

$$\mathbf{a} = (1/V^*)(\mathbf{b}^* \times \mathbf{c}^*) \quad (13-77a)$$

$$\mathbf{b} = (1/V^*)(\mathbf{c}^* \times \mathbf{a}^*) \quad (13-77b)$$

$$\mathbf{c} = (1/V^*)(\mathbf{a}^* \times \mathbf{b}^*) \quad (13-77c)$$

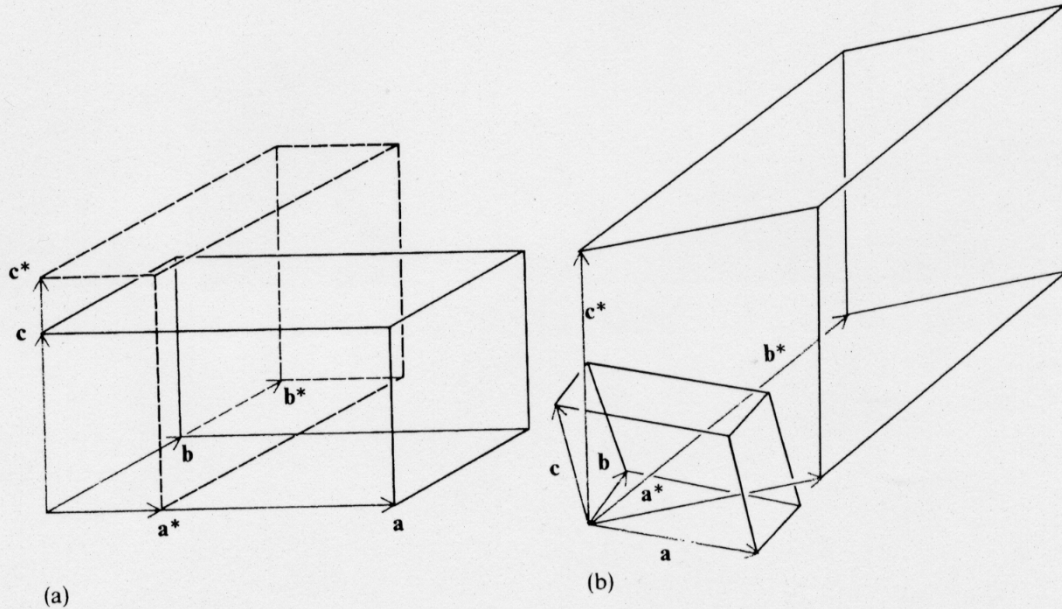


Figure 13-22

Comparisons of direct and reciprocal unit cells. (a) For an orthorhombic crystal. (b) For a triclinic crystal. [After G. H. Stout and L. M. Jensen, *X-Ray Structure Determination* (New York: Macmillan, 1968).]

Relations between the dimensions of the direct and reciprocal cells

Angular parameters

Linear parameters

$$\cos \alpha^* = \frac{\cos \beta \cos \gamma - \cos \alpha}{\sin \beta \sin \gamma}$$

$$a^* = \frac{bc \sin \alpha}{V}$$

$$\cos \beta^* = \frac{\cos \gamma \cos \alpha - \cos \beta}{\sin \gamma \sin \alpha}$$

$$b^* = \frac{ca \sin \beta}{V}$$

$$\cos \gamma^* = \frac{\cos \alpha \cos \beta - \cos \gamma}{\sin \alpha \sin \beta}$$

$$c^* = \frac{ab \sin \gamma}{V}$$

$$\cos \alpha = \frac{\cos \beta^* \cos \gamma^* - \cos \alpha^*}{\sin \beta^* \sin \gamma^*}$$

$$a = \frac{b^*c^* \sin \alpha^*}{V^*}$$

$$\cos \beta = \frac{\cos \gamma^* \cos \alpha^* - \cos \beta^*}{\sin \gamma^* \sin \alpha^*}$$

$$b = \frac{c^*a^* \sin \beta^*}{V^*}$$

$$\cos \gamma = \frac{\cos \alpha^* \cos \beta^* - \cos \gamma^*}{\sin \alpha^* \sin \beta^*}$$

$$c = \frac{a^*b^* \sin \gamma^*}{V^*}$$

Volume

$$V^* = a^*b^*c^* \sqrt{1 - \cos^2 \alpha^* - \cos^2 \beta^* - \cos^2 \gamma^* + 2 \cos \alpha^* \cos \beta^* \cos \gamma^*}$$

$$V = abc \sqrt{1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma}$$