# MSG No. 120.322 $I\bar{4}c21'$ [ Type II, tetragonal ]

Table 1: Wyckoff site: `4a`, site symmetry: `2.221'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0,\ 0,\ \frac{1}{4}\right]$ | `[1,2,3,4,17,18,19,20]` |
| 2 | $\left[0,\ 0,\ \frac{3}{4}\right]$ | `[5,6,7,8,21,22,23,24]` |
| 3 | $\left[\frac{1}{2},\ \frac{1}{2},\ \frac{3}{4}\right]$ | `[9,10,11,12,25,26,27,28]` |
| 4 | $\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[13,14,15,16,29,30,31,32]` |

Table 2: Wyckoff site: `4b`, site symmetry: `-4..1'`

| No. | position | mapping |
|---|---|---|
| 1 | $[0,\ 0,\ 0]$ | `[1,2,5,6,17,18,21,22]` |
| 2 | $\left[0,\ 0,\ \frac{1}{2}\right]$ | `[3,4,7,8,19,20,23,24]` |
| 3 | $\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$ | `[9,10,13,14,25,26,29,30]` |
| 4 | $\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$ | `[11,12,15,16,27,28,31,32]` |

Table 3: Wyckoff site: `4c`, site symmetry: `-4..1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0,\ \frac{1}{2},\ \frac{1}{4}\right]$ | `[1,2,13,14,17,18,29,30]` |
| 2 | $\left[\frac{1}{2},\ 0,\ \frac{1}{4}\right]$ | `[3,4,15,16,19,20,31,32]` |
| 3 | $\left[\frac{1}{2},\ 0,\ \frac{3}{4}\right]$ | `[5,6,9,10,21,22,25,26]` |
| 4 | $\left[0,\ \frac{1}{2},\ \frac{3}{4}\right]$ | `[7,8,11,12,23,24,27,28]` |

Table 4: Wyckoff site: `4d`, site symmetry: `2.221'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0,\ \frac{1}{2},\ 0\right]$ | `[1,2,11,12,17,18,27,28]` |
| 2 | $\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$ | `[3,4,9,10,19,20,25,26]` |
| 3 | $\left[\frac{1}{2},\ 0,\ 0\right]$ | `[5,6,15,16,21,22,31,32]` |
| 4 | $\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$ | `[7,8,13,14,23,24,29,30]` |

Table 5: Wyckoff site: `8e`, site symmetry: `..21'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\ x,\ \frac{1}{4}\right]$ | `[1,3,17,19]` |
| 2 | $\left[-x,\ -x,\ \frac{1}{4}\right]$ | `[2,4,18,20]` |

*continued ...*

Table 5

| No. | position | mapping |
|---|---|---|
| 3 | $\left[x,\, -x,\, \frac{3}{4}\right]$ | [5,8,21,24] |
| 4 | $\left[-x,\, x,\, \frac{3}{4}\right]$ | [6,7,22,23] |
| 5 | $\left[x+\frac{1}{2},\, x+\frac{1}{2},\, \frac{3}{4}\right]$ | [9,11,25,27] |
| 6 | $\left[\frac{1}{2}-x,\, \frac{1}{2}-x,\, \frac{3}{4}\right]$ | [10,12,26,28] |
| 7 | $\left[x+\frac{1}{2},\, \frac{1}{2}-x,\, \frac{1}{4}\right]$ | [13,16,29,32] |
| 8 | $\left[\frac{1}{2}-x,\, x+\frac{1}{2},\, \frac{1}{4}\right]$ | [14,15,30,31] |

Table 6: Wyckoff site: 8f, site symmetry: 2..1'

| No. | position | mapping |
|---|---|---|
| 1 | $[0,\, 0,\, z]$ | [1,2,17,18] |
| 2 | $\left[0,\, 0,\, \frac{1}{2}-z\right]$ | [3,4,19,20] |
| 3 | $[0,\, 0,\, -z]$ | [5,6,21,22] |
| 4 | $\left[0,\, 0,\, z+\frac{1}{2}\right]$ | [7,8,23,24] |
| 5 | $\left[\frac{1}{2},\, \frac{1}{2},\, z+\frac{1}{2}\right]$ | [9,10,25,26] |
| 6 | $\left[\frac{1}{2},\, \frac{1}{2},\, -z\right]$ | [11,12,27,28] |
| 7 | $\left[\frac{1}{2},\, \frac{1}{2},\, \frac{1}{2}-z\right]$ | [13,14,29,30] |
| 8 | $\left[\frac{1}{2},\, \frac{1}{2},\, z\right]$ | [15,16,31,32] |

