powder diffraction file

PDF

ICDD & PDF

ICDD - International Centre for Diffraction Data

- A non-profit scientific organization dedicated to collecting, editing, publishing, and distributing powder diffraction data for the identification of crystalline materials
- Joint Committee for Chemical Analysis by Powder Diffraction Methods ; founded in 1941.
- Joint Committee on Powder Diffraction Standards (JCPDS) ; established in 1969.
- Renamed to ICDD in 1978.

PDF - powder diffraction file

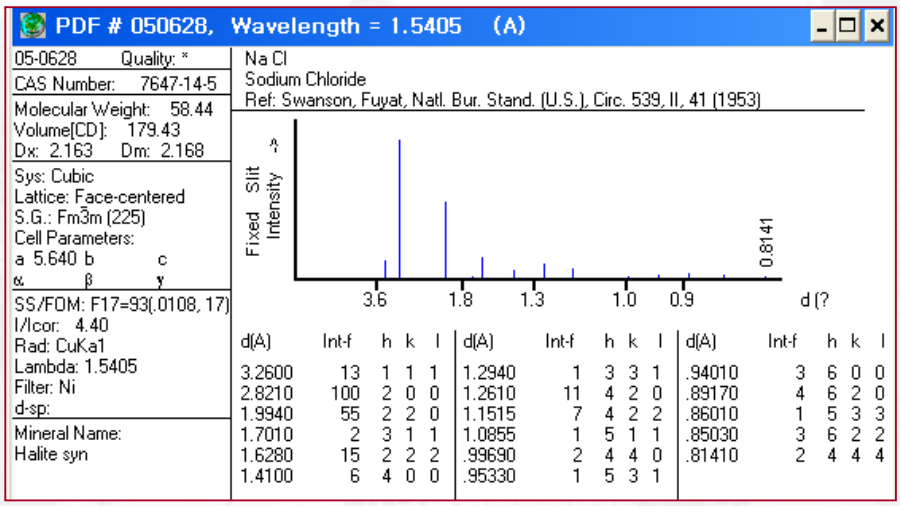
- a collection of single-phase XRPD patterns in the form of tables of characteristic **interplanar spacings (d's)** and corresponding **relative intensities (I's)** along with other pertinent physical and crystallographic properties
- dif file
- ###.dif

