

MSG No. 42.222  $Fm'm'2$  [ Type III, orthorhombic ]

Table 1: Wyckoff site: 4a, site symmetry:  $m'm'2$

| No. | position                            | mapping            |
|-----|-------------------------------------|--------------------|
| 1   | $[0, 0, z]$                         | $[1, 2, 3, 4]$     |
| 2   | $[0, \frac{1}{2}, z + \frac{1}{2}]$ | $[5, 6, 7, 8]$     |
| 3   | $[\frac{1}{2}, 0, z + \frac{1}{2}]$ | $[9, 10, 11, 12]$  |
| 4   | $[\frac{1}{2}, \frac{1}{2}, z]$     | $[13, 14, 15, 16]$ |

Table 2: Wyckoff site: 8b, site symmetry:  $. . 2$

| No. | position                                      | mapping   |
|-----|---|-----------|
| 1   | $[\frac{1}{4}, \frac{1}{4}, z]$               | $[1, 14]$ |
| 2   | $[\frac{3}{4}, \frac{3}{4}, z]$               | $[2, 13]$ |
| 3   | $[\frac{3}{4}, \frac{1}{4}, z]$               | $[3, 16]$ |
| 4   | $[\frac{1}{4}, \frac{3}{4}, z]$               | $[4, 15]$ |
| 5   | $[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$ | $[5, 10]$ |
| 6   | $[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}]$ | $[6, 9]$  |
| 7   | $[\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}]$ | $[7, 12]$ |
| 8   | $[\frac{1}{4}, \frac{1}{4}, z + \frac{1}{2}]$ | $[8, 11]$ |

Table 3: Wyckoff site: 8c, site symmetry:  $m' . .$

| No. | position                                | mapping    |
|-----|---|------------|
| 1   | $[0, y, z]$                             | $[1, 3]$   |
| 2   | $[0, -y, z]$                            | $[2, 4]$   |
| 3   | $[0, y + \frac{1}{2}, z + \frac{1}{2}]$ | $[5, 7]$   |
| 4   | $[0, \frac{1}{2} - y, z + \frac{1}{2}]$ | $[6, 8]$   |
| 5   | $[\frac{1}{2}, y, z + \frac{1}{2}]$     | $[9, 11]$  |
| 6   | $[\frac{1}{2}, -y, z + \frac{1}{2}]$    | $[10, 12]$ |
| 7   | $[\frac{1}{2}, y + \frac{1}{2}, z]$     | $[13, 15]$ |
| 8   | $[\frac{1}{2}, \frac{1}{2} - y, z]$     | $[14, 16]$ |

Table 4: Wyckoff site: 8d, site symmetry:  $.m' .$

| No. | position                                | mapping   |
|-----|---|-----------|
| 1   | $[x, 0, z]$                             | $[1, 4]$  |
| 2   | $[-x, 0, z]$                            | $[2, 3]$  |
| 3   | $[x, \frac{1}{2}, z + \frac{1}{2}]$     | $[5, 8]$  |
| 4   | $[-x, \frac{1}{2}, z + \frac{1}{2}]$    | $[6, 7]$  |
| 5   | $[x + \frac{1}{2}, 0, z + \frac{1}{2}]$ | $[9, 12]$ |

*continued ...*

Table 4

| No. | position                                | mapping  |
|-----|---|----------|
| 6   | $[\frac{1}{2} - x, 0, z + \frac{1}{2}]$ | [10, 11] |
| 7   | $[x + \frac{1}{2}, \frac{1}{2}, z]$     | [13, 16] |
| 8   | $[\frac{1}{2} - x, \frac{1}{2}, z]$     | [14, 15] |

Table 5: Wyckoff site: **16e**, 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]     |
| 5   | $[x, y + \frac{1}{2}, z + \frac{1}{2}]$  | [5]     |
| 6   | $[-x, \frac{1}{2} - y, z + \frac{1}{2}]$ | [6]     |
| 7   | $[-x, y + \frac{1}{2}, z + \frac{1}{2}]$ | [7]     |
| 8   | $[x, \frac{1}{2} - y, z + \frac{1}{2}]$  | [8]     |
| 9   | $[x + \frac{1}{2}, y, z + \frac{1}{2}]$  | [9]     |
| 10  | $[\frac{1}{2} - x, -y, z + \frac{1}{2}]$ | [10]    |
| 11  | $[\frac{1}{2} - x, y, z + \frac{1}{2}]$  | [11]    |
| 12  | $[x + \frac{1}{2}, -y, z + \frac{1}{2}]$ | [12]    |
| 13  | $[x + \frac{1}{2}, y + \frac{1}{2}, z]$  | [13]    |
| 14  | $[\frac{1}{2} - x, \frac{1}{2} - y, z]$  | [14]    |
| 15  | $[\frac{1}{2} - x, y + \frac{1}{2}, z]$  | [15]    |
| 16  | $[x + \frac{1}{2}, \frac{1}{2} - y, z]$  | [16]    |