1.45: Flack parameter

The Flack parameter is the molar fraction x in the defining equation $C = (1-x)X + x\bar{X}$, where C represents an oriented two-domain-structure crystal, twinned by inversion, consisting of an oriented domain structure X and an oriented inverted domain structure $\bar{X}$. In reciprocal space, the Flack parameter x is defined by the structure-amplitude equation

$$G^2(h,k,l,x) = (1-x)|F(h,k,l)|^2 + x|F(\bar{h},\bar{k},\bar{l})|^2 .$$

For a multidomain-structure twin of a chiral crystal structure, an equivalent Flack parameter may be calculated according to the method of Flack and Bernardinelli (1999).