

MSG No. 26.74 P_{Amc2_1} [Type IV, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: $\text{mm}'2'$

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

Table 2: Wyckoff site: 2b, site symmetry: $\text{mm}'2'$

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

Table 3: Wyckoff site: 4c, site symmetry: $.\text{m}'.$

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

Table 4: Wyckoff site: 4d, site symmetry: $\text{m}..$

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

Table 5: Wyckoff site: 4e, site symmetry: $\text{m}..$

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