# MSG No. 67.502 $Cmma1'$ [ Type II, orthorhombic ]

Table 1: Wyckoff site: `4a`, site symmetry: `2221'`

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

Table 2: Wyckoff site: `4b`, site symmetry: `2221'`

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

Table 3: Wyckoff site: `4c`, site symmetry: `2/m..1'`

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

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

| No. | position | mapping |
|---|---|---|
| 1 | $\left[0, 0, \frac{1}{2}\right]$ | `[1,2,5,6,17,18,21,22]` |
| 2 | $\left[\frac{1}{2}, 0, \frac{1}{2}\right]$ | `[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 | $\left[0, \frac{1}{2}, \frac{1}{2}\right]$ | `[11,12,15,16,27,28,31,32]` |

Table 5: Wyckoff site: `4e`, site symmetry: `.2/m.1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[\frac{1}{4}, \frac{1}{4}, 0\right]$ | `[1,3,13,15,17,19,29,31]` |
| 2 | $\left[\frac{1}{4}, \frac{3}{4}, 0\right]$ | `[2,4,14,16,18,20,30,32]` |

*continued ...*

Table 5

| No. | position | mapping |
|---|---|---|
| 3 | $\left[\frac{3}{4}, \frac{3}{4}, 0\right]$ | `[5,7,9,11,21,23,25,27]` |
| 4 | $\left[\frac{3}{4}, \frac{1}{4}, 0\right]$ | `[6,8,10,12,22,24,26,28]` |

Table 6: Wyckoff site: `4f`, site symmetry: `.2/m.1'`

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

Table 7: Wyckoff site: `4g`, site symmetry: `mm21'`

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

Table 8: Wyckoff site: `8h`, site symmetry: `2..1'`

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

Table 9: Wyckoff site: `8i`, site symmetry: `2..1'`

| No. | position | mapping |
|---|---|---|
| 1 | $\left[x, 0, \frac{1}{2}\right]$ | `[1,2,17,18]` |
| 2 | $\left[\frac{1}{2} - x, 0, \frac{1}{2}\right]$ | `[3,4,19,20]` |
| 3 | $\left[-x, 0, \frac{1}{2}\right]$ | `[5,6,21,22]` |

*continued ...*

Table 9

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

Table 10: Wyckoff site: 8j, site symmetry: .2.1'

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

Table 11: Wyckoff site: 8k, site symmetry: .2.1'

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

Table 12: Wyckoff site: 8l, site symmetry: ..21'

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

*continued ...*

Table 12

| No. | position | mapping |
|---|---|---|
| 7 | $\left[\frac{1}{4}, \frac{1}{2}, -z\right]$ | [13,16,29,32] |
| 8 | $\left[\frac{1}{4}, \frac{1}{2}, z\right]$ | [14,15,30,31] |

Table 13: Wyckoff site: 8m, site symmetry: m..1'

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

Table 14: Wyckoff site: 8n, site symmetry: .m.1'

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

Table 15: Wyckoff site: 16o, site symmetry: 11'

| No. | position | mapping |
|---|---|---|
| 1 | $[x, y, z]$ | [1,17] |
| 2 | $[x, -y, -z]$ | [2,18] |
| 3 | $\left[\frac{1}{2}-x, y, -z\right]$ | [3,19] |
| 4 | $\left[\frac{1}{2}-x, -y, z\right]$ | [4,20] |
| 5 | $[-x, -y, -z]$ | [5,21] |
| 6 | $[-x, y, z]$ | [6,22] |
| 7 | $\left[x+\frac{1}{2}, -y, z\right]$ | [7,23] |
| 8 | $\left[x+\frac{1}{2}, y, -z\right]$ | [8,24] |
| 9 | $\left[x+\frac{1}{2}, y+\frac{1}{2}, z\right]$ | [9,25] |

*continued ...*

Table 15

| No. | position | mapping |
|---|---|---|
| 10 | $\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$ | [10,26] |
| 11 | $\left[-x,\, y+\frac{1}{2},\, -z\right]$ | [11,27] |
| 12 | $\left[-x,\, \frac{1}{2}-y,\, z\right]$ | [12,28] |
| 13 | $\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, -z\right]$ | [13,29] |
| 14 | $\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z\right]$ | [14,30] |
| 15 | $\left[x,\, \frac{1}{2}-y,\, z\right]$ | [15,31] |
| 16 | $\left[x,\, y+\frac{1}{2},\, -z\right]$ | [16,32] |