

MSG No. 25.59 $Pm'm2'$ [Type III, orthorhombic]

Table 1: Wyckoff site: 1a, site symmetry: $m'm2'$

| No. | position | mapping |
|-----|-------------|----------------|
| 1 | $[0, 0, z]$ | $[1, 2, 3, 4]$ |

Table 2: Wyckoff site: 1b, site symmetry: $m'm2'$

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

Table 3: Wyckoff site: 1c, site symmetry: $m'm2'$

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

Table 4: Wyckoff site: 1d, site symmetry: $m'm2'$

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

Table 5: Wyckoff site: 2e, site symmetry: $.m.$

| No. | position | mapping |
|-----|--------------|----------|
| 1 | $[x, 0, z]$ | $[1, 2]$ |
| 2 | $[-x, 0, z]$ | $[3, 4]$ |

Table 6: Wyckoff site: 2f, site symmetry: $.m.$

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

Table 7: Wyckoff site: 2g, site symmetry: m' . .

| No. | position | mapping |
|-----|--------------|----------|
| 1 | $[0, y, z]$ | $[1, 4]$ |
| 2 | $[0, -y, z]$ | $[2, 3]$ |

Table 8: Wyckoff site: 2h, site symmetry: m' . .

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

Table 9: Wyckoff site: 4i, site symmetry: 1

| No. | position | mapping |
|-----|---------------|---------|
| 1 | $[x, y, z]$ | $[1]$ |
| 2 | $[x, -y, z]$ | $[2]$ |
| 3 | $[-x, -y, z]$ | $[3]$ |
| 4 | $[-x, y, z]$ | $[4]$ |