8.3. CONSTRAINTS AND RESTRAINTS IN REFINEMENT

Table 8.3.1.1. *Symmetry conditions for second-cumulant tensors*

If more than one condition is applicable for a space group, the site is identified by its Wyckoff notation following the space-group symbol. The stated conditions are valid only for the first equipoint listed for the position. For space groups with alternative choices of origin, the option with a centre of symmetry has been selected.

(*A*) Monoclinic

(1) Site symmetry m, 2, $2/m$ – four independent elements

(a) $\beta_{12} = \beta_{23} = 0$; one principal axis parallel to [010]
All groups with unique axis b

(b) $\beta_{13} = \beta_{23} = 0$; one principal axis parallel to [001]
All groups with unique axis c

(*B*) Orthorhombic

(1) Site symmetry m, 2, $2/m$ – four independent elements

(a) $\beta_{12} = \beta_{13} = 0$; one principal axis parallel to [100]
*P*222(i,j,k,l), *P*222$_1$(a,b), *C*222$_1$(a), *C*222(e,f), *F*222(e,j), *I*222(e,f), *I*2$_1$2$_1$2$_1$(a), *Pmm*2(g,h), *Pmc*2$_1$, *Pma*2(c), *Pmn*2$_1$, *Cmm*2(e), *Cmc*2$_1$, *Amm*2(d,e), *Ama*2(b), *Fmm*2(c), *Imm*2(d), *Ima*2(b), *Pmmm*(u,v), *Pnnn*(g,h), *Pccm*(i,j), *Pban*(g,h), *Pmma*(k), *Pnna*(d), *Pmna*(a,b,c,d,e,f,h), *Pbcm*(c), *Pmmn*(e), *Cmcm*(a,b,e,f), *Cmca*(a,b,d,f), *Cmmm*(n), *Cccm*(g), *Cmma*(c,d,h,i,m), *Ccca*(e), *Fmmm*(c,l,m), *Fddd*(e), *Immm*(l), *Ibam*(f), *Ibca*(c), *Imma*(a,b,f,h)

(b) $\beta_{12} = \beta_{23} = 0$; one principal axis parallel to [010]
*P*222(m,n,o,p), *P*222$_1$(c,d), *C*222$_1$(b), *C*222(g,h), *F*222(f,i), *I*222(g,h), *I*2$_1$2$_1$2$_1$(b), *Pmm*2(e,f), *Cmm*2(d), *Amm*2(c), *Abm*2(c), *Fmm*2(d), *Imm*2(c), *Pmmm*(w,x), *Pnnn*(i,j), *Pccm*(k,l), *Pban*(i,j), *Pmma*(a,b,c,d,g,h,i,j), *Pmna*(g), *Pcca*(c), *Pmmm*(f), *Pbcn*, *Pnma*, *Cmca*(e), *Cmmm*(o), *Cccm*(h), *Cmma*(e,f,j,k,n), *Ccca*(f), *Fmmm*(d,k,n), *Fddd*(f), *Immm*(m), *Ibam*(g), *Ibca*(d), *Imma*(c,d,g,i)

(c) $\beta_{13} = \beta_{23} = 0$; one principal axis parallel to [001]
*P*222(q,r,s,t), *P*2$_1$2$_1$2, *C*222(i,j,k), *F*222(g,h), *I*222(i,j), *I*2$_1$2$_1$2$_1$(c), *Pcc*2, *Pma*2(a,b), *Pnc*2, *Pba*2, *Pnn*2, *Cmm*2(c), *Ccc*2, *Abm*2(a,b), *Ama*2(a), *Aba*2, *Fmm*2(b), *Fdd*2, *Iba*2, *Ima*2(a), *Pmmm*(y,z), *Pnnn*(k,l), *Pccm*(a,b,c,d,m,n,o,p,q), *Pban*(k,l), *Pnna*(c), *Pcca*(d,e), *Pbam*, *Pccn*, *Pbcm*(d), *Pnnm*, *Cmcm*(g), *Cmmm*(e,f,m,p,q), *Cccm*(c,d,e,f,i,j,k,l), *Cmma*(l), *Ccca*(g,h), *Fmmm*(e,j,o), *Fddd*(g), *Immm*(n), *Ibam*(c,d,h,i,j), *Ibca*(e)

(2) Site symmetry $mm2$, 222, mmm – three independent elements

(a) $\beta_{12} = \beta_{13} = \beta_{23} = 0$ principal axes parallel to crystal axes
All space groups

