

MSG No. 126.382 $P4'/n'nc'$ [Type III, tetragonal]

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $22'2'$

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

Table 4: Wyckoff site: 4d, site symmetry: $-4..$

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

Table 5: Wyckoff site: 4e, site symmetry: $4'..$

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

Table 6: Wyckoff site: $8f$, site symmetry: $-1'$

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

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

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

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

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

Table 9: Wyckoff site: $8i$, site symmetry: $.2'$

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

continued ...

Table 9

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

Table 10: Wyckoff site: 8j, site symmetry: $.2'$.

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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