

MSG No. 120.325 $I\bar{4}c'2'$ [Type III, tetragonal]

Table 1: Wyckoff site: 4a, site symmetry: 2.2'2'

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

Table 2: Wyckoff site: 4b, site symmetry: -4..

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

Table 3: Wyckoff site: 4c, site symmetry: -4..

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

Table 4: Wyckoff site: 4d, site symmetry: 2.2'2'

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

Table 5: Wyckoff site: 8e, site symmetry: ..2'

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

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 2..

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

Table 7: Wyckoff site: 8g, site symmetry: 2..

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

Table 8: Wyckoff site: 8h, site symmetry: ..2'

| No. | position | mapping |
|-----|-------------------------------------|---------|
| 1 | $[x, x + \frac{1}{2}, 0]$ | [1,13] |
| 2 | $[-x, \frac{1}{2} - x, 0]$ | [2,14] |
| 3 | $[x + \frac{1}{2}, -x, 0]$ | [3,16] |
| 4 | $[\frac{1}{2} - x, x, 0]$ | [4,15] |
| 5 | $[x + \frac{1}{2}, x, \frac{1}{2}]$ | [5,9] |

continued ...

Table 8

| No. | position | mapping |
|-----|--------------------------------------|---------|
| 6 | $[\frac{1}{2} - x, -x, \frac{1}{2}]$ | [6,10] |
| 7 | $[-x, x + \frac{1}{2}, \frac{1}{2}]$ | [7,12] |
| 8 | $[x, \frac{1}{2} - x, \frac{1}{2}]$ | [8,11] |

Table 9: Wyckoff site: 16i, site symmetry: 1

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