

MSG No. 53.329  $Pm'n'a'$  [ Type III, orthorhombic ]

Table 1: Wyckoff site:  $2\mathbf{a}$ , site symmetry:  $2/m' \dots$

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

Table 2: Wyckoff site:  $2\mathbf{b}$ , site symmetry:  $2/m' \dots$

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

Table 3: Wyckoff site:  $2\mathbf{c}$ , site symmetry:  $2/m' \dots$

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

Table 4: Wyckoff site:  $2\mathbf{d}$ , site symmetry:  $2/m' \dots$

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

Table 5: Wyckoff site:  $4\mathbf{e}$ , site symmetry:  $2 \dots$

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

Table 6: Wyckoff site: 4f, site symmetry: 2..

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

Table 7: Wyckoff site: 4g, site symmetry: .2.

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

Table 8: Wyckoff site: 4h, site symmetry: m'..

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

Table 9: Wyckoff site: 8i, site symmetry: 1

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