

MSG No. 66.500 C_{Accm} [Type IV, orthorhombic]

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

| No. | position | mapping |
|-----|---|-------------------------|
| 1 | $[\frac{3}{4}, \frac{3}{4}, 0]$ | [1,8,12,13,18,23,27,30] |
| 2 | $[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$ | [2,7,11,14,17,24,28,29] |
| 3 | $[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$ | [3,6,10,15,20,21,25,32] |
| 4 | $[\frac{1}{4}, \frac{1}{4}, 0]$ | [4,5,9,16,19,22,26,31] |

Table 2: Wyckoff site: 4b, site symmetry: $m'm'm$

| No. | position | mapping |
|-----|---|-------------------------|
| 1 | $[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$ | [1,8,12,13,18,23,27,30] |
| 2 | $[\frac{3}{4}, \frac{1}{4}, 0]$ | [2,7,11,14,17,24,28,29] |
| 3 | $[\frac{1}{4}, \frac{3}{4}, 0]$ | [3,6,10,15,20,21,25,32] |
| 4 | $[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$ | [4,5,9,16,19,22,26,31] |

Table 3: Wyckoff site: 8c, site symmetry: $2/m'..$

| No. | position | mapping |
|-----|---|---------------|
| 1 | $[\frac{3}{4}, 0, \frac{1}{4}]$ | [1,2,29,30] |
| 2 | $[\frac{1}{4}, 0, \frac{1}{4}]$ | [3,4,31,32] |
| 3 | $[\frac{1}{4}, 0, \frac{3}{4}]$ | [5,6,25,26] |
| 4 | $[\frac{3}{4}, 0, \frac{3}{4}]$ | [7,8,27,28] |
| 5 | $[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$ | [9,10,21,22] |
| 6 | $[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$ | [11,12,23,24] |
| 7 | $[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}]$ | [13,14,17,18] |
| 8 | $[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}]$ | [15,16,19,20] |

Table 4: Wyckoff site: 8d, site symmetry: $.2/m'.$

| No. | position | mapping |
|-----|---|---------------|
| 1 | $[0, \frac{3}{4}, \frac{1}{4}]$ | [1,3,21,23] |
| 2 | $[0, \frac{1}{4}, \frac{1}{4}]$ | [2,4,22,24] |
| 3 | $[0, \frac{1}{4}, \frac{3}{4}]$ | [5,7,17,19] |
| 4 | $[0, \frac{3}{4}, \frac{3}{4}]$ | [6,8,18,20] |
| 5 | $[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$ | [9,11,29,31] |
| 6 | $[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$ | [10,12,30,32] |
| 7 | $[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$ | [13,15,25,27] |
| 8 | $[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$ | [14,16,26,28] |

Table 5: Wyckoff site: 8e, site symmetry: $\dots 2/m$

| No. | position | mapping |
|-----|---|--------------------|
| 1 | $[0, 0, 0]$ | $[1, 4, 5, 8]$ |
| 2 | $[0, 0, \frac{1}{2}]$ | $[2, 3, 6, 7]$ |
| 3 | $[\frac{1}{2}, \frac{1}{2}, 0]$ | $[9, 12, 13, 16]$ |
| 4 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | $[10, 11, 14, 15]$ |
| 5 | $[0, \frac{1}{2}, \frac{1}{2}]$ | $[17, 20, 21, 24]$ |
| 6 | $[0, \frac{1}{2}, 0]$ | $[18, 19, 22, 23]$ |
| 7 | $[\frac{1}{2}, 0, \frac{1}{2}]$ | $[25, 28, 29, 32]$ |
| 8 | $[\frac{1}{2}, 0, 0]$ | $[26, 27, 30, 31]$ |

Table 6: Wyckoff site: 8f, site symmetry: 222

| No. | position | mapping |
|-----|---|--------------------|
| 1 | $[0, 0, \frac{1}{4}]$ | $[1, 2, 3, 4]$ |
| 2 | $[0, 0, \frac{3}{4}]$ | $[5, 6, 7, 8]$ |
| 3 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$ | $[9, 10, 11, 12]$ |
| 4 | $[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$ | $[13, 14, 15, 16]$ |
| 5 | $[0, \frac{1}{2}, \frac{3}{4}]$ | $[17, 18, 19, 20]$ |
| 6 | $[0, \frac{1}{2}, \frac{1}{4}]$ | $[21, 22, 23, 24]$ |
| 7 | $[\frac{1}{2}, 0, \frac{3}{4}]$ | $[25, 26, 27, 28]$ |
| 8 | $[\frac{1}{2}, 0, \frac{1}{4}]$ | $[29, 30, 31, 32]$ |