XRPD; X-ray Powder Diffraction

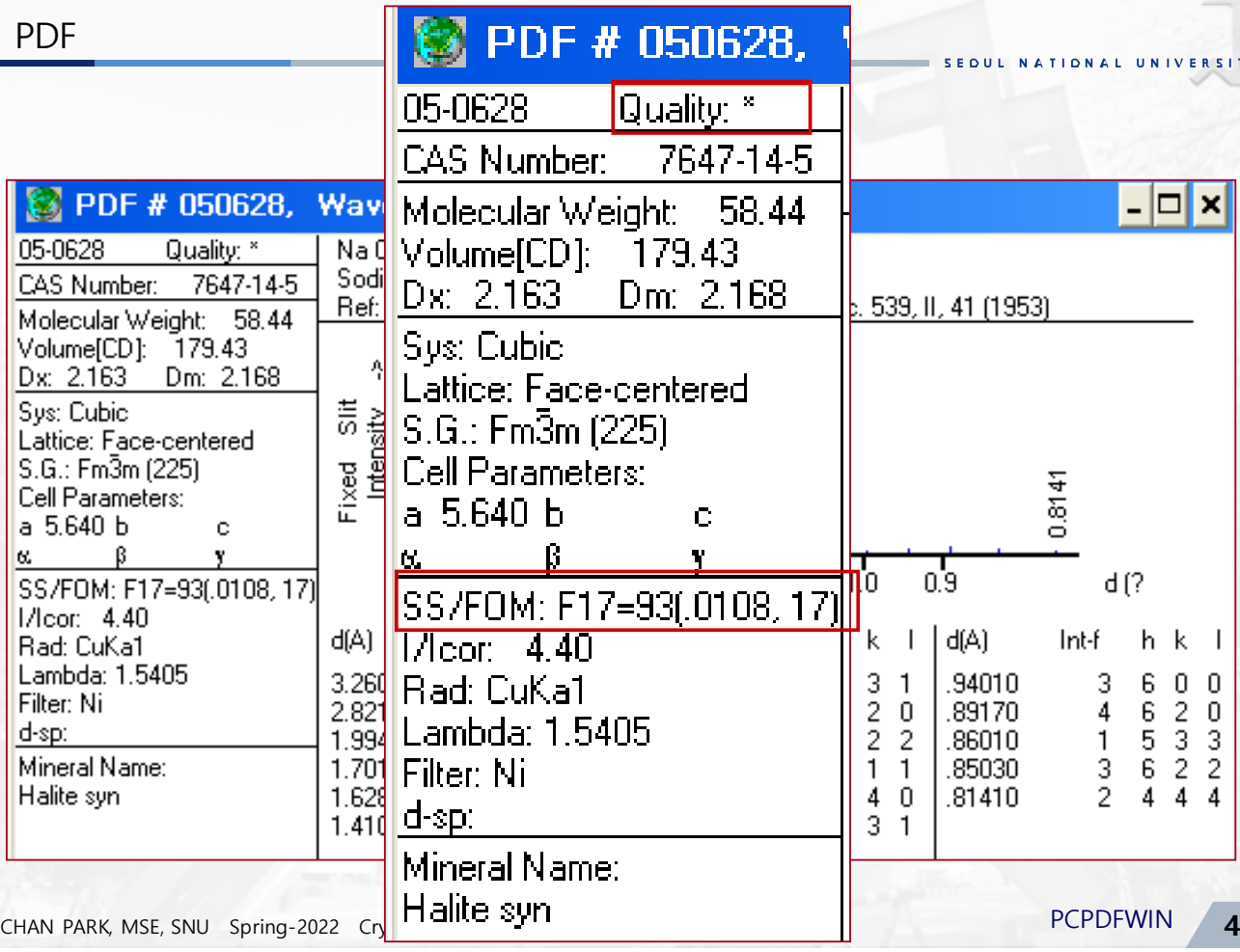
www.icdd.com

PDF - powder diffraction file

- a collection of single-phase X-ray powder diffraction patterns in the form of tables of characteristic interplanar spacings and corresponding relative intensities along with other pertinent physical and crystallographic properties
- a collection of single-phase X-ray powder diffraction patterns in the form of tables of characteristic d's & I's along with other pertinent physical and crystallographic properties



PDF



PDF card (in the past)

Quality mark
* Highest quality
i reasonable quality
o low quality
blank quality lower than o
c calculated data
r d's from Rietveld refinement

Set number
Add 1950 → year

Chemical formula
Chemical name
Mineral name

Experimental info
Types of X-ray
Wavelength
Monochromator/filter
Method of d measurement
Max measurable d-spacing
Method of I measurement
I/I(corundum)
Literature source

Physical data
Xtal system
International tables space group symbol
Axial lengths
Axial ratios
Interaxial angles
Number of chemical formulas in unit cell
Melting point
Literature source
X-ray density
Measured density
Figure of Merit

5- 628

NaCl

Sodium Chloride

Halite, syn

Rad. CuKα$_1$ λ 1.5405 **Filter** Ni **d-sp**
Cutoff **Int.** Diffractometer **I/I$_{cor}$**: 4.40
Ref. Swanson, Fuyai, *Natl. Burl. Stand. (U.S.), Circ. 539, II 41 (1953)*

Sys. Cubic **S.G.** Fm3m(225)
A 5.6402 **b** **c** **AC**
α β γ **Z** 4 **mp** 804
Ref. Ibid.
D$_x$ 2.16 **D$_m$** 2.17 **SS/FOM F$_{17}$**=93(.011,17)
εα ηωβ 1.542 εγ **Sign** **2V**
Ref. *Dana's System of Mineralogy, 7th Ed.*, II 4

