# MSG No. 85.59   $P4/n$   [ Type I, tetragonal ]

Table 1: Wyckoff site: 2a, site symmetry: -4..

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

Table 2: Wyckoff site: 2b, site symmetry: -4..

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

Table 3: Wyckoff site: 2c, site symmetry: 4..

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

Table 4: Wyckoff site: 4d, site symmetry: -1

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

Table 5: Wyckoff site: 4e, site symmetry: -1

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

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

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

Table 7: Wyckoff site: `8g`, site symmetry: `1`

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