

Hexagonal:

$$\cos \rho = \frac{h_1 h_2 + k_1 k_2 + \frac{1}{2}(h_1 k_2 + h_2 k_1) + (3a^2/4c^2)l_1 l_2}{\sqrt{\{[h_1^2 + k_1^2 + h_1 k_1 + (3a^2/4c^2)l_1^2][h_2^2 + k_2^2 + h_2 k_2 + (3a^2/4c^2)l_2^2]\}}}$$

Rhombohedral:

$$\cos \rho = (a^4 d_1 d_2 / V^2) [\sin^2 \alpha (h_1 h_2 + k_1 k_2 + l_1 l_2) + (\cos^2 \alpha - \cos \alpha)(k_1 l_2 + k_2 l_1 + l_1 h_2 + l_2 h_1 + h_1 k_2 + h_2 k_1)].$$

Monoclinic:

$$\cos \rho = \frac{d_1 d_2}{\sin^2 \beta} \left[ \frac{h_1 h_2}{a^2} + \frac{k_1 k_2 \sin^2 \beta}{b^2} + \frac{l_1 l_2}{c^2} - \frac{(l_1 h_2 + l_2 h_1) \cos \beta}{ac} \right].$$

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### A4.3 Volumes of unit cells

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Orthorhombic:

$$V = abc.$$

(Tetragonal:  $a = b$ ; cubic:  $a = b = c$ .)

Hexagonal:

$$V = \sqrt{3} a^2 c / 2 = 0.866 a^2 c.$$

Rhombohedral:

$$V = a^3 \sqrt{1 - 3 \cos^2 \alpha + 2 \cos^3 \alpha}.$$

Monoclinic:

$$V = abc \sin \beta.$$