Table 7: Wyckoff site: 8g, site symmetry: 2..1'

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0,\, \frac{1}{2},\, z\right]$ | [1,2,17,18] |
| 2 | $\left[\frac{1}{2},\, 0,\, \frac{1}{2}-z\right]$ | [3,4,19,20] |
| 3 | $\left[\frac{1}{2},\, 0,\, -z\right]$ | [5,6,21,22] |
| 4 | $\left[0,\, \frac{1}{2},\, z+\frac{1}{2}\right]$ | [7,8,23,24] |
| 5 | $\left[\frac{1}{2},\, 0,\, z+\frac{1}{2}\right]$ | [9,10,25,26] |
| 6 | $\left[0,\, \frac{1}{2},\, -z\right]$ | [11,12,27,28] |
| 7 | $\left[0,\, \frac{1}{2},\, \frac{1}{2}-z\right]$ | [13,14,29,30] |
| 8 | $\left[\frac{1}{2},\, 0,\, z\right]$ | [15,16,31,32] |

Table 8: Wyckoff site: 8h, site symmetry: ..21'

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x,\, x+\frac{1}{2},\, 0\right]$ | [1,11,17,27] |
| 2 | $\left[-x,\, \frac{1}{2}-x,\, 0\right]$ | [2,12,18,28] |
| 3 | $\left[x+\frac{1}{2},\, x,\, \frac{1}{2}\right]$ | [3,9,19,25] |
| 4 | $\left[\frac{1}{2}-x,\, -x,\, \frac{1}{2}\right]$ | [4,10,20,26] |
| 5 | $\left[x+\frac{1}{2},\, -x,\, 0\right]$ | [5,16,21,32] |

*continued ...*

Table 8

| No. | position | mapping |
|---|---|---|
| 6 | $\left[\frac{1}{2}-x,\, x,\, 0\right]$ | `[6,15,22,31]` |
| 7 | $\left[-x,\, x+\frac{1}{2},\, \frac{1}{2}\right]$ | `[7,14,23,30]` |
| 8 | $\left[x,\, \frac{1}{2}-x,\, \frac{1}{2}\right]$ | `[8,13,24,29]` |

Table 9: Wyckoff site: `16i`, site symmetry: `11'`

| No. | position | mapping |
|---|---|---|
| 1 | $[x,\, y,\, z]$ | `[1,17]` |
| 2 | $[-x,\, -y,\, z]$ | `[2,18]` |
| 3 | $\left[y,\, x,\, \frac{1}{2}-z\right]$ | `[3,19]` |
| 4 | $\left[-y,\, -x,\, \frac{1}{2}-z\right]$ | `[4,20]` |
| 5 | $[y,\, -x,\, -z]$ | `[5,21]` |
| 6 | $[-y,\, x,\, -z]$ | `[6,22]` |
| 7 | $\left[-x,\, y,\, z+\frac{1}{2}\right]$ | `[7,23]` |
| 8 | $\left[x,\, -y,\, z+\frac{1}{2}\right]$ | `[8,24]` |
| 9 | $\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$ | `[9,25]` |
| 10 | $\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$ | `[10,26]` |
| 11 | $\left[y+\frac{1}{2},\, x+\frac{1}{2},\, -z\right]$ | `[11,27]` |
| 12 | $\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, -z\right]$ | `[12,28]` |
| 13 | $\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$ | `[13,29]` |
| 14 | $\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$ | `[14,30]` |
| 15 | $\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z\right]$ | `[15,31]` |
| 16 | $\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z\right]$ | `[16,32]` |