# MSG No. 127.392 $P4'/m'b'm$ [ Type III, tetragonal ]

Table 1: Wyckoff site: 2a, site symmetry: 4'/m'..

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

Table 2: Wyckoff site: 2b, site symmetry: 4'/m'..

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: 4'..

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

Table 6: Wyckoff site: `4f`, site symmetry: `2.mm`

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `m'..`

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

Table 10: Wyckoff site: `8j`, site symmetry: `m'..`

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

Table 11: Wyckoff site: `8k`, site symmetry: `..m`

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

Table 12: Wyckoff site: `16l`, site symmetry: `1`

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