

1.3. TWINNING

Table 1.3.4.1. Possible twin operations for twins by merohedry *m* is the index of the point group in the corresponding holohedry; point groups allowing twins of type 2 are marked by an asterisk.

| Holohedry     | Bravais lattice       | Point group  | <i>m</i>  | Possible twin operations   |
|---------------|-----------------------|--|---|--|
| 1             | <i>aP</i>             | 1  | 2   | $\bar{1}$  |
| 2/ <i>m</i>   | <i>mP, mS</i>         | 2<br><i>m</i>  | 2<br>2  | $\bar{1}$<br>$\bar{1}$   |
| <i>mmm</i>    | <i>oP, oS, oI, oF</i> | 222<br><i>mm2</i>  | 2<br>2  | $\bar{1}$<br>$\bar{1}$   |
| 4/ <i>mmm</i> | <i>tP, tI</i>         | *4<br>*4<br>*4/ <i>m</i><br>422<br>4 <i>mm</i><br>42 <i>m</i> / $\bar{4}m2$  | 4<br>4<br>2<br>2<br>2<br>2                          | $\bar{1}, .m., .2.$<br>$\bar{1}, .m., .2.$<br><i>.m.</i><br>$\bar{1}$<br>$\bar{1}$<br>$\bar{1}$  |
| $\bar{3}m$    | <i>hR</i>             | *3<br>*3<br>32<br>3 <i>m</i>   | 4<br>2<br>2<br>2                                    | $\bar{1}, .m., .2$<br><i>.m</i><br>$\bar{1}$<br>$\bar{1}$  |
| 6/ <i>mmm</i> | <i>hP</i>             | *3<br>*3<br>*321/312<br>*3 <i>m</i> 1/31 <i>m</i><br>*3 <i>m</i> 1/ $\bar{3}1m$<br>*6<br>*6<br>*6/ <i>m</i><br>622<br>6 <i>mm</i><br>62 <i>m</i> / $\bar{6}m2$ | 8<br>4<br>4<br>4<br>2<br>4<br>4<br>2<br>2<br>2<br>2 | $\bar{1}, .m., .2., .m., .m., .2., .2$<br><i>.m., .m., .m</i><br>$\bar{1}, .m., .2/.2.$<br>$\bar{1}, .m., .m/.m.$<br><i>m.</i><br>$\bar{1}, .m., .2.$<br>$\bar{1}, .m., .m$<br><i>.m.</i><br>$\bar{1}$<br>$\bar{1}$<br>$\bar{1}$ |
| $m\bar{3}m$   | <i>cP, cI, cF</i>     | *23<br>* $\bar{m}\bar{3}$<br>432<br>43 <i>m</i>  | 4<br>2<br>2<br>2                                    | $\bar{1}, .m., .2$<br><i>.m</i><br>$\bar{1}$<br>$\bar{1}$  |

holohedry. Column 5 shows *m* – 1 possible twin operations referring to the different twin components. These twin operations are not uniquely defined (except for point group 1), but may be chosen arbitrarily from the corresponding right coset of the crystal point group in its holohedry. It is always possible, however, to choose an inversion, a reflection, or a twofold rotation as twin operation.

A twin that is not a twin by merohedry as defined above but, because of metrical specialization, has a twin lattice with twin index 1 is called a twin by pseudo-merohedry.

Two kinds of twins by merohedry may be distinguished.

Type 1: The twin can be described as an inversion twin. Then, only two twin components exist and the twin operation belongs to the Laue class of the crystal. As a consequence, the reciprocal lattices of the twin components are superimposed so that coinciding lattice points refer to Bragg reflections with the same  $|F|^2$  values as long as Friedel's law is valid. In that case, no differences with respect to symmetry, or to reflection conditions, or to relative intensities occur between two sets of Bragg

Table 1.3.4.2. Simulated Laue classes, extinction symbols, simulated 'possible space groups', and possible true space groups for crystals twinned by merohedry (type 2)