(*C*) Tetragonal

(1) Site symmetry m, 2, $2/m$ – four independent elements

(a) $\beta_{12} = \beta_{13} = 0$; one principal axis parallel to [100]
*P*422(l,m,n,o), *P*4$_2$22(j,k,l,m), *I*422(h,i), *I*4$_1$22(f), *I*4$_1$*md*, *P*$\bar{4}$2*m*(i,j,k,l), *P*$\bar{4}$2*c*(g,i), *I*$\bar{4}$2*m*(f,g), *I*$\bar{4}$2*d*(d), *P*4/*mcc*(k,l), *P*4/*nbm*(k,l), *P*4/*nnc*(i,j), *P*4/*nmm*(i), *P*4$_2$/*mmc*(o,p), *P*4$_2$/*mcm*(l,m), *P*4$_2$/*nbc*(h,i), *P*4$_2$/*nnm*(i,j), *P*4$_2$/*nmc*(g), *I*4/*mmm*(n), *I*4/*mcm*(j), *I*4$_1$/*amd*(c,d,f,h), *I*4$_1$/*acd*(e)

(b) $\beta_{12} = \beta_{23} = 0$; one principal axis parallel to [010]
*P*4$_1$22(a,b), *P*4$_3$22(a,b), *P*4*mm*(e,f), *P*4$_2$*mc*, *I*4*mm*(d), *P*$\bar{4}$2*c*(h,j), *P*$\bar{4}$*m*2(j,k), *I*$\bar{4}$*m*2(i), *P*4/*mmm*(s,t)

(c) $\beta_{13} = \beta_{23} = 0$; one principal axis parallel to [001]
*P*4, *P*4$_2$, *I*4, *I*4$_1$, *P*$\bar{4}$, *I*$\bar{4}$, *P*4/*m*, *P*4$_2$/*m*, *P*4/*n*, *P*4$_2$/*n*, *I*4/*m*, *I*4$_1$/*a*, *P*422(i), *P*42$_1$2(d), *P*4$_2$22(g,h,i), *P*4$_2$2$_1$2(c,d), *I*422(f), *I*4$_1$22(c), *P*4$_2$*cm*(c), *P*4$_2$*nm*(b), *P*4*cc*, *P*4*nc*, *P*4$_2$*bc*, *I*4$_1$*cd*, *P*$\bar{4}$2*m*(m), *P*$\bar{4}$2*c*(k,l,m), *P*$\bar{4}$2$_1$*m*(d), *P*$\bar{4}$21*c*, *P*$\bar{4}$*c*2(g,h,i), *P*$\bar{4}$*b*2(e,f), *P*$\bar{4}$*n*2(e,h), *I*$\bar{4}$*c*2(f,g), *I*$\bar{4}$2*m*(h), *I*$\bar{4}$2*d*(c), *P*4/*mmm*(p,q), *P*4/*mcc*(e,i,m), *P*4/*nnc*(g), *P*4/*mbm*(i,j), *P*4/*mnc*(c,f,h), *P*4/*ncc*(e), *P*42/*mmc*(q), *P*4$_2$/*mcm*(f,k,n), *P*4$_2$/*nbc*(f,g), *P*4$_2$/*nnm*(h), *P*4$_2$/*mbc*(a,c,e,f,h), *P*4$_2$/*mnm*(c,h,i), *P*4$_2$/*ncm*(f), *I*4/*mmm*(l), *I*4/*mcm*(k), *I*4$_1$/*acd*(d)

(d) $\beta_{11} = \beta_{22}$, $\beta_{13} = -\beta_{23}$ one principal axis parallel to [110]
*P*422(j,k), *P*42$_1$2(e,f), *P*4$_1$22(c), *P*4$_1$2$_1$2, *P*4$_2$22(n,o), *P*4$_2$2$_1$2(e,f), *P*4$_3$22(c), *P*4$_3$2$_1$2, *I*422(g,j), *I*4$_1$22(d), *P*$\bar{4}$*m*2(h,i), *P*$\bar{4}$*c*2(e,f), *P*$\bar{4}$*b*2(g,h), *P*$\bar{4}$*n*2(g), *I*$\bar{4}$*m*2(g,h), *I*$\bar{4}$*c*2(e,h), *P*4/*mcc*(j), *P*4/*nbm*(e,f,i,j,m), *P*4/*nnc*(h), *P*4/*mnc*(g), *P*4$_2$/*mmc*(n), *P*4$_2$/*nbc*(j), *P*4$_2$/*nnm*(e,f,k,l,m), *P*4$_2$/*mbc*(g), *I*4/*mmm*(k), *I*4/*mcm*(e,i), *I*4$_1$/*amd*(g), *I*4$_1$/*acd*(f)

