

MSG No. 16.1  $P222$  [ Type I, orthorhombic ]

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

| No. | position    | mapping        |
|-----|-------------|----------------|
| 1   | $[0, 0, 0]$ | $[1, 2, 3, 4]$ |

Table 2: Wyckoff site: 1b, site symmetry: 222

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

Table 3: Wyckoff site: 1c, site symmetry: 222

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

Table 4: Wyckoff site: 1d, site symmetry: 222

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

Table 5: Wyckoff site: 1e, site symmetry: 222

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

Table 6: Wyckoff site: 1f, site symmetry: 222

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

Table 7: Wyckoff site:  $1\mathbf{g}$ , site symmetry:  $222$ 

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

Table 8: Wyckoff site:  $1\mathbf{h}$ , site symmetry:  $222$ 

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

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

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

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

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

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

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

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

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

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

| No. | position     | mapping  |
|-----|--------------|----------|
| 1   | $[0, y, 0]$  | $[1, 3]$ |
| 2   | $[0, -y, 0]$ | $[2, 4]$ |

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

| No. | position               | mapping  |
|-----|------------------------|----------|
| 1   | $[0, y, \frac{1}{2}]$  | $[1, 3]$ |
| 2   | $[0, -y, \frac{1}{2}]$ | $[2, 4]$ |

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

| No. | position               | mapping  |
|-----|------------------------|----------|
| 1   | $[\frac{1}{2}, y, 0]$  | $[1, 3]$ |
| 2   | $[\frac{1}{2}, -y, 0]$ | $[2, 4]$ |

Table 16: Wyckoff site:  $2\mathbf{p}$ , site symmetry:  $.2$ .

| No. | position                         | mapping  |
|-----|----------------------------------|----------|
| 1   | $[\frac{1}{2}, y, \frac{1}{2}]$  | $[1, 3]$ |
| 2   | $[\frac{1}{2}, -y, \frac{1}{2}]$ | $[2, 4]$ |

Table 17: Wyckoff site:  $2\mathbf{q}$ , site symmetry:  $..2$ 

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

Table 18: Wyckoff site:  $2\mathbf{r}$ , site symmetry:  $..2$ 

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

Table 19: Wyckoff site:  $2\mathbf{s}$ , site symmetry:  $\dots 2$ 

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

Table 20: Wyckoff site:  $2\mathbf{t}$ , site symmetry:  $\dots 2$ 

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

Table 21: Wyckoff site:  $4\mathbf{u}$ , site symmetry:  $1$ 

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