

MSG No. 37.184 C_ccc2 [Type IV, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: $m'm'2$

| No. | position | mapping |
|-----|---|------------------|
| 1 | $[0, 0, z]$ | $[1, 2, 11, 12]$ |
| 2 | $[0, 0, z + \frac{1}{2}]$ | $[3, 4, 9, 10]$ |
| 3 | $[\frac{1}{2}, \frac{1}{2}, z]$ | $[5, 6, 15, 16]$ |
| 4 | $[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$ | $[7, 8, 13, 14]$ |

Table 2: Wyckoff site: 4b, site symmetry: $m'm'2$

| No. | position | mapping |
|-----|-------------------------------------|------------------|
| 1 | $[0, \frac{1}{2}, z]$ | $[1, 2, 11, 12]$ |
| 2 | $[0, \frac{1}{2}, z + \frac{1}{2}]$ | $[3, 4, 9, 10]$ |
| 3 | $[\frac{1}{2}, 0, z]$ | $[5, 6, 15, 16]$ |
| 4 | $[\frac{1}{2}, 0, z + \frac{1}{2}]$ | $[7, 8, 13, 14]$ |

Table 3: Wyckoff site: 8c, 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 | $[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}]$ | $[3, 8]$ |
| 4 | $[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$ | $[4, 7]$ |
| 5 | $[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$ | $[9, 14]$ |
| 6 | $[\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}]$ | $[10, 13]$ |
| 7 | $[\frac{3}{4}, \frac{1}{4}, z]$ | $[11, 16]$ |
| 8 | $[\frac{1}{4}, \frac{3}{4}, z]$ | $[12, 15]$ |

Table 4: Wyckoff site: 8d, site symmetry: $.m'.$

| No. | position | mapping |
|-----|---|-----------|
| 1 | $[x, 0, z]$ | $[1, 12]$ |
| 2 | $[-x, 0, z]$ | $[2, 11]$ |
| 3 | $[-x, 0, z + \frac{1}{2}]$ | $[3, 10]$ |
| 4 | $[x, 0, z + \frac{1}{2}]$ | $[4, 9]$ |
| 5 | $[x + \frac{1}{2}, \frac{1}{2}, z]$ | $[5, 16]$ |
| 6 | $[\frac{1}{2} - x, \frac{1}{2}, z]$ | $[6, 15]$ |
| 7 | $[\frac{1}{2} - x, \frac{1}{2}, z + \frac{1}{2}]$ | $[7, 14]$ |
| 8 | $[x + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$ | $[8, 13]$ |

Table 5: Wyckoff site: **8e**, site symmetry: **m'..**

| No. | position | mapping |
|-----|---|---------------|
| 1 | $[0, y, z]$ | [1,11] |
| 2 | $[0, -y, z]$ | [2,12] |
| 3 | $[0, y, z + \frac{1}{2}]$ | [3,9] |
| 4 | $[0, -y, z + \frac{1}{2}]$ | [4,10] |
| 5 | $[\frac{1}{2}, y + \frac{1}{2}, z]$ | [5,15] |
| 6 | $[\frac{1}{2}, \frac{1}{2} - y, z]$ | [6,16] |
| 7 | $[\frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$ | [7,13] |
| 8 | $[\frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$ | [8,14] |

Table 6: Wyckoff site: **16f**, site symmetry: **1**

| No. | position | mapping |
|-----|---|-------------|
| 1 | $[x, y, z]$ | [1] |
| 2 | $[-x, -y, z]$ | [2] |
| 3 | $[-x, y, z + \frac{1}{2}]$ | [3] |
| 4 | $[x, -y, z + \frac{1}{2}]$ | [4] |
| 5 | $[x + \frac{1}{2}, y + \frac{1}{2}, z]$ | [5] |
| 6 | $[\frac{1}{2} - x, \frac{1}{2} - y, z]$ | [6] |
| 7 | $[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$ | [7] |
| 8 | $[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$ | [8] |
| 9 | $[x, y, z + \frac{1}{2}]$ | [9] |
| 10 | $[-x, -y, z + \frac{1}{2}]$ | [10] |
| 11 | $[-x, y, z]$ | [11] |
| 12 | $[x, -y, z]$ | [12] |
| 13 | $[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$ | [13] |
| 14 | $[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$ | [14] |
| 15 | $[\frac{1}{2} - x, y + \frac{1}{2}, z]$ | [15] |
| 16 | $[x + \frac{1}{2}, \frac{1}{2} - y, z]$ | [16] |