

SG No. 128 D_{4h}^6 $P4/mnc$ [tetragonal]

* plus set: $+ [0, 0, 0]$

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

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

Table 2: Wyckoff site: 2b, site symmetry: $4/m..$

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

Table 3: Wyckoff site: 4c, site symmetry: $2/m..$

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

Table 4: Wyckoff site: 4d, site symmetry: $2..22$

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

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

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

Table 6: Wyckoff site: **8f**, 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 | $[0, \frac{1}{2}, \frac{1}{2} - z]$ | $[7, 8]$ |
| 5 | $[0, \frac{1}{2}, -z]$ | $[9, 10]$ |
| 6 | $[\frac{1}{2}, 0, -z]$ | $[11, 12]$ |
| 7 | $[\frac{1}{2}, 0, z + \frac{1}{2}]$ | $[13, 14]$ |
| 8 | $[0, \frac{1}{2}, z + \frac{1}{2}]$ | $[15, 16]$ |

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

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

Table 8: Wyckoff site: **8h**, site symmetry: $m..$

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

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

| No. | position | mapping |
|-----|---------------|---------|
| 1 | $[x, y, z]$ | $[1]$ |
| 2 | $[-x, -y, z]$ | $[2]$ |
| 3 | $[-y, x, z]$ | $[3]$ |

continued ...

Table 9

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