# MSG No. 53.332 $P_cmna$ [ Type IV, orthorhombic ]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `22'2'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{4}, 0, 0\right]$ | `[1,2,11,12]` |
| 2 | $\left[\frac{1}{4}, 0, \frac{1}{2}\right]$ | `[3,4,9,10]` |

*continued ...*

Table 5

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

Table 6: Wyckoff site: `4f`, site symmetry: `2'22'`

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

Table 7: Wyckoff site: `4g`, site symmetry: `22'2'`

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

Table 8: Wyckoff site: `4h`, site symmetry: `2'22'`

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

Table 9: Wyckoff site: `8i`, site symmetry: `..2'`

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

*continued ...*

Table 9

| No. | position | mapping |
|---|---|---|
| 8 | $\left[\frac{3}{4}, 0, \frac{1}{2} - z\right]$ | [8,13] |

Table 10: Wyckoff site: 8j, site symmetry: ..2'

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

Table 11: Wyckoff site: 8k, site symmetry: .2'.

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

Table 12: Wyckoff site: 8l, site symmetry: .2.

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

Table 13: Wyckoff site: `8m`, site symmetry: `2..`

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

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

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

Table 15: Wyckoff site: `8o`, site symmetry: `2..`

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

Table 16: Wyckoff site: `8p`, site symmetry: `2'..`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\ 0,\ \frac{1}{4}\right]$ | `[1,10]` |
| 2 | $\left[x,\ 0,\ \frac{3}{4}\right]$ | `[2,9]` |
| 3 | $\left[\frac{1}{2}-x,\ 0,\ \frac{1}{4}\right]$ | `[3,12]` |

*continued ...*

Table 16

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

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

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

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

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