

MSG No. 38.194 A_Bmm2 [Type IV, orthorhombic]

Table 1: Wyckoff site: **4a**, site symmetry: **mm2**

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

Table 2: Wyckoff site: **8b**, site symmetry: **..2'**

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

Table 3: Wyckoff site: **8c**, site symmetry: **m..**

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

Table 4: Wyckoff site: **8d**, site symmetry: **.m.**

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

continued ...

Table 4

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

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