# MSG No. 51.299 $P_bmma$ [ Type IV, orthorhombic ]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `mm2`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{4}, 0, z\right]$ | `[1,4,6,7]` |
| 2 | $\left[\frac{3}{4}, 0, -z\right]$ | `[2,3,5,8]` |

*continued ...*

Table 5

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

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

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

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

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

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

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

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

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

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

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

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

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

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 | $[-x,\ y,\ -z]$ | `[3]` |

*continued ...*

Table 12

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