Table 7: Wyckoff site: 8g, site symmetry: $2'm'm$

| No. | position | mapping |
|-----|---|--------------------|
| 1 | $[x, \frac{3}{4}, 0]$ | $[1, 8, 18, 23]$ |
| 2 | $[x, \frac{1}{4}, \frac{1}{2}]$ | $[2, 7, 17, 24]$ |
| 3 | $[-x, \frac{3}{4}, \frac{1}{2}]$ | $[3, 6, 20, 21]$ |
| 4 | $[-x, \frac{1}{4}, 0]$ | $[4, 5, 19, 22]$ |
| 5 | $[x + \frac{1}{2}, \frac{1}{4}, 0]$ | $[9, 16, 26, 31]$ |
| 6 | $[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{2}]$ | $[10, 15, 25, 32]$ |
| 7 | $[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{2}]$ | $[11, 14, 28, 29]$ |
| 8 | $[\frac{1}{2} - x, \frac{3}{4}, 0]$ | $[12, 13, 27, 30]$ |

Table 8: Wyckoff site: 8h, site symmetry: $m'2'm$

| No. | position | mapping |
|-----|----------------------------------|------------------|
| 1 | $[\frac{3}{4}, y, 0]$ | $[1, 8, 27, 30]$ |
| 2 | $[\frac{3}{4}, -y, \frac{1}{2}]$ | $[2, 7, 28, 29]$ |
| 3 | $[\frac{1}{4}, y, \frac{1}{2}]$ | $[3, 6, 25, 32]$ |

continued ...

Table 8

| No. | position | mapping |
|-----|---|---------------|
| 4 | $[\frac{1}{4}, -y, 0]$ | [4,5,26,31] |
| 5 | $[\frac{1}{4}, y + \frac{1}{2}, 0]$ | [9,16,19,22] |
| 6 | $[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{2}]$ | [10,15,20,21] |
| 7 | $[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{2}]$ | [11,14,17,24] |
| 8 | $[\frac{3}{4}, \frac{1}{2} - y, 0]$ | [12,13,18,23] |

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

| No. | position | mapping |
|-----|---|--------------|
| 1 | $[\frac{3}{4}, \frac{3}{4}, z]$ | [1,12,23,30] |
| 2 | $[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z]$ | [2,11,24,29] |
| 3 | $[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z]$ | [3,10,21,32] |
| 4 | $[\frac{1}{4}, \frac{1}{4}, z]$ | [4,9,22,31] |
| 5 | $[\frac{1}{4}, \frac{1}{4}, -z]$ | [5,16,19,26] |
| 6 | $[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}]$ | [6,15,20,25] |
| 7 | $[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}]$ | [7,14,17,28] |
| 8 | $[\frac{3}{4}, \frac{3}{4}, -z]$ | [8,13,18,27] |

Table 10: Wyckoff site: 16j, site symmetry: $\dots 2$

| No. | position | mapping |
|-----|---|---------|
| 1 | $[0, 0, z]$ | [1,4] |
| 2 | $[0, 0, \frac{1}{2} - z]$ | [2,3] |
| 3 | $[0, 0, -z]$ | [5,8] |
| 4 | $[0, 0, z + \frac{1}{2}]$ | [6,7] |
| 5 | $[\frac{1}{2}, \frac{1}{2}, z]$ | [9,12] |
| 6 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$ | [10,11] |
| 7 | $[\frac{1}{2}, \frac{1}{2}, -z]$ | [13,16] |
| 8 | $[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$ | [14,15] |
| 9 | $[0, \frac{1}{2}, z + \frac{1}{2}]$ | [17,20] |
| 10 | $[0, \frac{1}{2}, -z]$ | [18,19] |
| 11 | $[0, \frac{1}{2}, \frac{1}{2} - z]$ | [21,24] |
| 12 | $[0, \frac{1}{2}, z]$ | [22,23] |
| 13 | $[\frac{1}{2}, 0, z + \frac{1}{2}]$ | [25,28] |
| 14 | $[\frac{1}{2}, 0, -z]$ | [26,27] |
| 15 | $[\frac{1}{2}, 0, \frac{1}{2} - z]$ | [29,32] |
| 16 | $[\frac{1}{2}, 0, z]$ | [30,31] |

Table 11: Wyckoff site: 16k, site symmetry: .2.

