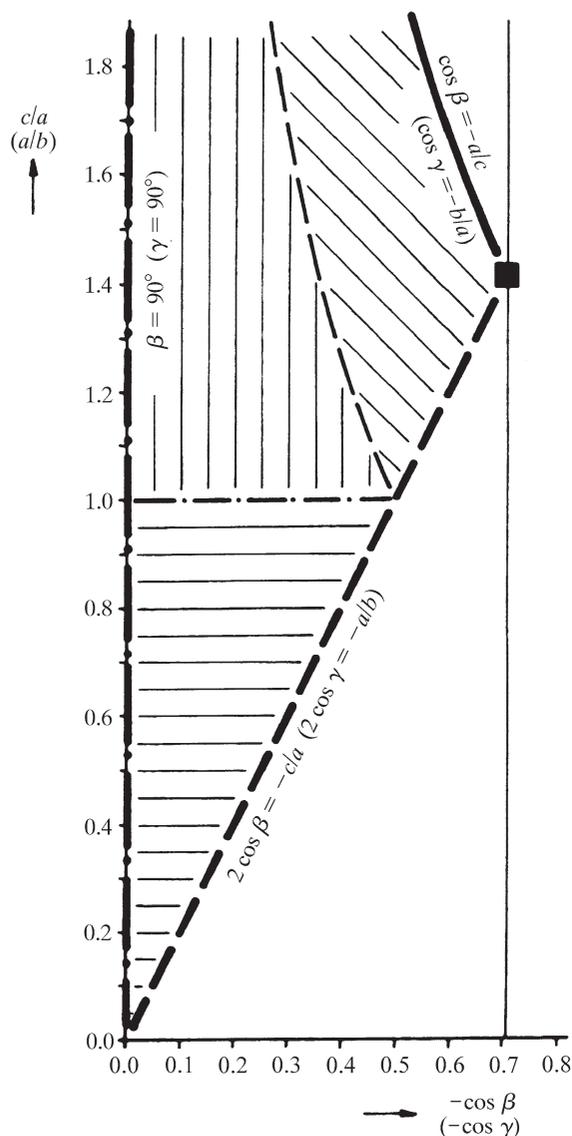


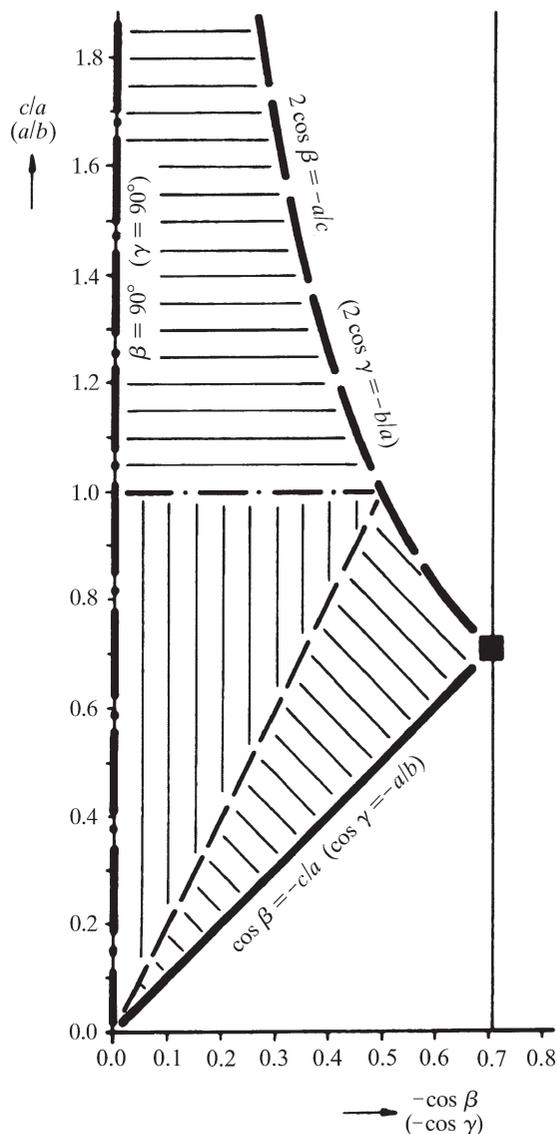
## 3. ADVANCED TOPICS ON SPACE-GROUP SYMMETRY

