

MSG No. 35.168 $Cm'm'2$ [Type III, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: $m'm'2$

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $\dots 2$

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

Table 4: Wyckoff site: 4d, site symmetry: $.m'.$

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

Table 5: Wyckoff site: 4e, site symmetry: $m'..$

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

Table 6: Wyckoff site: **8f**, 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] |
| 5 | $[x + \frac{1}{2}, y + \frac{1}{2}, z]$ | [5] |
| 6 | $[\frac{1}{2} - x, \frac{1}{2} - y, z]$ | [6] |
| 7 | $[\frac{1}{2} - x, y + \frac{1}{2}, z]$ | [7] |
| 8 | $[x + \frac{1}{2}, \frac{1}{2} - y, z]$ | [8] |