(e) $\beta_{11} = \beta_{22}$, $\beta_{13} = \beta_{23}$; one principal axis parallel to [1$\bar{1}$0]
*I*4$_1$22(e), *P*4*mm*(d), *P*4*bm*, *P*4$_2$*cm*(d), *P*4$_2$*nm*(c), *I*4*mm*(c), *I*4*cm*, *P*$\bar{4}$2*m*(n), *P*$\bar{4}$2$_1$*m*(e), *P*$\bar{4}$*n*2(f), *I*$\bar{4}$2*m*(i), *P*4/*mmm*(r), *P*4/*mbm*(k), *P*4/*nmm*(d,e,g,h,j), *P*4/*ncc*(f), *P*4$_2$/*mcm*(o), *P*4$_2$/*mnm*(j), *P*4$_2$/*nmc*(f), *P*4$_2$/*ncm*(c,d,g,h,i), *I*4/*mmm*(f,m), *I*4/*mcm*(l)

(2) Site symmetry $mm2$, 222, mmm – three independent elements

(a) $\beta_{12} = \beta_{13} = \beta_{23} = 0$; principal axes parallel to crystal axes
*P*422, *P*4$_2$22(a,b,c,d), *I*422(c), *P*4*mm*, *P*4$_2$*mc*, *I*4*mm*, *I*4$_1$*md*, *P*$\bar{4}$2*m*(e,f), *P*$\bar{4}$2*c*, *P*$\bar{4}$*m*2, *I*$\bar{4}$*m*2, *I*$\bar{4}$2*m*(c), *P*4/*mmm*(e,f,i,l,m,n,o), *P*4/*mcc*, *P*4/*nnc*, *P*4/*nmm*, *P*4$_2$/*mmc*, *P*4$_2$/*mcm*(e), *P*4$_2$/*nbc*(a,b), *P*4$_2$/*nnm*(c), *P*4$_2$/*nmc*, *I*4/*mmm*(c,g,i,j), *I*4$_1$/*amd*

Table 8.3.1.1. *Symmetry conditions for second-cumulant tensors (cont.)*

(*C*) Tetragonal (*cont.*)

(*b*) $\beta_{11} = \beta_{22}$, $\beta_{13} = \beta_{23} = 0$; principal axes parallel to [110], [1$\bar{1}$0] and [001]
*P*42$_1$2, *P*4$_2$22(*e*,*f*), *P*4$_2$2$_1$2, *I*422(*d*), *I*4$_1$22, *P*4*bm*, *P*4$_2$*cm*, *P*4$_2$*nm*, *I*4*cm*, *P*$\bar{4}$2*m*(*g*, *h*), *P*$\bar{4}$2$_1$*m*, *P*$\bar{4}$*c*2, *P*$\bar{4}$*b*2, *P*$\bar{4}$*n*2, *I*$\bar{4}$*c*2, *I*$\bar{4}$2*m*(*e*), *P*4/*mmm*(*j*, *k*), *P*4/*nbm*, *P*4/*mbm*, *P*4/*mnc*, *P*4/*ncc*, *P*4$_2$/*mcm*(*a*, *c*, *g*, *h*, *i*, *j*), *P*4$_2$/*nbc*(*c*), *P*4$_2$/*nnm*(*d*, *g*), *P*4$_2$/*mbc*, *P*4$_2$/*mnm*, *P*4$_2$/*ncm*, *I*4/*mmm*(*h*), *I*4/*mcm*, *I*4$_1$/*acd*

(3) Site symmetry 4, $\bar{4}$, 4/*m*, 4*mm*, $\bar{4}$2*m*, 422, 4/*mmm* – two independent elements

(*a*) $\beta_{11} = \beta_{22}$, $\beta_{12} = \beta_{13} = \beta_{23} = 0$; uniaxial with unique axis parallel to [001]
All space groups

(*D*) Trigonal (hexagonal axes) and hexagonal

(1) Site symmetry *m*, 2, 2/*m* – four independent elements

(*a*) $\beta_{13} = \beta_{23} = 0$; one principal axis parallel to [001]
*P*6, *P*6$_2$, *P*6$_4$, *P*$\bar{6}$, *P*6/*m*, *P*6$_3$/*m*, *P*622(*i*), *P*6$_2$22(*e*,*f*), *P*6$_4$22(*e*,*f*), *P*6*cc*, *P*$\bar{6}$*m*2(*l*, *m*), *P*$\bar{6}$*c*2(*k*), *P*$\bar{6}$2*m*(*j*, *k*), *P*$\bar{6}$2*c*(*h*), *P*6/*mmm*(*p*, *q*), *P*6/*mcc*(*g*, *i*, *l*), *P*6$_3$/*mcm*(*j*), *P*6$_3$/*mmc*(*j*)

