

MSG No. 84.51  $P4_2/m$  [ Type I, tetragonal ]

Table 1: Wyckoff site: 2a, site symmetry:  $2/m..$

| No. | position              | mapping        |
|-----|-----------------------|----------------|
| 1   | $[0, 0, 0]$           | $[1, 4, 5, 8]$ |
| 2   | $[0, 0, \frac{1}{2}]$ | $[2, 3, 6, 7]$ |

Table 2: Wyckoff site: 2b, site symmetry:  $2/m..$

| No. | position                                  | mapping        |
|-----|---|----------------|
| 1   | $[\frac{1}{2}, \frac{1}{2}, 0]$           | $[1, 4, 5, 8]$ |
| 2   | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | $[2, 3, 6, 7]$ |

Table 3: Wyckoff site: 2c, site symmetry:  $2/m..$

| No. | position                        | mapping        |
|-----|---------------------------------|----------------|
| 1   | $[0, \frac{1}{2}, 0]$           | $[1, 4, 5, 8]$ |
| 2   | $[\frac{1}{2}, 0, \frac{1}{2}]$ | $[2, 3, 6, 7]$ |

Table 4: Wyckoff site: 2d, site symmetry:  $2/m..$

| No. | position                        | mapping        |
|-----|---------------------------------|----------------|
| 1   | $[0, \frac{1}{2}, \frac{1}{2}]$ | $[1, 4, 5, 8]$ |
| 2   | $[\frac{1}{2}, 0, 0]$           | $[2, 3, 6, 7]$ |

Table 5: Wyckoff site: 2e, site symmetry:  $-4..$

| No. | position              | mapping        |
|-----|-----------------------|----------------|
| 1   | $[0, 0, \frac{1}{4}]$ | $[1, 4, 6, 7]$ |
| 2   | $[0, 0, \frac{3}{4}]$ | $[2, 3, 5, 8]$ |

Table 6: Wyckoff site: 2f, site symmetry:  $-4..$

| No. | position                                  | mapping        |
|-----|---|----------------|
| 1   | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$ | $[1, 4, 6, 7]$ |
| 2   | $[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$ | $[2, 3, 5, 8]$ |

Table 7: Wyckoff site:  $4\mathbf{g}$ , site symmetry:  $2..$ 

| No. | position                  | mapping  |
|-----|---------------------------|----------|
| 1   | $[0, 0, z]$               | $[1, 4]$ |
| 2   | $[0, 0, z + \frac{1}{2}]$ | $[2, 3]$ |
| 3   | $[0, 0, -z]$              | $[5, 8]$ |
| 4   | $[0, 0, \frac{1}{2} - z]$ | $[6, 7]$ |

Table 8: Wyckoff site:  $4\mathbf{h}$ , site symmetry:  $2..$ 

| No. | position                                      | mapping  |
|-----|---|----------|
| 1   | $[\frac{1}{2}, \frac{1}{2}, z]$               | $[1, 4]$ |
| 2   | $[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$ | $[2, 3]$ |
| 3   | $[\frac{1}{2}, \frac{1}{2}, -z]$              | $[5, 8]$ |
| 4   | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$ | $[6, 7]$ |

Table 9: Wyckoff site:  $4\mathbf{i}$ , site symmetry:  $2..$ 

| No. | position                            | mapping  |
|-----|-------------------------------------|----------|
| 1   | $[0, \frac{1}{2}, z]$               | $[1, 4]$ |
| 2   | $[\frac{1}{2}, 0, z + \frac{1}{2}]$ | $[2, 3]$ |
| 3   | $[0, \frac{1}{2}, -z]$              | $[5, 8]$ |
| 4   | $[\frac{1}{2}, 0, \frac{1}{2} - z]$ | $[6, 7]$ |

Table 10: Wyckoff site:  $4\mathbf{j}$ , site symmetry:  $\mathbf{m}..$ 

| No. | position               | mapping  |
|-----|------------------------|----------|
| 1   | $[x, y, 0]$            | $[1, 8]$ |
| 2   | $[-y, x, \frac{1}{2}]$ | $[2, 7]$ |
| 3   | $[y, -x, \frac{1}{2}]$ | $[3, 6]$ |
| 4   | $[-x, -y, 0]$          | $[4, 5]$ |

Table 11: Wyckoff site:  $8\mathbf{k}$ , site symmetry:  $1$ 

| No. | position                   | mapping |
|-----|----------------------------|---------|
| 1   | $[x, y, z]$                | $[1]$   |
| 2   | $[-y, x, z + \frac{1}{2}]$ | $[2]$   |
| 3   | $[y, -x, z + \frac{1}{2}]$ | $[3]$   |
| 4   | $[-x, -y, z]$              | $[4]$   |

*continued ...*

Table 11

| No. | position                   | mapping |
|-----|----------------------------|---------|
| 5   | $[-x, -y, -z]$             | [5]     |
| 6   | $[y, -x, \frac{1}{2} - z]$ | [6]     |
| 7   | $[-y, x, \frac{1}{2} - z]$ | [7]     |
| 8   | $[x, y, -z]$               | [8]     |