

MSG No. 66.493  $Cc'cm$  [ Type III, orthorhombic ]

Table 1: Wyckoff site: **4a**, site symmetry:  $22'2'$

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

Table 2: Wyckoff site: **4b**, site symmetry:  $22'2'$

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

Table 3: Wyckoff site: **4c**, site symmetry:  $\dots 2^1/m$

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

Table 4: Wyckoff site: **4d**, site symmetry:  $\dots 2^1/m$

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

Table 5: Wyckoff site: **4e**, site symmetry:  $\dots 2^1/m$

| No. | position                                  | mapping          |
|-----|---|------------------|
| 1   | $[\frac{1}{4}, \frac{1}{4}, 0]$           | $[1, 4, 14, 15]$ |
| 2   | $[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$ | $[2, 3, 13, 16]$ |

*continued ...*

Table 5

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

Table 6: Wyckoff site: 4f, site symmetry:  $\dots 2^3/m$ 

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

Table 7: Wyckoff site: 8g, site symmetry:  $2\ldots$ 

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

Table 8: Wyckoff site: 8h, site symmetry:  $.2^3.$ 

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

Table 9: Wyckoff site: 8i, site symmetry:  $\dots 2'$ 

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

Table 10: Wyckoff site: 8j, site symmetry:  $\dots 2'$ 

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

Table 11: Wyckoff site: 8k, site symmetry:  $\dots 2'$ 

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

Table 12: Wyckoff site: 8l, site symmetry:  $\dots m$ 

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

*continued ...*

Table 12

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

Table 13: Wyckoff site: 16m, site symmetry: 1

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