# MSG No. 119.318 $I\bar{4}'m2'$ [ Type III, tetragonal ]

Table 1: Wyckoff site: `2a`, site symmetry: `-4'm2'`

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

Table 2: Wyckoff site: `2b`, site symmetry: `-4'm2'`

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

Table 3: Wyckoff site: `2c`, site symmetry: `-4'm2'`

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

Table 4: Wyckoff site: `2d`, site symmetry: `-4'm2'`

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

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

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

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

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

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

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

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

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

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

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

*continued ...*

Table 9

| No. | position | mapping |
|---|---|---|
| 8 | $\left[\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$ | `[14,15]` |

Table 10: Wyckoff site: `16j`, site symmetry: `1`

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