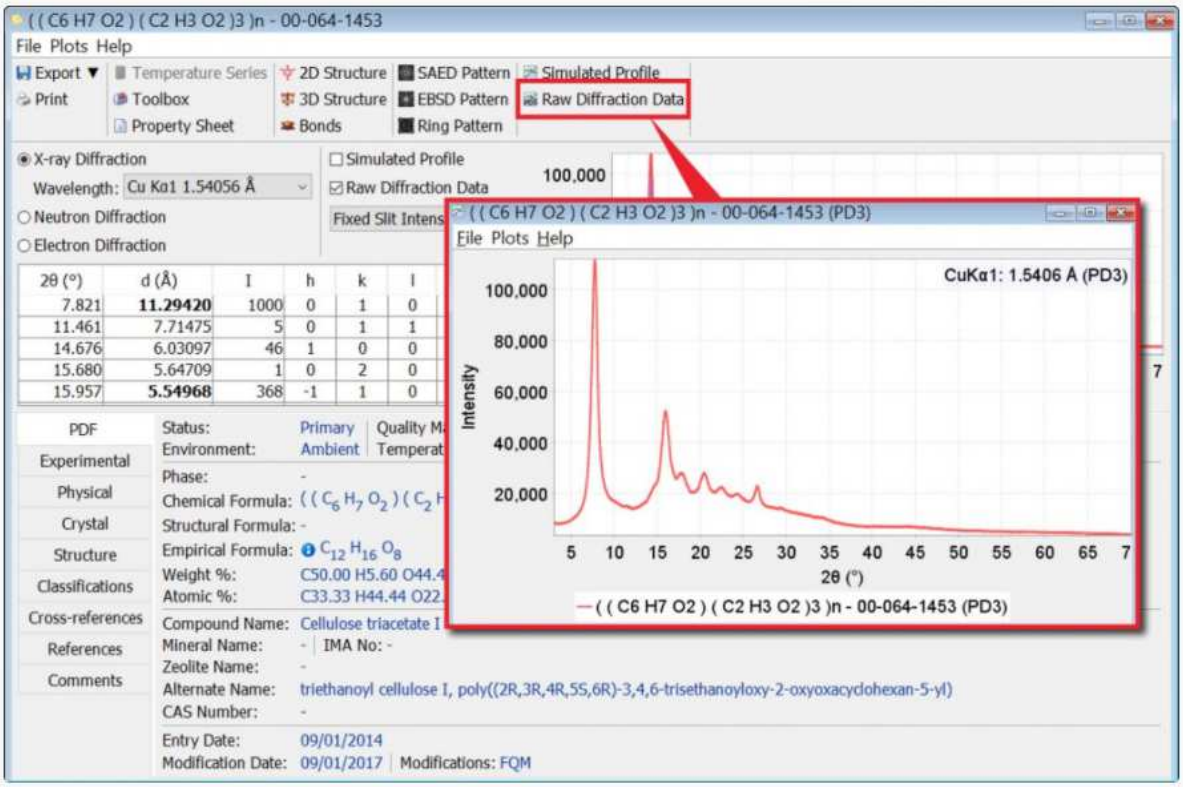
Color Colorless
Pattern taken at 26 C. CAS#: 7647-14-5. An ACS reagent grade sample recrystallized twice from hydrochloric acid. Halite group, halite subgroup. PSC: cF8.

d Å	Int	h k l	d Å	Int	h k l
3.26	13	111			
2.821	100	200			
1.994	55	220			
1.701	2	311			
1.628	15	222			
1.410	6	400			
1.294	1	331			
1.261	11	420			
1.1515	7	422			
1.0855	1	511			
0.9969	2	440			
0.9533	1	531			
0.9401	3	600			
0.8917	4	620			
0.8601	1	533			
0.8503	32	622			
0.8141	2	444			

General comments

D's, I's and Miller indices

PDF card (2021)



- The initial term of the license for PDF-2 and SIeve is five (5) years from the license registration key date.
- All PDF-4 products are licensed for 12 months.

