

MSG No. 25.63  $P_Cmm2$  [ Type IV, orthorhombic ]

Table 1: Wyckoff site: 2a, site symmetry:  $mm2$

| 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:  $mm2$

| 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:  $. . 2'$

| 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]     |