

MSG No. 13.70  $P_a2/c$  [ Type IV, monoclinic ]

Table 1: Wyckoff site: 4a, site symmetry:  $-1$

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

Table 2: Wyckoff site: 4b, site symmetry:  $-1'$

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

Table 3: Wyckoff site: 4c, site symmetry:  $-1$

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

Table 4: Wyckoff site: 4d, site symmetry:  $-1'$

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

Table 5: Wyckoff site: 4e, site symmetry: 2

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

*continued ...*

Table 5

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

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

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

Table 7: Wyckoff site: 8g, site symmetry: 1

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