

1. INTRODUCTION TO SPACE-GROUP SYMMETRY

**Table 1.6.4.16**

Reflection conditions and possible space groups with Bravais lattice  $tI$  and Laue class  $4/mmm$ ;  $hk$  are permutable; Patterson symmetry  $I4/mmm$

| Reflection conditions |        |        |            |        |       |            | Space group             | No. | Space group  | No. | Space group  | No. |
|-----------------------|--------|--------|------------|--------|-------|------------|-------------------------|-----|--------------|-----|--------------|-----|
| $hkl$                 | $hk0$  | $0kl$  | $h \pm hl$ | $00l$  | $h00$ | $h \pm h0$ |                         |     |              |     |              |     |
| $h+k+l$               | $h+k$  | $k+l$  | $l$        | $l$    | $h$   |            | <b>I422</b>             | 97  | $I4mm$       | 107 | $I\bar{4}m2$ | 119 |
|                       |        |        |            |        |       |            | $I\bar{4}2m$            | 121 | $I4/mmm$     | 139 |              |     |
| $h+k+l$               | $h+k$  | $k+l$  | $l$        | $l=4n$ | $h$   |            | <b>I4<sub>1</sub>22</b> | 98  |              |     |              |     |
| $h+k+l$               | $h+k$  | $k+l$  | $2h+l=4n$  | $l=4n$ | $h$   | $h$        | $I4_1md$                | 109 | $I\bar{4}2d$ | 122 |              |     |
| $h+k+l$               | $h+k$  | $k, l$ | $l$        | $l$    | $h$   |            | $I4cm$                  | 108 | $I\bar{4}c2$ | 120 | $I4/mcm$     | 140 |
| $h+k+l$               | $h+k$  | $k, l$ | $2h+l=4n$  | $l=4n$ | $h$   | $h$        | $I4_1cd$                | 110 |              |     |              |     |
| $h+k+l$               | $h, k$ | $k+l$  | $2h+l=4n$  | $l=4n$ | $h$   | $h$        | $I4_1/amd$              | 141 |              |     |              |     |
| $h+k+l$               | $h, k$ | $k, l$ | $2h+l=4n$  | $l=4n$ | $h$   | $h$        | $I4_1/acd$              | 142 |              |     |              |     |

**Table 1.6.4.17**

Reflection conditions and possible space groups with Bravais lattice  $hP$  and Laue class  $\bar{3}$ ;  $hki$  are permutable; Patterson symmetry  $P\bar{3}$

| Reflection conditions |              |        | Space group           | No. | Space group           | No. |
|-----------------------|--------------|--------|-----------------------|-----|-----------------------|-----|
| $hh\bar{2}hl$         | $h\bar{h}0l$ | $000l$ |                       |     |                       |     |
|                       |              |        | <b>P3</b>             | 143 | $P\bar{3}$            | 147 |
|                       |              | $l=3n$ | <b>P3<sub>1</sub></b> | 144 | <b>P3<sub>2</sub></b> | 145 |

**Table 1.6.4.18**

Reflection conditions and possible space groups with Bravais lattice  $hP$  and Laue classes  $\bar{3}1m$  and  $\bar{3}m1$ ;  $hki$  are permutable; Patterson symmetry  $P\bar{3}1m$  and  $P\bar{3}m1$

| Reflection conditions |              |        | Class $\bar{3}1m$       |     | Class $\bar{3}m1$       |     |
|-----------------------|--------------|--------|-------------------------|-----|-------------------------|-----|
| $hh\bar{2}hl$         | $h\bar{h}0l$ | $000l$ | Space group             | No. | Space group             | No. |
|                       |              |        | <b>P312</b>             | 149 | <b>P321</b>             | 150 |
|                       |              |        | $P31m$                  | 157 | $P3m1$                  | 156 |
|                       |              |        | $P\bar{3}1m$            | 162 | $P\bar{3}m1$            | 164 |
|                       |              | $l=3n$ | <b>P3<sub>1</sub>12</b> | 151 | <b>P3<sub>1</sub>21</b> | 152 |
|                       |              |        | <b>P3<sub>2</sub>12</b> | 153 | <b>P3<sub>2</sub>21</b> | 154 |
| $l$                   |              | $l$    | $P31c$                  | 159 |                         |     |
|                       |              |        | $P\bar{3}1c$            | 163 |                         |     |
|                       | $l$          | $l$    |                         |     | $P3c1$                  | 158 |
|                       |              |        |                         |     | $P\bar{3}c1$            | 165 |

**Table 1.6.4.19**

Reflection conditions and possible space groups with Bravais lattice  $hP$  and Laue class  $6/m$ ;  $hki$  are permutable; Patterson symmetry  $P6/m$

| Reflection conditions |              |        | Space group           | No. | Space group           | No. | Space group | No. |
|-----------------------|--------------|--------|-----------------------|-----|-----------------------|-----|-------------|-----|
| $hh\bar{2}hl$         | $h\bar{h}0l$ | $000l$ |                       |     |                       |     |             |     |
|                       |              |        | <b>P6</b>             | 168 | $P\bar{6}$            | 174 | $P6/m$      | 175 |
|                       |              | $l$    | <b>P6<sub>3</sub></b> | 173 | $P6_3/m$              | 176 |             |     |
|                       |              | $l=3n$ | <b>P6<sub>2</sub></b> | 171 | <b>P6<sub>4</sub></b> | 172 |             |     |
|                       |              | $l=6n$ | <b>P6<sub>1</sub></b> | 169 | <b>P6<sub>5</sub></b> | 170 |             |     |