| No. | position | mapping |
|-----|---|---------|
| 1 | $[0, y, \frac{1}{4}]$ | [1,3] |
| 2 | $[0, -y, \frac{1}{4}]$ | [2,4] |
| 3 | $[0, -y, \frac{3}{4}]$ | [5,7] |
| 4 | $[0, y, \frac{3}{4}]$ | [6,8] |
| 5 | $[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{4}]$ | [9,11] |
| 6 | $[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{4}]$ | [10,12] |
| 7 | $[\frac{1}{2}, \frac{1}{2} - y, \frac{3}{4}]$ | [13,15] |
| 8 | $[\frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$ | [14,16] |
| 9 | $[0, y + \frac{1}{2}, \frac{3}{4}]$ | [17,19] |
| 10 | $[0, \frac{1}{2} - y, \frac{3}{4}]$ | [18,20] |
| 11 | $[0, \frac{1}{2} - y, \frac{1}{4}]$ | [21,23] |
| 12 | $[0, y + \frac{1}{2}, \frac{1}{4}]$ | [22,24] |
| 13 | $[\frac{1}{2}, y, \frac{3}{4}]$ | [25,27] |
| 14 | $[\frac{1}{2}, -y, \frac{3}{4}]$ | [26,28] |
| 15 | $[\frac{1}{2}, -y, \frac{1}{4}]$ | [29,31] |
| 16 | $[\frac{1}{2}, y, \frac{1}{4}]$ | [30,32] |

Table 12: Wyckoff site: 16l, site symmetry: 2..

| No. | position | mapping |
|-----|---|---------|
| 1 | $[x, 0, \frac{1}{4}]$ | [1,2] |
| 2 | $[-x, 0, \frac{1}{4}]$ | [3,4] |
| 3 | $[-x, 0, \frac{3}{4}]$ | [5,6] |
| 4 | $[x, 0, \frac{3}{4}]$ | [7,8] |
| 5 | $[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$ | [9,10] |
| 6 | $[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{4}]$ | [11,12] |
| 7 | $[\frac{1}{2} - x, \frac{1}{2}, \frac{3}{4}]$ | [13,14] |
| 8 | $[x + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$ | [15,16] |
| 9 | $[x, \frac{1}{2}, \frac{3}{4}]$ | [17,18] |
| 10 | $[-x, \frac{1}{2}, \frac{3}{4}]$ | [19,20] |
| 11 | $[-x, \frac{1}{2}, \frac{1}{4}]$ | [21,22] |
| 12 | $[x, \frac{1}{2}, \frac{1}{4}]$ | [23,24] |
| 13 | $[x + \frac{1}{2}, 0, \frac{3}{4}]$ | [25,26] |
| 14 | $[\frac{1}{2} - x, 0, \frac{3}{4}]$ | [27,28] |
| 15 | $[\frac{1}{2} - x, 0, \frac{1}{4}]$ | [29,30] |
| 16 | $[x + \frac{1}{2}, 0, \frac{1}{4}]$ | [31,32] |

Table 13: Wyckoff site: 16m, site symmetry: m'..

| No. | position | mapping |
|-----|-----------------------|---------|
| 1 | $[\frac{3}{4}, y, z]$ | [1,30] |

continued ...

Table 13

| No. | position | mapping |
|-----|---|---------|
| 2 | $[\frac{3}{4}, -y, \frac{1}{2} - z]$ | [2,29] |
| 3 | $[\frac{1}{4}, y, \frac{1}{2} - z]$ | [3,32] |
| 4 | $[\frac{1}{4}, -y, z]$ | [4,31] |
| 5 | $[\frac{1}{4}, -y, -z]$ | [5,26] |
| 6 | $[\frac{1}{4}, y, z + \frac{1}{2}]$ | [6,25] |
| 7 | $[\frac{3}{4}, -y, z + \frac{1}{2}]$ | [7,28] |
| 8 | $[\frac{3}{4}, y, -z]$ | [8,27] |
| 9 | $[\frac{1}{4}, y + \frac{1}{2}, z]$ | [9,22] |
| 10 | $[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{2} - z]$ | [10,21] |
| 11 | $[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{2} - z]$ | [11,24] |
| 12 | $[\frac{3}{4}, \frac{1}{2} - y, z]$ | [12,23] |
| 13 | $[\frac{3}{4}, \frac{1}{2} - y, -z]$ | [13,18] |
| 14 | $[\frac{3}{4}, y + \frac{1}{2}, z + \frac{1}{2}]$ | [14,17] |
| 15 | $[\frac{1}{4}, \frac{1}{2} - y, z + \frac{1}{2}]$ | [15,20] |
| 16 | $[\frac{1}{4}, y + \frac{1}{2}, -z]$ | [16,19] |

Table 14: Wyckoff site: 16n, site symmetry: .m'.

