

MSG No. 59.416  $P_{I}mmn$  [ Type IV, orthorhombic ]

Table 1: Wyckoff site: 2a, site symmetry:  $mmm'$

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

Table 2: Wyckoff site: 2b, site symmetry:  $mmm'$

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

Table 3: Wyckoff site: 2c, site symmetry:  $mmm'$

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

Table 4: Wyckoff site: 2d, site symmetry:  $mmm'$

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

Table 5: Wyckoff site: 4e, site symmetry:  $mm2$

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

Table 6: Wyckoff site: 4f, site symmetry: mm2

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

Table 7: Wyckoff site: 4g, site symmetry: 2'mm'

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

Table 8: Wyckoff site: 4h, site symmetry: 2'mm'

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

Table 9: Wyckoff site: 4i, site symmetry: m2'm'

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

Table 10: Wyckoff site: 4j, site symmetry: m2'm'

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

Table 11: Wyckoff site:  $8k$ , site symmetry:  $-1$ 

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

Table 12: Wyckoff site:  $8l$ , site symmetry:  $. . m'$ 

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

Table 13: Wyckoff site:  $8m$ , site symmetry:  $m . .$ 

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

Table 14: Wyckoff site:  $8n$ , site symmetry:  $. . m$ .

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

*continued ...*

Table 14

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

Table 15: Wyckoff site: 16o, site symmetry: 1

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