| Twinned crystal      |  |  | Single crystal  |
|----------------------|--|--|---|
| Simulated Laue class | Twin extinction symbol   | Simulated 'possible space groups'  | Possible true space groups  |
| 4/ <i>mmm</i>        | <i>P</i> ---<br><i>P</i> <sub>2</sub> --<br><i>P</i> <sub>4</sub> --<br><i>P</i> <i>n</i> --<br><i>P</i> <sub>4</sub> / <i>n</i> --<br><i>I</i> ---  | <i>P</i> 422, <i>P</i> 4 <i>mm</i> , <i>P</i> $\bar{4}2m$ ,<br><i>P</i> $\bar{4}m2$ , <i>P</i> 4/ <i>mmm</i><br><i>P</i> <sub>4</sub> 222<br><i>P</i> <sub>4</sub> 122, <i>P</i> <sub>4</sub> 322<br><i>P</i> 4/ <i>nmm</i><br>-<br><i>I</i> 422, <i>I</i> 4 <i>mm</i> , <i>I</i> $\bar{4}2m$ ,<br><i>I</i> $\bar{4}m2$ , <i>I</i> 4/ <i>mmm</i><br><i>I</i> 4122<br>- | <i>P</i> 4, <i>P</i> $\bar{4}$ , <i>P</i> 4/ <i>m</i><br><i>P</i> <sub>4</sub> 2, <i>P</i> <sub>4</sub> 2/ <i>m</i><br><i>P</i> <sub>4</sub> 1, <i>P</i> <sub>4</sub> 3<br><i>P</i> 4/ <i>n</i><br><i>P</i> <sub>4</sub> 2/ <i>n</i><br><i>I</i> 4, <i>I</i> $\bar{4}$ , <i>I</i> 4/ <i>m</i><br><i>I</i> 4 <sub>1</sub><br><i>I</i> 4 <sub>1</sub> / <i>a</i>  |
| $\bar{3}m1$          | <i>P</i> ---<br><i>P</i> <sub>3</sub> --   | <i>P</i> 321, <i>P</i> 3 <i>m</i> 1, <i>P</i> $\bar{3}m1$<br><i>P</i> <sub>3</sub> 121, <i>P</i> <sub>3</sub> 221  | <i>P</i> 3, <i>P</i> $\bar{3}$<br><i>P</i> <sub>3</sub> 1, <i>P</i> <sub>3</sub> 2  |
| $\bar{3}1m$          | <i>P</i> ---<br><i>P</i> <sub>3</sub> --   | <i>P</i> 312, <i>P</i> 31 <i>m</i> , <i>P</i> $\bar{3}1m$<br><i>P</i> <sub>3</sub> 112, <i>P</i> <sub>3</sub> 212  | <i>P</i> 3, <i>P</i> $\bar{3}$<br><i>P</i> <sub>3</sub> 1, <i>P</i> <sub>3</sub> 2  |
| $\bar{3}m$           | <i>R</i> --  | <i>R</i> 32, <i>R</i> 3 <i>m</i> , <i>R</i> $\bar{3}m$   | <i>R</i> 3, <i>R</i> $\bar{3}$  |
| 6/ <i>m</i>          | <i>P</i> ---<br><i>P</i> <sub>6</sub> --   | <i>P</i> 6, <i>P</i> $\bar{6}$ , <i>P</i> 6/ <i>m</i><br><i>P</i> <sub>6</sub> 2, <i>P</i> <sub>6</sub> 4  | <i>P</i> 3, <i>P</i> $\bar{3}$<br><i>P</i> <sub>3</sub> 1, <i>P</i> <sub>3</sub> 2  |
| 6/ <i>mmm</i>        | <i>P</i> ---<br><i>P</i> <sub>6</sub> 3--<br><i>P</i> <sub>6</sub> 2--   | <i>P</i> 622, <i>P</i> 6 <i>mm</i> , <i>P</i> $\bar{6}m2$ ,<br><i>P</i> $\bar{6}2m$ , <i>P</i> 6/ <i>mmm</i><br><br><i>P</i> 6 <sub>3</sub> 22<br><i>P</i> 6 <sub>2</sub> 22, <i>P</i> 6 <sub>4</sub> 22   | <i>P</i> 3, <i>P</i> $\bar{3}$ , <i>P</i> 321,<br><i>P</i> 312, <i>P</i> 3 <i>m</i> 1,<br><i>P</i> 31 <i>m</i> , <i>P</i> $\bar{3}m1$ ,<br><i>P</i> $\bar{3}1m$ , <i>P</i> 6, <i>P</i> $\bar{6}$ ,<br><i>P</i> 6/ <i>m</i><br><i>P</i> 6 <sub>3</sub> , <i>P</i> 6 <sub>3</sub> / <i>m</i><br><i>P</i> <sub>3</sub> 1, <i>P</i> <sub>3</sub> 2,<br><i>P</i> <sub>3</sub> 121, <i>P</i> <sub>3</sub> 221,<br><i>P</i> <sub>3</sub> 12, <i>P</i> <sub>3</sub> 212,<br><i>P</i> 6 <sub>2</sub> , <i>P</i> 6 <sub>4</sub><br><i>P</i> 6 <sub>1</sub> , <i>P</i> 6 <sub>5</sub><br><i>P</i> 31 <i>c</i> , <i>P</i> $\bar{3}1c$ |
| $m\bar{3}m$          | <i>P</i> ---<br><i>P</i> <sub>4</sub> 2--<br><i>P</i> <i>n</i> --<br><i>I</i> ---<br><i>I</i> <i>a</i> --<br><i>F</i> ---<br><i>F</i> <i>d</i> --<br><i>P</i> <sub>2</sub> 1/ <i>a, b</i> -- | <i>P</i> 432, <i>P</i> $\bar{4}3m$ , <i>P</i> $m\bar{3}m$<br><i>P</i> 4 <sub>3</sub> 32<br><i>P</i> <i>n</i> $\bar{3}m$<br><i>I</i> 432, <i>I</i> 43 <i>m</i> , <i>I</i> $m\bar{3}m$<br>-<br><i>F</i> 432, <i>F</i> $\bar{4}3m$ , <i>F</i> $m\bar{3}m$<br><i>F</i> $d\bar{3}m$<br>-  | <i>P</i> 23, <i>P</i> $m\bar{3}$<br><i>P</i> 2 <sub>1</sub> 3<br><i>P</i> <i>n</i> $\bar{3}$<br><i>I</i> 23, <i>I</i> 2 <sub>1</sub> 3, <i>I</i> $m\bar{3}$<br><i>I</i> $a\bar{3}$<br><i>F</i> 23, <i>F</i> $m\bar{3}$<br><i>F</i> $d\bar{3}$<br><i>P</i> $a\bar{3}$  |

intensities measured from a single crystal on the one hand and from a twin on the other hand (whether or not the twin components differ in their volumes). If anomalous scattering is observed and the twin components differ in size, the intensities of Bragg reflections are changed in comparison with the untwinned crystal but the symmetry of the diffraction pattern is unchanged. For equal volumes of the twin components, however, the diffraction pattern is centrosymmetric again. The occurrence of anomalous scattering does not produce additional difficulties for space-group determination. The change of the