Chemical and Structural Classifications
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.
Example:
Cu3 As, cl64, 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
Information about the structure & its classification are found under the Miscellaneous tab of the PDF card window.

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

Zeolite Classification

• Zeolite Name
• Framework Code


- For more information
  http://www.iza-online.org
Zeolite Names Example
Aluminum Silicate

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

<table>
<thead>
<tr>
<th>Compound Name</th>
<th>Mineral Name</th>
<th>Common Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum Silicate</td>
<td>Multinitie, syn</td>
<td>ZSM-5</td>
</tr>
</tbody>
</table>
Zeolite Classification Example

Aluminum Silicate

$[\text{Al}_2\text{O}_3 \times 54\text{SiO}_2]$
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.

Push this button for a list of prototype structures.
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.
Zeolite & Mineral Classification Menus

Zeolite Classification

- ABW - Li-A(BW)
- ACO - ACP-1
- AIZ - AIOPO4-18
- AEL - AIOPO4-11
- AEN - AIOPO4-EN3
- AET - AIOPO4-8
- AFG - Afghanistan
- AFI - AIOPO4-5
- AFN - AIOPO4-14
- AFO - AIOPO4-41
- AFR - SAPO-40
- AFS - MAPSO-46
- AFT - AIOPO4-52
-AFX - SAPO-56
- AFY - CoAPO-50
- AHT - AIOPO4-H2
- AHA - AIOPO4
- APC - AIOPO4-C
- APB - AIOPO4-B
- APW - AIOPO4-W
- APX - AIOPO4-X

Mineral Classification

- AEN - Aenigmatite (Group)
- APL - Alunite (Group)
- APM - Ambygongite (Group)
- AMP - Amphibole (Family)
- ANC - Analcime (Superclass)
- AMY - Analcylite (Superclass)
- ADA - Andalusite (Group)
- ANT - Anatase (Group)
- APA - Apatite (Group)
- APH - Asphalite (Superclass)
- APO - Apophyllite (Superclass)
- ARA - Aragonite (Group)
- ARC - Acanite (Group)
- ARG - Argyrodite (Superclass)
- AS5 - Arseniosodite (Group)

Structure: Please select a class
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.
Formula Type (ANX) panel

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

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