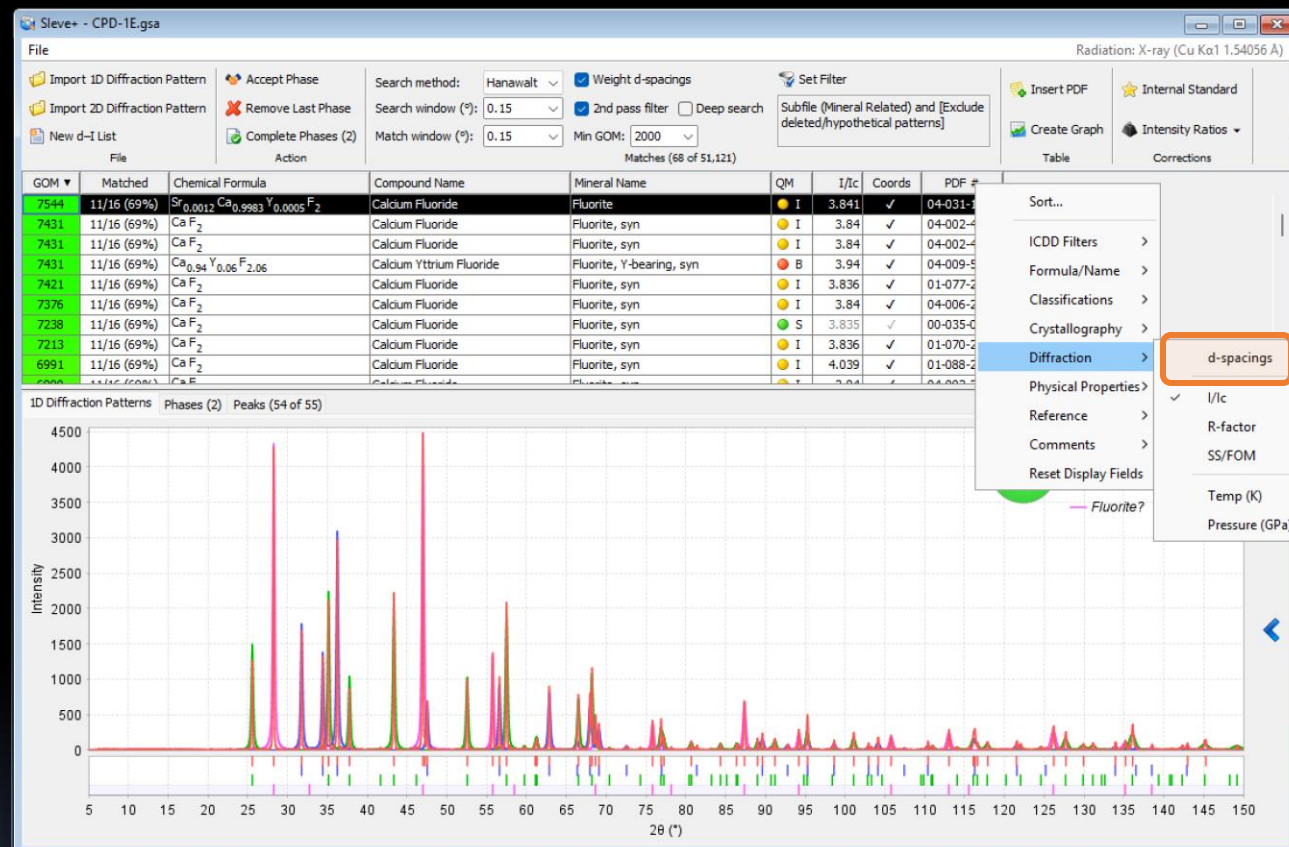
_chemical_name_systematic 'Silicon Oxide'
_chemical_name_mineral    Quartz
_chemical_name_common     'quartz enfume'
_chemical_formula_moiety  'Si O2'
_chemical_formula_sum      'O2 Si'
_chemical_formula_weight  60.08

_cell_length_a            4.9134
_cell_length_b            4.9134
_cell_length_c            5.4046
_cell_angle_alpha         90
_cell_angle_beta          90
_cell_angle_gamma         120
_cell_formula_units_Z     3
_cell_volume              112.99
_symmetry_cell_setting    hexagonal
_symmetry_space_group_name_H-M P3121
_symmetry_Int_Tables_number 152
```



New Sleeve+ Features

- Import NeXus (.nxs) diffraction patterns
 - HDF5 format
- Show/hide d-spacing columns in the Matches table
- Show alternate names in the graph phase list



New Raman Metadata

- **Objective** – Microscope objective used (e.g., 50×, NA value)
- **Orientation** – Orientation of the sample relative to the laser or polarization
- **Resolution** – Spectral resolution of the spectrometer (cm^{-1})
- **Exposure time** – Detector integration time per scan
- **Accumulations** – Number of scans summed/averaged to produce the final spectrum

