

Important Crystallography Formulas PDF



Formulas Examples with Units

List of 13 Important Crystallography Formulas

1) Body Centered Cubic Formulas

1.1) Atomic Radius in BCC Formula

Formula

$$r = \frac{\sqrt{3}}{4} \cdot a_{\text{BCC}}$$

Example with Units

$$1.3597 \text{ \AA} = \frac{\sqrt{3}}{4} \cdot 3.14 \text{ \AA}$$

Evaluate Formula

1.2) Lattice Constant of BCC Formula

Formula

$$a_{\text{BCC}} = \frac{4}{\sqrt{3}} \cdot r$$

Example with Units

$$3.1177 \text{ \AA} = \frac{4}{\sqrt{3}} \cdot 1.35 \text{ \AA}$$

Evaluate Formula

1.3) Total Volume of Atoms in BCC Formula

Formula

$$V_a = \frac{8}{3} \cdot \pi \cdot r^3$$

Example with Units

$$20.612 \text{ \AA}^3 = \frac{8}{3} \cdot 3.1416 \cdot 1.35 \text{ \AA}^3$$

Evaluate Formula

2) Face Centered Crystal Formulas

2.1) Atomic Radius in FCC Formula

Formula

$$r = \frac{a_{\text{FCC}}}{2 \cdot \sqrt{2}}$$

Example with Units

$$1.35 \text{ \AA} = \frac{3.818377 \text{ \AA}}{2 \cdot \sqrt{2}}$$

Evaluate Formula

2.2) Lattice Constant of FCC Formula

Formula

$$a_{\text{FCC}} = 2 \cdot \sqrt{2} \cdot r$$

Example with Units

$$3.8184 \text{ \AA} = 2 \cdot \sqrt{2} \cdot 1.35 \text{ \AA}$$

Evaluate Formula

2.3) Volume of Atoms in FCC Formula

Formula

$$V_a = \frac{16}{3} \cdot \pi \cdot r^3$$

Example with Units

$$41.224 \text{ \AA}^3 = \frac{16}{3} \cdot 3.1416 \cdot 1.35 \text{ \AA}^3$$

Evaluate Formula



3) Gibbs Phase Rule Formulas

3.1) Degree of Freedom Formula

Formula

$$F = C - p + 2$$

Example

$$5 = 7 - 4 + 2$$

Evaluate Formula 

3.2) Number of Components Formula

Formula

$$C = F + p - 2$$

Example

$$7 = 5 + 4 - 2$$

Evaluate Formula 

3.3) Number of Phases Formula

Formula

$$p = C - F + 2$$

Example

$$4 = 7 - 5 + 2$$

Evaluate Formula 

3.4) Total Number of Variables in System Formula

Formula

$$T_v = p \cdot (C - 1) + 2$$

Example

$$26 = 4 \cdot (7 - 1) + 2$$

Evaluate Formula 

4) Simple Cubic Cell Formulas

4.1) Atomic Radius in SCC Formula

Formula

$$r = \frac{a}{2}$$

Example with Units

$$1.35 \text{ \AA} = \frac{2.7 \text{ \AA}}{2}$$

Evaluate Formula 

4.2) Lattice Constant of SCC Formula

Formula

$$a = 2 \cdot r$$

Example with Units

$$2.7 \text{ \AA} = 2 \cdot 1.35 \text{ \AA}$$

Evaluate Formula 

4.3) Total Volume of Atoms in SCC Formula

Formula

$$V_a = \frac{4}{3} \cdot \pi \cdot r^3$$

Example with Units

$$10.306 \text{ \AA}^3 = \frac{4}{3} \cdot 3.1416 \cdot 1.35 \text{ \AA}^3$$

Evaluate Formula 



Variables used in list of Crystallography Formulas above

- **a** Lattice Parameter (Angstrom)
- **a_{BCC}** Lattice Parameter of BCC (Angstrom)
- **a_{FCC}** Lattice Parameter of FCC (Angstrom)
- **C** Number of Components in System
- **F** Degree of Freedom
- **p** Number of Phases
- **r** Atomic Radius (Angstrom)
- **T_v** Total Number of Variables in System
- **V_a** Volume of Atoms in Unit Cell (Cubic Angstrom)

Constants, Functions, Measurements used in list of Crystallography Formulas above

- **constant(s):** **pi**,
3.14159265358979323846264338327950288
Archimedes' constant
- **Functions:** **sqrt**, sqrt(Number)
A square root function is a function that takes a non-negative number as an input and returns the square root of the given input number.
- **Measurement: Length** in Angstrom (A)
Length Unit Conversion 
- **Measurement: Volume** in Cubic Angstrom (A³)
Volume Unit Conversion 



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