# MSG No. 131.437 $P4_2/m'mc$ [ Type III, tetragonal ]

Table 1: Wyckoff site: `2a`, site symmetry: `m'mm`.

| No. | position | mapping |
|---|---|---|
| 1 | $[0, 0, 0]$ | `[1,4,5,6,9,10,13,16]` |
| 2 | $\left[0, 0, \frac{1}{2}\right]$ | `[2,3,7,8,11,12,14,15]` |

Table 2: Wyckoff site: `2b`, site symmetry: `m'mm`.

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{2}, \frac{1}{2}, 0\right]$ | `[1,4,5,6,9,10,13,16]` |
| 2 | $\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$ | `[2,3,7,8,11,12,14,15]` |

Table 3: Wyckoff site: `2c`, site symmetry: `m'mm`.

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0, \frac{1}{2}, 0\right]$ | `[1,4,5,6,9,10,13,16]` |
| 2 | $\left[\frac{1}{2}, 0, \frac{1}{2}\right]$ | `[2,3,7,8,11,12,14,15]` |

Table 4: Wyckoff site: `2d`, site symmetry: `m'mm`.

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0, \frac{1}{2}, \frac{1}{2}\right]$ | `[1,4,5,6,9,10,13,16]` |
| 2 | $\left[\frac{1}{2}, 0, 0\right]$ | `[2,3,7,8,11,12,14,15]` |

Table 5: Wyckoff site: `2e`, site symmetry: `-4'm2'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0, 0, \frac{1}{4}\right]$ | `[1,4,5,6,11,12,14,15]` |
| 2 | $\left[0, 0, \frac{3}{4}\right]$ | `[2,3,7,8,9,10,13,16]` |

Table 6: Wyckoff site: `2f`, site symmetry: `-4'm2'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$ | `[1,4,5,6,11,12,14,15]` |
| 2 | $\left[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$ | `[2,3,7,8,9,10,13,16]` |

Table 7: Wyckoff site: `4g`, site symmetry: `2mm`.

| No. | position | mapping |
|---|---|---|
| 1 | $[0,\ 0,\ z]$ | `[1,4,5,6]` |
| 2 | $\left[0,\ 0,\ z+\frac{1}{2}\right]$ | `[2,3,7,8]` |
| 3 | $[0,\ 0,\ -z]$ | `[9,10,13,16]` |
| 4 | $\left[0,\ 0,\ \frac{1}{2}-z\right]$ | `[11,12,14,15]` |

Table 8: Wyckoff site: `4h`, site symmetry: `2mm`.

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{2},\ \frac{1}{2},\ z\right]$ | `[1,4,5,6]` |
| 2 | $\left[\frac{1}{2},\ \frac{1}{2},\ z+\frac{1}{2}\right]$ | `[2,3,7,8]` |
| 3 | $\left[\frac{1}{2},\ \frac{1}{2},\ -z\right]$ | `[9,10,13,16]` |
| 4 | $\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-z\right]$ | `[11,12,14,15]` |

Table 9: Wyckoff site: `4i`, site symmetry: `2mm`.

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0,\ \frac{1}{2},\ z\right]$ | `[1,4,5,6]` |
| 2 | $\left[\frac{1}{2},\ 0,\ z+\frac{1}{2}\right]$ | `[2,3,7,8]` |
| 3 | $\left[0,\ \frac{1}{2},\ -z\right]$ | `[9,10,13,16]` |
| 4 | $\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$ | `[11,12,14,15]` |

Table 10: Wyckoff site: `4j`, site symmetry: `m'2'm`.

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\ 0,\ 0]$ | `[1,6,9,16]` |
| 2 | $\left[0,\ x,\ \frac{1}{2}\right]$ | `[2,8,11,15]` |
| 3 | $\left[0,\ -x,\ \frac{1}{2}\right]$ | `[3,7,12,14]` |
| 4 | $[-x,\ 0,\ 0]$ | `[4,5,10,13]` |

Table 11: Wyckoff site: `4k`, site symmetry: `m'2'm`.

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\ \frac{1}{2},\ \frac{1}{2}\right]$ | `[1,6,9,16]` |
| 2 | $\left[\frac{1}{2},\ x,\ 0\right]$ | `[2,8,11,15]` |
| 3 | $\left[\frac{1}{2},\ -x,\ 0\right]$ | `[3,7,12,14]` |
| 4 | $\left[-x,\ \frac{1}{2},\ \frac{1}{2}\right]$ | `[4,5,10,13]` |

Table 12: Wyckoff site: `4l`, site symmetry: `m'2'm`.

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\ 0,\ \frac{1}{2}\right]$ | `[1,6,9,16]` |
| 2 | $[0,\ x,\ 0]$ | `[2,8,11,15]` |
| 3 | $[0,\ -x,\ 0]$ | `[3,7,12,14]` |
| 4 | $\left[-x,\ 0,\ \frac{1}{2}\right]$ | `[4,5,10,13]` |

Table 13: Wyckoff site: `4m`, site symmetry: `m'2'm`.

