

Appendix B

Calculation of unit cell volume

The equations of calculation of the unit cell volume depend on crystal system :

Crystal system	Equation
Cubic	$V = a^3$
Tetragonal	$V = a^2 c$
Orthorhombic	$V = abc$
Hexagonal	$V = 0.866a^2 c$
Monoclinic	$V = abc \sin\beta$
Triclinic	$V = abc (1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2\cos\alpha \cdot \cos\beta \cdot \cos\gamma)^{1/2}$

Calculation of number of molecules per unit cell (Z)

$$Z = \frac{D \times V \times N}{Fw}$$

D = Density of crystal (g/cm^3)

V = Volume of unit cell (cm^3)

N = Avogadro number ($6.02 \times 10^{23} \text{ mol}^{-1}$)

Fw = Formula weight