**Figure 3.5.2.3**

Parameter range for space groups of types  $C2$ ,  $Pc$ ,  $Cm$ ,  $Cc$ ,  $C2/m$ ,  $P2/c$ ,  $P2_1/c$  and  $C2/c$ :

- unique axis  $b$ , cell choice 1:  $P1c1$ ,  $P12/c1$ ,  $P12_1/c1$ ;
- unique axis  $b$ , cell choice 2:  $A121$ ,  $A1m1$ ,  $A1n1$ ,  $A12/m1$ ,  $A12/n1$ ;
- unique axis  $c$ , cell choice 1:  $P11a$ ,  $P112/a$ ,  $P112_1/a$ ;
- unique axis  $c$ , cell choice 2:  $B112$ ,  $B11m$ ,  $B11n$ ,  $B112/m$ ,  $B112/n$ .

The information in parentheses refers to unique axis  $c$ .

**Figure 3.5.2.4**

Parameter range for space groups of types  $C2$ ,  $Pc$ ,  $Cm$ ,  $Cc$ ,  $C2/m$ ,  $P2/c$ ,  $P2_1/c$  and  $C2/c$ :

- unique axis  $b$ , cell choice 1:  $C121$ ,  $C1m1$ ,  $C1c1$ ,  $C12/m1$ ,  $C12/c1$ ;
- unique axis  $b$ , cell choice 3:  $P1a1$ ,  $P12/a1$ ,  $P12_1/a1$ ,  $C12/c1$ ;
- unique axis  $c$ , cell choice 1:  $A112$ ,  $A11m$ ,  $A11a$ ,  $A112/m$ ,  $A112/a$ ;
- unique axis  $c$ , cell choice 3:  $P11b$ ,  $P112/b$ ,  $P112_1/b$ ,  $A112/a$ .

The information in parentheses refers to unique axis  $c$ .

section and gives rise to a symmetry enhancement of the respective Euclidean normalizer.

For each of the other eight types of monoclinic space groups, *i.e.*  $C2$ ,  $Pc$ ,  $Cm$ ,  $Cc$ ,  $C2/m$ ,  $P2/c$ ,  $P2_1/c$  and  $C2/c$ , and for each setting three possibilities of cell choice are listed in Chapter 2.3, which can be distinguished by different space-group symbols (example:  $C12/m1$ ,  $A12/m1$ ,  $I12/m1$ ,  $A112/m$ ,  $B112/m$ ,  $I112/m$ ). For each setting, there exist two ways to choose a suitable range for the metrical parameters such that each group corresponds to exactly one point:

- (i) One arbitrarily restricts oneself to cell choice 1, 2 or 3. Then, the suitable parameter range (displayed in one of the Figs. 3.5.2.2, 3.5.2.3 or 3.5.2.4) is larger than the range shown in Fig. 3.5.2.1 because, in contrast to the space-group types discussed above, some of the possible metrical specializations do not give rise to any symmetry enhancement of the Euclidean normalizers. These special metrical cases refer to the light lines subdividing the parameter regions of Figs. 3.5.2.2 to

3.5.2.4. Again, all inner points of these regions correspond to space groups with Euclidean normalizers without enhanced symmetry, and all points on the heavy-line boundaries refer to space groups, the Euclidean normalizers of which show symmetry enhancement.

- (ii) For all types of monoclinic space groups, one regards only the small parameter region shown in Fig. 3.5.2.1, but in return takes into consideration all three possibilities for the cell choice. Then, however, not all boundaries of this small parameter region correspond to Euclidean normalizers with enhanced symmetry. (Similar considerations are true for oblique plane groups.)

For triclinic space groups, five metrical parameters are necessary and, therefore, it is impossible to describe the special metrical cases in an analogous way.

In general, between a space group (or plane group)  $\mathcal{G}$  and its Euclidean normalizer  $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ , two uniquely defined intermediate groups  $\mathcal{K}(\mathcal{G})$  and  $\mathcal{L}(\mathcal{G})$  exist, such that