

MSG No. 93.121 $P4_2'22'$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 222.

| No. | position | mapping |
|-----|-----------------------|----------------|
| 1 | $[0, 0, 0]$ | $[1, 2, 3, 4]$ |
| 2 | $[0, 0, \frac{1}{2}]$ | $[5, 6, 7, 8]$ |

Table 2: Wyckoff site: 2b, site symmetry: 222.

| No. | position | mapping |
|-----|---|----------------|
| 1 | $[\frac{1}{2}, \frac{1}{2}, 0]$ | $[1, 2, 3, 4]$ |
| 2 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | $[5, 6, 7, 8]$ |

Table 3: Wyckoff site: 2c, site symmetry: 222.

| No. | position | mapping |
|-----|---------------------------------|----------------|
| 1 | $[0, \frac{1}{2}, 0]$ | $[1, 2, 3, 4]$ |
| 2 | $[\frac{1}{2}, 0, \frac{1}{2}]$ | $[5, 6, 7, 8]$ |

Table 4: Wyckoff site: 2d, site symmetry: 222.

| No. | position | mapping |
|-----|---------------------------------|----------------|
| 1 | $[0, \frac{1}{2}, \frac{1}{2}]$ | $[1, 2, 3, 4]$ |
| 2 | $[\frac{1}{2}, 0, 0]$ | $[5, 6, 7, 8]$ |

Table 5: Wyckoff site: 2e, site symmetry: 2.2'2'

| No. | position | mapping |
|-----|-----------------------|----------------|
| 1 | $[0, 0, \frac{1}{4}]$ | $[1, 4, 7, 8]$ |
| 2 | $[0, 0, \frac{3}{4}]$ | $[2, 3, 5, 6]$ |

Table 6: Wyckoff site: 2f, site symmetry: 2.2'2'

| No. | position | mapping |
|-----|---|----------------|
| 1 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$ | $[1, 4, 7, 8]$ |
| 2 | $[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$ | $[2, 3, 5, 6]$ |

Table 7: Wyckoff site: $4\mathbf{g}$, site symmetry: $2..$

| No. | position | mapping |
|-----|---------------------------|----------|
| 1 | $[0, 0, z]$ | $[1, 4]$ |
| 2 | $[0, 0, -z]$ | $[2, 3]$ |
| 3 | $[0, 0, z + \frac{1}{2}]$ | $[5, 6]$ |
| 4 | $[0, 0, \frac{1}{2} - z]$ | $[7, 8]$ |

Table 8: Wyckoff site: $4\mathbf{h}$, site symmetry: $2..$

| No. | position | mapping |
|-----|---|----------|
| 1 | $[\frac{1}{2}, \frac{1}{2}, z]$ | $[1, 4]$ |
| 2 | $[\frac{1}{2}, \frac{1}{2}, -z]$ | $[2, 3]$ |
| 3 | $[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$ | $[5, 6]$ |
| 4 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$ | $[7, 8]$ |

Table 9: Wyckoff site: $4\mathbf{i}$, site symmetry: $2..$

| No. | position | mapping |
|-----|-------------------------------------|----------|
| 1 | $[0, \frac{1}{2}, z]$ | $[1, 4]$ |
| 2 | $[0, \frac{1}{2}, -z]$ | $[2, 3]$ |
| 3 | $[\frac{1}{2}, 0, z + \frac{1}{2}]$ | $[5, 6]$ |
| 4 | $[\frac{1}{2}, 0, \frac{1}{2} - z]$ | $[7, 8]$ |

Table 10: Wyckoff site: $4\mathbf{j}$, site symmetry: $.2.$

| No. | position | mapping |
|-----|------------------------|----------|
| 1 | $[x, 0, 0]$ | $[1, 2]$ |
| 2 | $[-x, 0, 0]$ | $[3, 4]$ |
| 3 | $[0, x, \frac{1}{2}]$ | $[5, 7]$ |
| 4 | $[0, -x, \frac{1}{2}]$ | $[6, 8]$ |

Table 11: Wyckoff site: $4\mathbf{k}$, site symmetry: $.2.$

| No. | position | mapping |
|-----|----------------------------------|----------|
| 1 | $[x, \frac{1}{2}, \frac{1}{2}]$ | $[1, 2]$ |
| 2 | $[-x, \frac{1}{2}, \frac{1}{2}]$ | $[3, 4]$ |
| 3 | $[\frac{1}{2}, x, 0]$ | $[5, 7]$ |
| 4 | $[\frac{1}{2}, -x, 0]$ | $[6, 8]$ |

Table 12: Wyckoff site: $4\mathbf{l}$, site symmetry: $.2$.

| No. | position | mapping |
|-----|------------------------|----------|
| 1 | $[x, 0, \frac{1}{2}]$ | $[1, 2]$ |
| 2 | $[-x, 0, \frac{1}{2}]$ | $[3, 4]$ |
| 3 | $[0, x, 0]$ | $[5, 7]$ |
| 4 | $[0, -x, 0]$ | $[6, 8]$ |

Table 13: Wyckoff site: $4\mathbf{m}$, site symmetry: $.2$.

| No. | position | mapping |
|-----|----------------------------------|----------|
| 1 | $[x, \frac{1}{2}, 0]$ | $[1, 2]$ |
| 2 | $[-x, \frac{1}{2}, 0]$ | $[3, 4]$ |
| 3 | $[\frac{1}{2}, x, \frac{1}{2}]$ | $[5, 7]$ |
| 4 | $[\frac{1}{2}, -x, \frac{1}{2}]$ | $[6, 8]$ |

Table 14: Wyckoff site: $4\mathbf{n}$, site symmetry: $.2'$

| No. | position | mapping |
|-----|-------------------------|----------|
| 1 | $[x, x, \frac{1}{4}]$ | $[1, 7]$ |
| 2 | $[x, -x, \frac{3}{4}]$ | $[2, 6]$ |
| 3 | $[-x, x, \frac{3}{4}]$ | $[3, 5]$ |
| 4 | $[-x, -x, \frac{1}{4}]$ | $[4, 8]$ |

Table 15: Wyckoff site: $4\mathbf{o}$, site symmetry: $.2'$

| No. | position | mapping |
|-----|-------------------------|----------|
| 1 | $[x, x, \frac{3}{4}]$ | $[1, 7]$ |
| 2 | $[x, -x, \frac{1}{4}]$ | $[2, 6]$ |
| 3 | $[-x, x, \frac{1}{4}]$ | $[3, 5]$ |
| 4 | $[-x, -x, \frac{3}{4}]$ | $[4, 8]$ |

Table 16: Wyckoff site: $8\mathbf{p}$, site symmetry: 1

| No. | position | mapping |
|-----|---------------|---------|
| 1 | $[x, y, z]$ | $[1]$ |
| 2 | $[x, -y, -z]$ | $[2]$ |
| 3 | $[-x, y, -z]$ | $[3]$ |
| 4 | $[-x, -y, z]$ | $[4]$ |

continued ...

Table 16

| No. | position | mapping |
|-----|-----------------------------|---------|
| 5 | $[-y, x, z + \frac{1}{2}]$ | [5] |
| 6 | $[y, -x, z + \frac{1}{2}]$ | [6] |
| 7 | $[y, x, \frac{1}{2} - z]$ | [7] |
| 8 | $[-y, -x, \frac{1}{2} - z]$ | [8] |