

MSG No. 114.276 $P\bar{4}2_1c1'$ [Type II, tetragonal]

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

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

Table 2: Wyckoff site: 2b, site symmetry: $-4..1'$

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

Table 3: Wyckoff site: 4c, site symmetry: $2..1'$

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

Table 4: Wyckoff site: 4d, site symmetry: $2..1'$

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

Table 5: Wyckoff site: 8e, site symmetry: $11'$

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

continued ...

Table 5

| No. | position | mapping |
|-----|---|-----------|
| 7 | $[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$ | $[7, 15]$ |
| 8 | $[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$ | $[8, 16]$ |