# MSG No. 57.388 $P_cbcm$ [ Type IV, orthorhombic ]

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

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `..2'/m`

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

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

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

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

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

*continued ...*

Table 5

| No. | position | mapping |
|---|---|---|
| 3 | $\left[-x,\ \frac{3}{4},\ \frac{3}{4}\right]$ | `[3,6,12,13]` |
| 4 | $\left[-x,\ \frac{3}{4},\ \frac{1}{4}\right]$ | `[4,5,11,14]` |

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

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

Table 7: Wyckoff site: `8g`, site symmetry: `..2'`

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

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

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

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

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

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

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

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

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

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

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\, y,\, z]$ | `[1]` |
| 2 | $\left[x,\, \frac{1}{2}-y,\, -z\right]$ | `[2]` |
| 3 | $\left[-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$ | `[3]` |

*continued ...*

Table 12

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