ICDD® 2022 Product Summary

Data Entry Source	PDF-4+ 2022 PDF-4+/Web 2022	PDF-4/ Axiom 2022	PDF-4/ Minerals 2022	PDF-4/ Organics 2022	PDF-2 2022
00- ICDD	122,611	36,257	12,805	43,162	122,611
01- FIZ	84,354	13,448	13,987	17,378	194,077
02- CCDC	0	0	0	444,125	0
03- NIST	2,862	412	229	283	10,067
04- MPDS	250,258	51,856	22,819	0	0
05- ICDD Crystal Data	869	0	75	55,247	869
Total No. of Entries	460,954	101,973	49,915	560,195	327,624
Subfile Distribution:					
Inorganic	438,726	92,727	49,861	324,259	305,502
Organic	51,414	11,978	732	548,959	49,726
New Entries	16,187	4,184	969	12,900	10,804
Rietveld—No. with atomic coordinates	353,330	71,560	41,376	156,107	0
Reference Intensity Ratio (RIR)—I/I_c	358,223	73,144	38,387	525,705	224,922
Experimental Digital Patterns	17,053	7,535	169	9,167	0

All ICDD databases combine the power of both powder diffraction and crystal structure reference data. We are the only crystallographic database in the world with quality marks and quality review processes that are ISO certified. Each PDF® database includes our integrated data mining software.

https://www.icdd.com/assets/files/2022-Product-Summary.pdf

WHICH ICDD DATABASE IS RIGHT FOR YOU?

https://www.icdd.com/assets/files/2022-Which-Database-Flyer.pdf

	PDF-4+ 2022	PDF-4+/ WEB 2022	PDF-4/ AXIOM 2022	PDF-4/ MINERALS 2022	PDF-4/ ORGANICS 2022	PDF-2 2022
I WORK PRIMARILY WITH INORGANIC COMPOUNDS	✔	✔	✔			✔
I WORK PRIMARILY WITH ORGANIC COMPOUNDS					✔	
I WORK PRIMARILY WITH MINERALS				✔		
I WORK WITH ELECTRON DIFFRACTION/SYNCHROTRON	✔	✔		✔	✔	
I NEED TO WORK AT THE OFFICE AND HOME		✔				
I NEED TO DO QUANTITATIVE ANALYSIS						
RIETVELD	✔ *	✔ *	✔ *	✔ *	✔ *	
REFERENCE INTENSITY RATIO (RIR)	✔ †	✔ †	✔ *	✔ †	✔ †	✔ †
PATTERN FITTING	✔ *	✔ *	✔ *	✔ *	✔ *	
I NEED A DATABASE WITH ATOMIC COORDINATES	✔	✔	✔	✔	✔	
HOW MANY ENTRIES ARE IN THE DATABASE?	460,954	460,954	101,973	49,915	560,195	327,624
HOW MANY ENTRIES ARE NEW?	16,821	16,821	4,184	969	12,900	10,804
I am using vendor software for my analysis. Which databases will work with my vendor software? Global software vendors provide search/match software that interfaces with our databases. Please check with your software vendor for compatibility.	✔	✔	✔	✔	✔	✔
WHAT IS THE LICENSE TERM FOR THE DATABASE?	1 YEAR	1 YEAR	3 YEAR	1 YEAR	1 YEAR	5 YEAR
MULTI-YEAR LICENSE AVAILABLE	✔	✔		✔	✔	
SITE LICENSE AVAILABLE	✔	✔			✔	✔

* Using diffraction equipment manufacturer or vendor software.
† Using SIeve or SIeve+, diffraction equipment manufacturer or vendor software.
NEW- Extended multi-year license terms – let us know what you need!

