Crystal Structure and Unit Cell

Talk to a Teacher
http://spoken-tutorial.org
National Mission on Education through ICT
http://sakshat.ac.in

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Learning Objectives

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- **Download CIF (Crystallographic Information File) from Crystallography Open Database (COD)**

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- **Display unit cell and unit cell parameters on Jmol panel**

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- **Display crystal structures of different crystal systems Example Cubic, Hexagonal and Rhombohedral**

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- **Mozilla Firefox Browser 35.0**

Crystal Systems

system	Lattice parameter	Interfacial angles	Examples
Cubic or regular	a=b=c	$\alpha = \beta = \gamma = 90^0$	Nacl, KCl, Diamond
Tetragonal	a=b ≠ c	$\alpha = \beta = \gamma = 90^0$	SiO_2, $Ti0_2$
Hexagonal	a=b ≠ c	$\alpha = \beta = 90^0$, $\gamma = 120^0$	Graphite, ZnO
Trigonal Rhombohedral	a=b=c	$\alpha = \beta = 90^0$, $\gamma \neq 90^0$	Calcite; $NaNO_3$
orthorhombic	a ≠ b ≠ c	$\alpha = \beta = \gamma = 90^0$	KNO_3
Monoclinic	a ≠ b ≠ c	$\alpha = \beta = 90^0$, $\gamma \neq 90^0$	$Na_2SO_4.10H_2O$
Triclinic	a ≠ b ≠ c	$\alpha \neq \beta \neq \gamma \neq 90^0$	$CuSO_4.5H_2O$

Crystallographic Information File (CIF)

- **Crystallographic Information File (CIF) is a standard text file format for representing crystallographic information**
- **CIF format has the file extension .cif**

Crystallography Open Database (COD)

- **Crystallography Open Database (COD) is an open-access database**
- **The downloadable CIF are available at COD website**
- **www.crystallography.net**

Unit Cell

- **Unit cell is the smallest repeating unit in a crystal**
- **Stacking of these unit cells in 3 dimensions will form the basis of the crystal structure**

Summary

- **Download CIF from Crystallography Open Database (COD)**
- **Open CIF in Jmol**
- **Display unit cell and unit cell parameters**

Summary

- **Display crystal structures of sodium chloride, graphite and calcite**

Assignment

- **Download CIF for quartz crystal from COD database**
- **Display unitcell on Jmol panel and explore the symmetry options**

About the Spoken Tutorial Project

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The Spoken Tutorial Project Team

- **Conducts workshops using spoken tutorials**
- **Gives certificates to those who pass an online test**
- **For more details, please write to contact@spoken-tutorial.org**

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- More information on this Mission is available at http://spoken-tutorial.org/NMEICT-Intro