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\ \frac{1}{2},\ 0\right]$ | `[1,6,9,16]` |
| 2 | $\left[\frac{1}{2},\ x,\ \frac{1}{2}\right]$ | `[2,8,11,15]` |
| 3 | $\left[\frac{1}{2},\ -x,\ \frac{1}{2}\right]$ | `[3,7,12,14]` |
| 4 | $\left[-x,\ \frac{1}{2},\ 0\right]$ | `[4,5,10,13]` |

Table 14: Wyckoff site: `8n`, site symmetry: `..2'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\ x,\ \frac{1}{4}\right]$ | `[1,11]` |
| 2 | $\left[-x,\ x,\ \frac{3}{4}\right]$ | `[2,10]` |
| 3 | $\left[x,\ -x,\ \frac{3}{4}\right]$ | `[3,9]` |
| 4 | $\left[-x,\ -x,\ \frac{1}{4}\right]$ | `[4,12]` |
| 5 | $\left[-x,\ x,\ \frac{1}{4}\right]$ | `[5,15]` |
| 6 | $\left[x,\ -x,\ \frac{1}{4}\right]$ | `[6,14]` |
| 7 | $\left[-x,\ -x,\ \frac{3}{4}\right]$ | `[7,13]` |
| 8 | $\left[x,\ x,\ \frac{3}{4}\right]$ | `[8,16]` |

Table 15: Wyckoff site: `8o`, site symmetry: `.m.`

| No. | position | mapping |
|---|---|---|
| 1 | $[0,\ y,\ z]$ | `[1,5]` |
| 2 | $\left[-y,\ 0,\ z+\frac{1}{2}\right]$ | `[2,7]` |
| 3 | $\left[y,\ 0,\ z+\frac{1}{2}\right]$ | `[3,8]` |
| 4 | $[0,\ -y,\ z]$ | `[4,6]` |
| 5 | $[0,\ -y,\ -z]$ | `[9,13]` |
| 6 | $[0,\ y,\ -z]$ | `[10,16]` |
| 7 | $\left[y,\ 0,\ \frac{1}{2}-z\right]$ | `[11,14]` |
| 8 | $\left[-y,\ 0,\ \frac{1}{2}-z\right]$ | `[12,15]` |

Table 16: Wyckoff site: `8p`, site symmetry: `.m.`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{2}, y, z\right]$ | `[1,5]` |
| 2 | $\left[-y, \frac{1}{2}, z+\frac{1}{2}\right]$ | `[2,7]` |
| 3 | $\left[y, \frac{1}{2}, z+\frac{1}{2}\right]$ | `[3,8]` |
| 4 | $\left[\frac{1}{2}, -y, z\right]$ | `[4,6]` |
| 5 | $\left[\frac{1}{2}, -y, -z\right]$ | `[9,13]` |
| 6 | $\left[\frac{1}{2}, y, -z\right]$ | `[10,16]` |
| 7 | $\left[y, \frac{1}{2}, \frac{1}{2}-z\right]$ | `[11,14]` |
| 8 | $\left[-y, \frac{1}{2}, \frac{1}{2}-z\right]$ | `[12,15]` |

Table 17: Wyckoff site: `8q`, site symmetry: `m'..`

| No. | position | mapping |
|---|---|---|
| 1 | $[x, y, 0]$ | `[1,16]` |
| 2 | $\left[-y, x, \frac{1}{2}\right]$ | `[2,15]` |
| 3 | $\left[y, -x, \frac{1}{2}\right]$ | `[3,14]` |
| 4 | $[-x, -y, 0]$ | `[4,13]` |
| 5 | $[-x, y, 0]$ | `[5,10]` |
| 6 | $[x, -y, 0]$ | `[6,9]` |
| 7 | $\left[-y, -x, \frac{1}{2}\right]$ | `[7,12]` |
| 8 | $\left[y, x, \frac{1}{2}\right]$ | `[8,11]` |

Table 18: Wyckoff site: `16r`, site symmetry: `1`

| No. | position | mapping |
|---|---|---|
| 1 | $[x, y, z]$ | `[1]` |
| 2 | $\left[-y, x, z+\frac{1}{2}\right]$ | `[2]` |
| 3 | $\left[y, -x, z+\frac{1}{2}\right]$ | `[3]` |
| 4 | $[-x, -y, z]$ | `[4]` |
| 5 | $[-x, y, z]$ | `[5]` |
| 6 | $[x, -y, z]$ | `[6]` |
| 7 | $\left[-y, -x, z+\frac{1}{2}\right]$ | `[7]` |
| 8 | $\left[y, x, z+\frac{1}{2}\right]$ | `[8]` |
| 9 | $[x, -y, -z]$ | `[9]` |
| 10 | $[-x, y, -z]$ | `[10]` |
| 11 | $\left[y, x, \frac{1}{2}-z\right]$ | `[11]` |
| 12 | $\left[-y, -x, \frac{1}{2}-z\right]$ | `[12]` |
| 13 | $[-x, -y, -z]$ | `[13]` |
| 14 | $\left[y, -x, \frac{1}{2}-z\right]$ | `[14]` |
| 15 | $\left[-y, x, \frac{1}{2}-z\right]$ | `[15]` |
| 16 | $[x, y, -z]$ | `[16]` |