# MSG No. 136.497 $P4_2/m'nm$ [ Type III, tetragonal ]

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

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

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

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

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

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

Table 4: Wyckoff site: `4d`, site symmetry: `-4'..`

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

Table 5: Wyckoff site: `4e`, site symmetry: `2.mm`

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

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

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

Table 7: Wyckoff site: `4g`, site symmetry: `m'.m2'`

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

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

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

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

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

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

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

Table 11: Wyckoff site: `16k`, site symmetry: `1`

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