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# Crystallography Formulas

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# List of 14 Crystallography Formulas

## Crystallography

### 1) Atomic Packing Factor

$$\text{fx } APF = \frac{V_{\text{atoms}}}{V_{\text{unit cell}}}$$

[Open Calculator !\[\]\(a870788d6ed9b8fd294b7654a8c8526b\_img.jpg\)](#)

$$\text{ex } 0.552381 = \frac{58A^3}{105A^3}$$

## Body Centered Cubic

### 2) Atomic Radius in BCC

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

[Open Calculator !\[\]\(6a9b39b98eb945faa14c645ec99e4eaa\_img.jpg\)](#)

$$\text{ex } 1.35966A = \frac{\sqrt{3}}{4} \cdot 3.14A$$

### 3) Lattice Constant of BCC

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

[Open Calculator !\[\]\(f1c5da15572e3e09d343161be98f508d\_img.jpg\)](#)

$$\text{ex } 2.863657A = \frac{4}{\sqrt{3}} \cdot 1.24A$$




4) Total Volume of Atoms in BCC 

$$\text{fx } V_{\text{atoms}} = \frac{8}{3} \cdot \pi \cdot r^3$$

Open Calculator 

$$\text{ex } 15.9729\text{\AA}^3 = \frac{8}{3} \cdot \pi \cdot (1.24\text{\AA})^3$$

Face Centered Crystal 5) Atomic Radius in FCC 

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

Open Calculator 

$$\text{ex } 1.237437\text{\AA} = \frac{3.5\text{\AA}}{2 \cdot \sqrt{2}}$$

6) Lattice Constant of FCC 

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

Open Calculator 

$$\text{ex } 3.50725\text{\AA} = 2 \cdot \sqrt{2} \cdot 1.24\text{\AA}$$

7) Volume of Atoms in FCC 

$$\text{fx } V_{\text{atoms}} = \frac{16}{3} \cdot \pi \cdot r^3$$

Open Calculator 

$$\text{ex } 31.94579\text{\AA}^3 = \frac{16}{3} \cdot \pi \cdot (1.24\text{\AA})^3$$



## Gibbs Phase Rule

### 8) Degree of Freedom

$$f_x F = C - P + 2$$

[Open Calculator !\[\]\(23d9fc146e83b5c3013cfa32c784f8d5\_img.jpg\)](#)

$$ex \quad 5 = 5 - 2 + 2$$

### 9) Number of Components

$$f_x C = F + P - 2$$

[Open Calculator !\[\]\(aa53ad6fea213b8b2226d3077e30533a\_img.jpg\)](#)

$$ex \quad 3 = 3 + 2 - 2$$

### 10) Number of Phases

$$f_x P = C - F + 2$$

[Open Calculator !\[\]\(626ce8ac21792b9405bfddfea8e0c96a\_img.jpg\)](#)

$$ex \quad 4 = 5 - 3 + 2$$

### 11) Total Number of Variables in System

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

[Open Calculator !\[\]\(c1168d6a8b365d11e842ece304635fa7\_img.jpg\)](#)

$$ex \quad 10 = 2 \cdot (5 - 1) + 2$$



## Simple Cubic Cell

### 12) Atomic Radius in SCC

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

[Open Calculator !\[\]\(74d4806277d7e73349d8e8c0897931e9\_img.jpg\)](#)

$$\text{ex } 1.25\text{\AA} = \frac{2.5\text{\AA}}{2}$$

### 13) Lattice Constant of SCC

$$\text{fx } a = 2 \cdot r$$

[Open Calculator !\[\]\(8bba887393ca45b761e5cb49e755e762\_img.jpg\)](#)

$$\text{ex } 2.48\text{\AA} = 2 \cdot 1.24\text{\AA}$$

### 14) Total Volume of Atoms in SCC

$$\text{fx } V_{\text{atoms}} = \frac{4}{3} \cdot \pi \cdot r^3$$

[Open Calculator !\[\]\(0fb13ad0bfa3d86868cdd3883e5665b3\_img.jpg\)](#)

$$\text{ex } 7.986448\text{\AA}^3 = \frac{4}{3} \cdot \pi \cdot (1.24\text{\AA})^3$$





## Variables Used

- **a** Lattice Parameter (*Angstrom*)
- **a<sub>BCC</sub>** Lattice Parameter of BCC (*Angstrom*)
- **a<sub>FCC</sub>** Lattice Parameter of FCC (*Angstrom*)
- **APF** Atomic Packing Factor
- **C** Number of Components in System
- **F** Degree of Freedom
- **P** Number of Phases
- **r** Atomic Radius (*Angstrom*)
- **T<sub>v</sub>** Total Number of Variables in System
- **V<sub>atoms</sub>** Volume of Atoms in Unit Cell (*Cubic Angstrom*)
- **V<sub>unit cell</sub>** Volume of Unit Cell (*Cubic Angstrom*)



## Constants, Functions, Measurements used

- **Constant:** **pi**, 3.14159265358979323846264338327950288  
*Archimedes' constant*
- **Function:** **sqrt**, sqrt(Number)  
*Square root function*
- **Measurement:** **Length** in Angstrom (A)  
*Length Unit Conversion* 
- **Measurement:** **Volume** in Cubic Angstrom (A<sup>3</sup>)  
*Volume Unit Conversion* 



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- [Basics Formulas](#) 
- [Crystallography Formulas](#) 
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