| No. | position | mapping |
|-----|---|---------|
| 1 | $[x, \frac{3}{4}, z]$ | [1,23] |
| 2 | $[x, \frac{1}{4}, \frac{1}{2} - z]$ | [2,24] |
| 3 | $[-x, \frac{3}{4}, \frac{1}{2} - z]$ | [3,21] |
| 4 | $[-x, \frac{1}{4}, z]$ | [4,22] |
| 5 | $[-x, \frac{1}{4}, -z]$ | [5,19] |
| 6 | $[-x, \frac{3}{4}, z + \frac{1}{2}]$ | [6,20] |
| 7 | $[x, \frac{1}{4}, z + \frac{1}{2}]$ | [7,17] |
| 8 | $[x, \frac{3}{4}, -z]$ | [8,18] |
| 9 | $[x + \frac{1}{2}, \frac{1}{4}, z]$ | [9,31] |
| 10 | $[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{2} - z]$ | [10,32] |
| 11 | $[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{2} - z]$ | [11,29] |
| 12 | $[\frac{1}{2} - x, \frac{3}{4}, z]$ | [12,30] |
| 13 | $[\frac{1}{2} - x, \frac{3}{4}, -z]$ | [13,27] |
| 14 | $[\frac{1}{2} - x, \frac{1}{4}, z + \frac{1}{2}]$ | [14,28] |
| 15 | $[x + \frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}]$ | [15,25] |
| 16 | $[x + \frac{1}{2}, \frac{1}{4}, -z]$ | [16,26] |

Table 15: Wyckoff site: 16o, site symmetry: ..m

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

continued ...

Table 15

| No. | position | mapping |
|-----|---|---------|
| 4 | $[-x, -y, 0]$ | [4,5] |
| 5 | $[x + \frac{1}{2}, y + \frac{1}{2}, 0]$ | [9,16] |
| 6 | $[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$ | [10,15] |
| 7 | $[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2}]$ | [11,14] |
| 8 | $[\frac{1}{2} - x, \frac{1}{2} - y, 0]$ | [12,13] |
| 9 | $[x, y + \frac{1}{2}, \frac{1}{2}]$ | [17,24] |
| 10 | $[x, \frac{1}{2} - y, 0]$ | [18,23] |
| 11 | $[-x, y + \frac{1}{2}, 0]$ | [19,22] |
| 12 | $[-x, \frac{1}{2} - y, \frac{1}{2}]$ | [20,21] |
| 13 | $[x + \frac{1}{2}, y, \frac{1}{2}]$ | [25,32] |
| 14 | $[x + \frac{1}{2}, -y, 0]$ | [26,31] |
| 15 | $[\frac{1}{2} - x, y, 0]$ | [27,30] |
| 16 | $[\frac{1}{2} - x, -y, \frac{1}{2}]$ | [28,29] |

Table 16: Wyckoff site: 32p, site symmetry: 1

| No. | position | mapping |
|-----|---|---------|
| 1 | $[x, y, z]$ | [1] |
| 2 | $[x, -y, \frac{1}{2} - z]$ | [2] |
| 3 | $[-x, y, \frac{1}{2} - z]$ | [3] |
| 4 | $[-x, -y, z]$ | [4] |
| 5 | $[-x, -y, -z]$ | [5] |
| 6 | $[-x, y, z + \frac{1}{2}]$ | [6] |
| 7 | $[x, -y, z + \frac{1}{2}]$ | [7] |
| 8 | $[x, y, -z]$ | [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 | $[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$ | [11] |
| 12 | $[\frac{1}{2} - x, \frac{1}{2} - y, z]$ | [12] |
| 13 | $[\frac{1}{2} - x, \frac{1}{2} - y, -z]$ | [13] |
| 14 | $[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$ | [14] |
| 15 | $[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$ | [15] |
| 16 | $[x + \frac{1}{2}, y + \frac{1}{2}, -z]$ | [16] |
| 17 | $[x, y + \frac{1}{2}, z + \frac{1}{2}]$ | [17] |
| 18 | $[x, \frac{1}{2} - y, -z]$ | [18] |
| 19 | $[-x, y + \frac{1}{2}, -z]$ | [19] |
| 20 | $[-x, \frac{1}{2} - y, z + \frac{1}{2}]$ | [20] |
| 21 | $[-x, \frac{1}{2} - y, \frac{1}{2} - z]$ | [21] |
| 22 | $[-x, y + \frac{1}{2}, z]$ | [22] |
| 23 | $[x, \frac{1}{2} - y, z]$ | [23] |
| 24 | $[x, y + \frac{1}{2}, \frac{1}{2} - z]$ | [24] |
| 25 | $[x + \frac{1}{2}, y, z + \frac{1}{2}]$ | [25] |
| 26 | $[x + \frac{1}{2}, -y, -z]$ | [26] |
| 27 | $[\frac{1}{2} - x, y, -z]$ | [27] |

continued ...

Table 16

| No. | position | mapping |
|-----|--|---------|
| 28 | $[\frac{1}{2} - x, -y, z + \frac{1}{2}]$ | [28] |
| 29 | $[\frac{1}{2} - x, -y, \frac{1}{2} - z]$ | [29] |
| 30 | $[\frac{1}{2} - x, y, z]$ | [30] |
| 31 | $[x + \frac{1}{2}, -y, z]$ | [31] |
| 32 | $[x + \frac{1}{2}, y, \frac{1}{2} - z]$ | [32] |