

Chemical and Structural Classifications

Chemical and Structural Classification

What?

Materials can be classified by their chemistry and structure.

There are three main types of structural classifications:

1. Prototype Structure

- Structure prototyping is a well-known concept in inorganic chemistry where, often, a large number of compounds crystallize with very similar atomic arrangements.

2. Mineral Classification

- Based on the crystal chemistry characteristics and used to assist in the identification of mineral phases

3. Zeolite Classification

- Based on the zeolite name and framework type code (FTC)

Chemical and Structural Classification

Prototype Structures

ICDD Traditional Prototype Structure Notation

Based on the unit cell, axial ratios, Pearson Symbol and chemistry (usually assigned semi-automatically by comparing crystal chemistry and diffraction patterns)

ANX Formula

Based on the type of ion and its site occupation

Example :

Ca Ti O₃ is of ABX₃ type

Fe₃O₄ is of AB₂X₄ type

LPF Prototype Structure

Based on the method proposed by Parthe of comparing the standardized crystal structures of isopointal groups.

(*Acta Cryst.* (1984) A40, 169-183)

Example:

Cu₃As, cI64, 220

(Structure Type Formula, Pearson Symbol, Space Group Number)

Chemical and Structural Classification

Mineral Classification

- Family

Related by partial structural similarities
such as framework, chain, etc.

- Subfamily

Collection within the family based on specific similarities

Chemical and Structural Classification

Mineral Classification Breakdown

- Supergroup

Highest symmetry phase in which the structural arrangement remains unchanged

- Group

Composed of isostructural phase

- Subgroup

Groups further classified based on chemistry

(oxides, sulfides)

- ❖ Related Structures

Based on structural distortions from the group structure

Example Zinc Sulfide (ZnS)

Information about the structure & its classification are found under the **Miscellaneous** tab of the PDF card window.

PDF Card - 00-005-0566

File Edit d-Spacings Tools Help

Wavelength: Cu Kα1 1.54056Å

Intensity: Fixed Slit Variable Slit Integrated

2θ	d(Å)	I	h	k	l
28.5584	3.123	100	1	1	1
33.0892	2.705	10	2	0	0
47.515	1.912	51	2	2	0
56.2889	1.633	30	3	1	1
59.1356	1.561	2	2	2	2
69.5221	1.351	6	4	0	0
76.8067	1.24	9	3	3	1
79.155	1.209	2	4	2	0

PDF Experimental Physical Crystal Optical Structure **Miscellaneous** Comments

CAS: Former PDF #:

Pearson: **cf8.00**

Pearson w/o H:

Prototype Structure: **Zn S**

PDF Prototype Structure:

Mineral Classification: **Diamond (Supergroup), 2C-chalcogenide (Group)**

Zeolite Classification:

Subfile(s): Common Phase, Corrosion, Educational Pattern, Forensic, Inorganic, Metals & Alloys, Mineral Related (Mineral), NBS Pattern, Primary Pattern

Entry Date: Last Modification Date: 01/24/2006

The Pearson Symbol, Prototype Structure & Mineral Classification are all given here.

Chemical and Structural Classification

Zeolite Classification

- Zeolite Name
- Framework Code
 - Based on topologically distinct tetrahedral TO_4 framework (T=Si, Al, P, Ga, B, etc.) as per "Atlas of Zeolite Framework Types", 5th edition, Ch. Baerlocher, W.M. Meier & D.H. Olson, Amsterdam: Elsevier (2001)
 - For more information

<http://www.iza-online.org>

Zeolite Names Example

Aluminum Silicate

PDF Card - 00-044-0002

File Edit d-Spacings Tools Window Help

Wavelength: Cu Kα1 1.54056Å

Intensity: Fixed Slit Variable Slit Integrated

2θ	d(Å)	I	h	k	l
7.9868	11.0606...	69	1	0	1
8.8848	9.944670	52	2	0	0
9.1348	9.673060	12	1	1	1
9.9247	8.904820	3	2	1	0
11.9247	7.415460	6	2	1	1
12.5397	7.053130	2	2	2	0
13.2297	6.686790	1	0	0	2
13.9626	6.337370	10	1	0	2

Intensity vs 1/d plot showing peaks at various 1/d values. Legend: 00-044-0002 (Fixed Slit Intensity)

PDF Experimental Physical Crystal Optical Structure Miscellaneous Comments

PDF #: 00-044-0002 Status: Primary QM: Indexed (I)

Pressure/Temperature: Ambient

Chemical Formula: Al₂O₃ · 54 SiO₂

Weight %: Al1.61 O53.07 Si45.32

Atomic %: Al1.20 O66.47 Si32.34

Compound Name: Aluminum Silicate

Mineral Name: Mutinaite, syn

Common Name: ZSM-5

The possible names are found at the bottom of the **PDF** pane.

