

MSG No. 36.179 C_Amc2_1 [Type IV, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: mm'2'

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

Table 2: Wyckoff site: 8b, site symmetry: $\dots 2'$

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

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

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

Table 4: Wyckoff site: 8d, site symmetry: $.\text{m}'.$

| No. | position | mapping |
|-----|--------------------------------------|---------|
| 1 | $[x, \frac{3}{4}, z]$ | [1,12] |
| 2 | $[-x, \frac{1}{4}, z + \frac{1}{2}]$ | [2,11] |
| 3 | $[-x, \frac{3}{4}, z]$ | [3,10] |
| 4 | $[x, \frac{1}{4}, z + \frac{1}{2}]$ | [4,9] |
| 5 | $[x + \frac{1}{2}, \frac{1}{4}, z]$ | [5,16] |

continued ...

Table 4

| No. | position | mapping |
|-----|---|---------|
| 6 | $[\frac{1}{2} - x, \frac{3}{4}, z + \frac{1}{2}]$ | [6,15] |
| 7 | $[\frac{1}{2} - x, \frac{1}{4}, z]$ | [7,14] |
| 8 | $[x + \frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}]$ | [8,13] |

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