# MSG No. 108.238 $I_c4cm$ [ Type IV, tetragonal ]

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

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

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

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

Table 3: Wyckoff site: `8c`, site symmetry: `2.mm`

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

Table 4: Wyckoff site: `16d`, site symmetry: `.m'.`

| No. | position | mapping |
|---|---|---|
| 1 | $[0,\ y,\ z]$ | `[1,21]` |
| 2 | $[-y,\ 0,\ z]$ | `[2,23]` |
| 3 | $[y,\ 0,\ z]$ | `[3,24]` |
| 4 | $[0,\ -y,\ z]$ | `[4,22]` |
| 5 | $\left[0,\ y,\ z+\frac{1}{2}\right]$ | `[5,17]` |
| 6 | $\left[0,\ -y,\ z+\frac{1}{2}\right]$ | `[6,20]` |
| 7 | $\left[-y,\ 0,\ z+\frac{1}{2}\right]$ | `[7,18]` |
| 8 | $\left[y,\ 0,\ z+\frac{1}{2}\right]$ | `[8,19]` |
| 9 | $\left[\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$ | `[9,29]` |

*continued ...*

Table 4

| No. | position | mapping |
|---|---|---|
| 10 | $\left[\frac{1}{2}-y,\ \frac{1}{2},\ z+\frac{1}{2}\right]$ | [10,31] |
| 11 | $\left[y+\frac{1}{2},\ \frac{1}{2},\ z+\frac{1}{2}\right]$ | [11,32] |
| 12 | $\left[\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$ | [12,30] |
| 13 | $\left[\frac{1}{2},\ y+\frac{1}{2},\ z\right]$ | [13,25] |
| 14 | $\left[\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$ | [14,28] |
| 15 | $\left[\frac{1}{2}-y,\ \frac{1}{2},\ z\right]$ | [15,26] |
| 16 | $\left[y+\frac{1}{2},\ \frac{1}{2},\ z\right]$ | [16,27] |

Table 5: Wyckoff site: 16e, site symmetry: ..m'

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

Table 6: Wyckoff site: 16f, site symmetry: ..m

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

*continued ...*

Table 6

| No. | position | mapping |
|---|---|---|
| 12 | $\left[-x,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$ | [20,31] |
| 13 | $\left[-x,\ x+\frac{1}{2},\ z\right]$ | [21,26] |
| 14 | $\left[x,\ \frac{1}{2}-x,\ z\right]$ | [22,27] |
| 15 | $\left[\frac{1}{2}-x,\ -x,\ z\right]$ | [23,28] |
| 16 | $\left[x+\frac{1}{2},\ x,\ z\right]$ | [24,25] |

Table 7: Wyckoff site: 32g, site symmetry: 1

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