

# SG No. 89 $D_4^1$ $P422$ [ tetragonal ]

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

Table 1: Wyckoff site: 1a, site symmetry: 422

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

Table 2: Wyckoff site: 1b, site symmetry: 422

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

Table 3: Wyckoff site: 1c, site symmetry: 422

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

Table 4: Wyckoff site: 1d, site symmetry: 422

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

Table 5: Wyckoff site: 2e, site symmetry: 222.

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

Table 6: Wyckoff site: 2f, site symmetry: 222.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

*continued ...*

Table 16

| No. | position       | mapping |
|-----|----------------|---------|
| 5   | $[-x, y, -z]$  | [5]     |
| 6   | $[x, -y, -z]$  | [6]     |
| 7   | $[y, x, -z]$   | [7]     |
| 8   | $[-y, -x, -z]$ | [8]     |