Zeolite Classification Example

Aluminum Silicate

[Al₂O₃ * 54SiO₂]

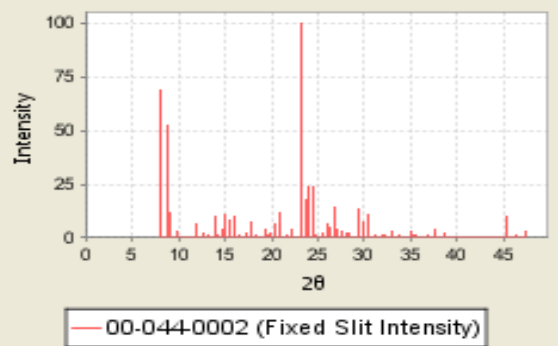
PDF Card - 00-044-0002

File Edit d-Spacings Tools Help

Wavelength: Cu Kα1 1.54056Å

Intensity: Fixed Slit Variable Slit Integrated

2θ	d(Å)	I	h	k	l
7.9868	11.0606	69	1	0	1
8.8847	9.9447	52	2	0	0
9.1347	9.6731	12	1	1	1
9.9248	8.9048	3	2	1	0
11.9246	7.4155	6	2	1	1
12.5397	7.0531	2	2	2	0
13.2296	6.6868	1	0	0	2
13.9626	6.3374	10	1	0	2



PDF Experimental Physical Crystal Optical Structure **Miscellaneous** Comments

CAS: Former PDF #:

Pearson: tP? Cross-Ref PDF #'s (0)

Pearson w/o H:

Prototype Structure:

LPF Prototype Structure:

Mineral Classification: Zeolite (Family), other zeolites

Zeolite Classification: MFI (ZSM-5)

Subfile(s): Inorganic, Mineral Related (Mineral), Primary Pattern, Zeolite

Entry Date: 12/14/1993 Last Modification Date: 01/24/2006

The Zeolite Classification is found on the **Miscellaneous** pane of the PDF card.

Chemical and Structural Classification

Why?

- Deriving a Starting Model for Rietveld Refinements
 - Traditionally the starting models for Rietveld refinements were developed based on chemical/crystallographic intuition. In other words, the individual's knowledge of structure types was used.
 - Databases with Structure Type information can make seminal contributions to this effort. The Powder Diffraction File, in particular, offers several advantages as one can perform a search match based on the user's diffraction pattern to explore possible models.

Chemical and Structural Classification

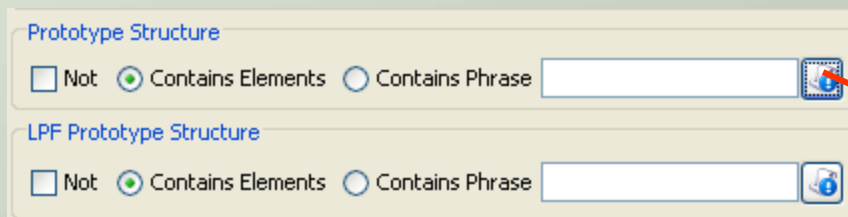
Why?

- Structural chemistry information
 - Database search results can be sorted based on structural chemistry.
 - Can be used to explore the database from the materials design point of view.
 - 3D crystalline structure related properties
 - Ferroelectric, Piezoelectric, Non Linear Optics Transport
 - Mineral and Zeolite classifications are extremely useful as database search filters.

Chemical and Structural Classification

How?

- Prototype structure search option
 1. Click on Structures tab on the main search window.
 2. The LPF prototype & prototype structure selection panes are located at the bottom of the window.



Prototype Structure

Not Contains Elements Contains Phrase

LPF Prototype Structure

Not Contains Elements Contains Phrase

**Push this button
for a list of
prototype
structures.**

Chemical and Structural Classification

How?

- Mineral and Zeolite classification search option
 1. Click on Names tab on the main search window.
 2. Choose the mineral or zeolite classification codes of interest from the menu as shown in the following slide.

Search

Global Operator Numeric Input Help

Subfiles/Database Filters Periodic Table Elements **Names** References Structures Miscellaneous

Compound Name
 Not Contains Words Contains Phrase

Common Name
 Not Contains Words Contains Phrase

Mineral Name
 Not Contains Words Contains Phrase

All Names
 Not Contains Words Contains Phrase

Zeolite Classification

Not Or

- ABW - Li-A(BW)
- ACO - ACP-1
- AEI - AlPO4-18
- AEL - AlPO4-11
- AEN - AlPO-EN3
- AET - AlPO4-8
- AFG - Afghanite
- AFI - AlPO4-5
- AFN - AlPO-14
- AFO - AlPO4-41
- AFR - SAPO-40
- AFS - MAPSO-46
- AFT - AlPO4-52
- AFX - SAPO-56
- AFY - CoAPO-50
- AHT - AlPO4-H2
- ANA - Analcime
- APC - AlPO4-C

Mineral Classification

Not Or

- + AEN - Aenigmatite (Group)
- + VRL - Alluaudite (Group)
- + ALM - Alum (Group)
- + ALN - Alunite (Supergroup)
- + AMB - Amblygonite (Group)
- + AMP - Amphibole (Family)
- + ANC - Analcime (Supergroup)
- + ANY - Ancylicite (Supergroup)
- + ADA - Andalusite (Group)
- + ANT - Antlerite (Group)
- + APA - Apatite (Group)
- + APH - Aphaniticite (Supergroup)
- + APO - Apophyllite (Supergroup)
- + ARA - Aragonite (Group)
- + ARC - Arcanite (Group)
- + ARG - Argyrodite (Supergroup)
- + ASS - Arseniosiderite (Group)
- + APT - Arthursite (Group)

Structure: Please select a class

 Show Results

Zeolite & Mineral Classification Menus

Chemical and Structural Classification

How?

- ANX formula search option
 1. Click on Elements tab on the main search window.
 2. Type in the ANX formula or select from the ANX list displayed using the lookup button.



Thank you for viewing our tutorial.
Additional tutorials are available at the ICDD website
(www.icdd.com).

International Centre for Diffraction Data

12 Campus Boulevard

Newtown Square, PA 19073

Phone: 610.325.9814

Fax: 610.325.9823