

MSG No. 51.289 *Pmma* [ Type I, orthorhombic ]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 2e, site symmetry:  $mm2$

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

Table 6: Wyckoff site: 2f, site symmetry:  $mm2$

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

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

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

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

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

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

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

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

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

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

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

Table 12: Wyckoff site: **81**, site symmetry: **1**

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