PDF-4+ 2021

PDF-4+ Purchase Options

https://www.icdd.com/assets/files/2021-Purchase-Options.pdf

PDF-4+ 2021	DVD CODE	USB CODE	2020 –2021 LIST $	2020 –2021 ACADEMIC $
New - Single License	F4D21	F4S21	$8,910	$5,925
Renewal from 2020 to 2021	F4RD21	F4RS21	$1,960	$1,250
PDF-4+ and JADE Pro Bundle*				
New - Single License	BUJPF4D21	BUJPF4S21	$15,648	$10,986
*Purchase a new license for PDF-4+ and JADE Pro				
PDF-4+ 2021 Multi-year License*				
Renewal - 3 year license	F4D22MR24	F4S22MR24	$5,290	$3,375
Renewal - 5 year license	F4D22MR26	F4S22MR26	$8,330	$5,315
PDF-4+Scholar 2021 (10-Year License Package)*				
PDF-4+ New – Single License	F4D21	F4S21	NA	$5,925
Sleve+ – New Single License	SWS421N	SWS421N	NA	$500
Scholar Multi-year	F4SPD22MR26	F4SPS22MR26	NA	$6,125
				$12,550
Save Money! Take advantange of ICDD's Combo Site License – Request a quote today!				
PDF-4+ 2021 Site License*				
New Master License	F4D21M	F4S21M	$8,910	$5,925
New - additional licenses, each	F4D21C	F4S21C	$1,960	$1,250
Renewal - Yearly Master License	F4RD21M	F4RS21M	$1,960	$1,250
Renewal - additional licenses, each	F4RD21C	F4RS21C	$750	$495
PDF-4+ 2021 Site/Multi-year License*				
Renewal - 3 year Master Site License	F4D22MR24M	F4S22MR24M	$5,290	$3,375
Renewal - 3 year additional licenses, each	F4D22MR24C	F4S22MR24C	$2,250	$1,485
Renewal - 5 year Master Site License	F4D22MR26M	F4S22MR26M	$8,330	$5,315
Renewal - 5 year additional licenses, each	F4D22MR26C	F4S22MR26C	$3,750	$2,475
PDF-2 to PDF-4+ Conversion				
PDF-2 2020 to PDF-4+ 2021	F2420RDU21	F2420RSU21	$1,960	$1,250
PDF-2 2019 to PDF-4+ 2021	F2419RDU21	F2419RSU21	$3,920	$2,500
PDF-2 2018 to PDF-4+ 2021	F2418RDU21	F2418RSU21	$5,880	$3,750
PDF-2 2016 to PDF-4+ 2021	F2416RDU21	F2416RSU21	$7,840	$5,000

PDF - Quality Mark & Figure of Merit

Quality Mark

- * highest quality - average Δ2θ < 0.03 degree, all lines were indexed, I measured quantitatively
- i reasonable quality - average Δ2θ < 0.06 degree, indexed with no more than two lines being unaccounted for, I measured quantitatively
- o low quality - low precision, poorly characterized, no unit cell data
- **blank** quality lower than o
- c calculated data
- r d's from Rietveld refinement
- h (hypothetical)

www.icdd.com/resources/webpdf/explain.htm
"Evaluating Data Quality" from ICDD

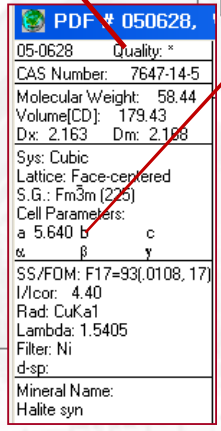


Figure of Merit

- To quantify better the quality of a given set of d-spacings
- To judge the credibility and worth of the results
- To evaluate the quality of d measurements
- The higher, the better

< 20 → poor quality

SS/FOM

(Smith & Snyder FOM)

$$F_N = \frac{1}{|\Delta 2\theta|} \frac{N_{obs}}{N_{poss}}$$

F_N	=	Figure of merit
$\Delta 2\theta$	=	The average error in 2θ
N_{obs}	=	The number of lines observed
N_{poss}	=	Number of lines possible

Jenkins & Snyder page 315

Quality Mark of PDF

- A reliability index used in Powder Diffraction File (PDF)
- Plays an important role in interpreting search match results.
- Data validation and the assignment of the quality mark are the most important steps in the editorial process of PDF.
- The criteria for the assignment of the quality marks differ between patterns obtained experimentally and those determined from the crystal structure (calculated patterns).
- Editorial comments describing the quality of the pattern are extremely useful in evaluating and eventually accepting the search/match results.