

MSG No. 129.422 P_I4/nmm [Type IV, tetragonal]

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: $m'mm$.

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

Table 4: Wyckoff site: 4d, site symmetry: $-4m2$

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

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

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

Table 6: Wyckoff site: 8f, site symmetry: $\dots 2/m$

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

Table 7: Wyckoff site: 8g, site symmetry: $2mm$.

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

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

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

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

| No. | position | mapping |
|-----|---|--------------|
| 1 | $[x, \frac{1}{4}, \frac{3}{4}]$ | [1,13,20,30] |
| 2 | $[\frac{1}{4}, x, \frac{3}{4}]$ | [2,16,23,27] |
| 3 | $[\frac{1}{4}, \frac{1}{2} - x, \frac{3}{4}]$ | [3,15,24,26] |

continued ...

Table 9

| No. | position | mapping |
|-----|---|--------------|
| 4 | $[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$ | [4,14,17,29] |
| 5 | $[-x, \frac{3}{4}, \frac{1}{4}]$ | [5,9,22,28] |
| 6 | $[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$ | [6,12,21,25] |
| 7 | $[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}]$ | [7,11,18,32] |
| 8 | $[\frac{3}{4}, -x, \frac{1}{4}]$ | [8,10,19,31] |

Table 10: Wyckoff site: 8j, site symmetry: $m'2'm$.

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

Table 11: Wyckoff site: 16k, site symmetry: $\dots 2$

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

Table 12: Wyckoff site: 16l, site symmetry: $\text{m}'\dots$

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

Table 13: Wyckoff site: 16m, site symmetry: $\dots\text{m}$

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

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

| No. | position | mapping |
|-----|-----------------------|---------|
| 1 | $[\frac{1}{4}, y, z]$ | [1,12] |

continued ...

Table 14

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

Table 15: Wyckoff site: 32o, site symmetry: 1

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

continued ...

Table 15

| No. | position | mapping |
|-----|---|---------|
| 26 | $[y, \frac{1}{2} - x, \frac{1}{2} - z]$ | [26] |
| 27 | $[\frac{1}{2} - y, x, \frac{1}{2} - z]$ | [27] |
| 28 | $[-x, y + \frac{1}{2}, z + \frac{1}{2}]$ | [28] |
| 29 | $[x + \frac{1}{2}, -y, z + \frac{1}{2}]$ | [29] |
| 30 | $[x, y, \frac{1}{2} - z]$ | [30] |
| 31 | $[-y, -x, z + \frac{1}{2}]$ | [31] |
| 32 | $[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$ | [32] |