# MSG No. 58.402 $P_Bnnm$ [ Type IV, orthorhombic ]

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

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

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

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

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

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

Table 4: Wyckoff site: `8d`, site symmetry: `-1'`

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

Table 5: Wyckoff site: `8e`, site symmetry: `..2`

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

Table 6: Wyckoff site: `8f`, site symmetry: `..m`

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

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

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

Table 8: Wyckoff site: `16h`, site symmetry: `1`

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

*continued ...*

Table 8

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