(*b*) $\beta_{11} = \beta_{22}$, $\beta_{13} = -\beta_{23}$ one principal axis parallel to [110]
*P*3*m*1, *R*3*m*, *P*$\bar{3}$*m*1(*i*), *R*$\bar{3}$*m*(*h*), *P*6*mm*(*e*), *P*6$_3$*mc*, *P*$\bar{6}$*m*2(*n*)

(*c*) $\beta_{11} = \beta_{22}$, $\beta_{13} = \beta_{23}$; one principal axis parallel to [2$\bar{1}$0]
*P*312, *P*3$_1$12, *P*3$_2$12, *P*$\bar{3}$1*m*(*i*, *j*), *P*$\bar{3}$1*c*, *P*622(*l*, *m*), *P*$\bar{6}$*c*2(*j*)

(*d*) $\beta_{22} = 2\beta_{12}$, $2\beta_{13} = \beta_{23}$; one principal axis parallel to [100]
*P*321, *P*3$_1$21, *P*3$_2$21, *R*32, *P*$\bar{3}$*m*1(*e*, *f*, *g*, *h*), *P*$\bar{3}$*c*1, *R*$\bar{3}$*m*(*d*, *e*, *f*, *g*), *R*$\bar{3}$*c*, *P*622(*j*, *k*), *P*6$_1$22(*a*), *P*6$_5$22(*a*), *P*6$_2$22(*g*, *h*), *P*6$_4$22(*g*, *h*), *P*6$_3$22(*g*), *P*$\bar{6}$2*c*(*g*), *P*6/*mmm*(*o*), *P*6/*mcc*(*j*), *P*6$_3$/*mmc*(*g*, *i*, *k*)

(*e*) $\beta_{22} = 2\beta_{12}$, $\beta_{23} = 0$; one principal axis parallel to [210]
*P*31*m*, *P*$\bar{3}$1*m*(*f*, *g*, *k*), *P*6$_1$22(*b*), *P*6$_5$22(*b*), *P*6$_2$22(*i*, *j*), *P*6$_4$22(*i*, *j*), *P*6$_3$22(*h*), *P*6*mm*(*d*), *P*6$_3$*cm*, *P*$\bar{6}$2*m*(*i*), *P*6/*mmm*(*n*), *P*6/*mcc*(*k*), *P*6$_3$/*mcm*(*f*, *i*, *k*)

(2) Site symmetry *mm*2, 222, *mmm* – three independent elements

(*a*) $\beta_{22} = 2\beta_{12}$, $\beta_{13} = \beta_{23} = 0$; principal axes parallel to [100] and [001]
*P*622, *P*6$_2$22, *P*6$_4$22, *P*6*mm*, *P*$\bar{6}$2*m*, *P*6/*mmm*, *P*6/*mcc*, *P*6$_3$/*mcm*, *P*6$_3$/*mmc*

(*b*) $\beta_{11} = \beta_{22}$, $\beta_{13} = \beta_{23} = 0$; principal axes parallel to [110], [2$\bar{1}$0] and [001]
P$\bar{6}$*m*2

(3) Site symmetry 3, $\bar{3}$, 3*m*, 32, $\bar{3}$*m*, $\bar{6}$, 6, 6/*m*, $\bar{6}$*m*2, 6*mm*, 622, 6/*mmm* – two independent elements

(*a*) $\beta_{11} = \beta_{22} = 2\beta_{12}$, $\beta_{13} = \beta_{23} = 0$; unique axis parallel to **c**
All space groups

(*E*) Cubic

(1) Site symmetry *m*, 2, 2/*m* – four independent elements

(*a*) $\beta_{12} = \beta_{13} = 0$; one principal axis parallel to [100]
*P*23, *F*23, *I*23, *I*2$_1$3, *Pm*$\bar{3}$, *Pn*$\bar{3}$, *Fm*$\bar{3}$, *Fd*$\bar{3}$, *Im*$\bar{3}$, *Ia*$\bar{3}$, *P*432(*h*), *P*4$_2$32(*h*, *i*, *j*), *F*432(*i*), *F*4$_1$32(*f*), *I*432(*g*), *I*4$_1$32(*f*), *P*$\bar{4}$3*m*(*h*), *I*$\bar{4}$3*m*(*f*), *P*$\bar{4}$3*n*, *F*$\bar{4}$3*c*, *I*$\bar{4}$3*d*, *Pm*$\bar{3}$*m*(*k*, *l*), *Pn*$\bar{3}$*n*(*g*), *Pm*$\bar{3}$*n*(*k*), *Pn*$\bar{3}$*m*(*h*), *Fm*$\bar{3}$*m*(*j*), *Fm*$\bar{3}$*c*(*i*), *Fd*$\bar{3}$*c*(*f*), *Im*$\bar{3}$*m*(*j*), *Ia*$\bar{3}$*d*(*f*)

(*b*) $\beta_{11} = \beta_{22}$, $\beta_{13} = \beta_{23}$; one principal axis parallel to [1$\bar{1}$0]
P$\bar{4}$3*m*(*i*), *F*$\bar{4}$3*m*, *I*$\bar{4}$3*m*(*g*), *Pm*$\bar{3}$*m*(*m*), *Pn*$\bar{3}$*m*(*k*), *Fm*$\bar{3}$*m*(*k*), *Fd*$\bar{3}$*m*(*g*), *Im*$\bar{3}$*m*(*k*)

(*c*) $\beta_{22} = \beta_{33}$, $\beta_{12} = -\beta_{13}$; one principal axis parallel to [011]
*P*432(*i*, *j*), *P*4$_2$32(*l*), *F*432(*g*, *h*), *I*432(*h*), *P*4$_1$32, *I*4$_1$32(*g*), *Pn*$\bar{3}$*n*(*h*), *Pm*$\bar{3}$*n*(*j*), *Pn*$\bar{3}$*m*(*j*), *Fm*$\bar{3}$*c*(*h*)

(*d*) $\beta_{22} = \beta_{33}$, $\beta_{12} = \beta_{13}$; one principal axis parallel to [01$\bar{1}$]
*P*4$_2$32(*k*), *F*4$_1$32(*g*), *I*432(*i*), *P*4$_3$32, *I*4$_1$32(*h*), *Pn*$\bar{3}$*m*(*i*), *Fd*$\bar{3}$*m*(*h*, *i*), *Fd*$\bar{3}$*c*(*g*), *Im*$\bar{3}$*m*(*i*), *Ia*$\bar{3}$*d*(*g*)

(2) Site symmetry *mm*2, 222, *mmm* – three independent elements

(*a*) $\beta_{12} = \beta_{13} = \beta_{23} = 0$; principal axes parallel to crystal axes
*P*23, *I*23, *Pm*$\bar{3}$, *Pn*$\bar{3}$, *Fm*$\bar{3}$, *Im*$\bar{3}$, *P*4$_2$32(*d*), *P*$\bar{4}$3*n*, *Pm*$\bar{3}$*m*(*h*), *Pm*$\bar{3}$*n*, *Fm*$\bar{3}$*c*, *Im*$\bar{3}$*m*(*g*)

(*b*) $\beta_{22} = \beta_{33}$, $\beta_{12} = \beta_{13} = 0$; principal axes parallel to [011], [01$\bar{1}$] and [100]
*P*4$_2$32(*e*,*f*), *F*432, *I*432, *I*4$_1$32, *P*$\bar{4}$3*m*, *F*$\bar{4}$3*m*, *I*$\bar{4}$3*m*, *Pm*$\bar{3}$*m*(*i*, *j*), *Pn*$\bar{3}$*m*, *Fm*$\bar{3}$*m*, *Fd*$\bar{3}$*m*, *Im*$\bar{3}$*m*(*h*), *Ia*$\bar{3}$*d*

(3) Site symmetry 3, $\bar{3}$, 3*m*, 32, $\bar{3}$*m*, $\bar{6}$, 6, 6/*m*, $\bar{6}$*m*2, 6*mm*, 622, 6/*mmm* – two independent elements

(*a*) $\beta_{11} = \beta_{22} = \beta_{33}$, $\beta_{12} = \beta_{13} = \beta_{23}$; unique axis parallel to [111]
All space groups

(4) Site symmetry 4, $\bar{4}$, 4/*m*, 4*mm*, $\bar{4}$2*m*, 422, 4/*mmm* – two independent elements

(*a*) $\beta_{22} = \beta_{33}$, $\beta_{12} = \beta_{13} = \beta_{23} = 0$; uniaxial with unique axis parallel to [100]
All space groups

(5) Site symmetry 23, *m*3, $\bar{4}$3*m*, 432, *m*3*m* – one independent element

(*a*) $\beta_{11} = \beta_{22} = \beta_{33}$, $\beta_{12} = \beta_{13} = \beta_{23} = 0$; isotropic
All space groups

references