

Table 1: Wyckoff site: 2a, site symmetry: 23 .

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

Table 2: Wyckoff site: 4b, site symmetry: $.32'$

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

Table 3: Wyckoff site: 4c, site symmetry: $.32'$

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

Table 4: Wyckoff site: 6d, site symmetry: $222..$

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

Table 5: Wyckoff site: 6e, site symmetry: $2.2'2'$

| No. | position | mapping |
|-----|---------------------------------|------------------|
| 1 | $[\frac{1}{4}, 0, \frac{1}{2}]$ | $[1, 2, 21, 22]$ |
| 2 | $[\frac{3}{4}, 0, \frac{1}{2}]$ | $[3, 4, 13, 14]$ |

continued ...

Table 5

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

Table 6: Wyckoff site: 6f, site symmetry: $2.2'2'$

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

Table 7: Wyckoff site: 8g, site symmetry: $.3.$

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

Table 8: Wyckoff site: 12h, site symmetry: $2..$

| No. | position | mapping |
|-----|---|----------|
| 1 | $[x, 0, 0]$ | [1, 2] |
| 2 | $[-x, 0, 0]$ | [3, 4] |
| 3 | $[0, x, 0]$ | [5, 12] |
| 4 | $[0, 0, x]$ | [6, 9] |
| 5 | $[0, 0, -x]$ | [7, 11] |
| 6 | $[0, -x, 0]$ | [8, 10] |
| 7 | $[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$ | [13, 14] |
| 8 | $[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$ | [15, 24] |
| 9 | $[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$ | [16, 23] |

continued ...

Table 8

| No. | position | mapping |
|-----|---|----------|
| 10 | $[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$ | [17, 19] |
| 11 | $[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$ | [18, 20] |
| 12 | $[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$ | [21, 22] |

Table 9: Wyckoff site: 12i, site symmetry: 2. .

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

Table 10: Wyckoff site: 12j, site symmetry: 2. .

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

Table 11: Wyckoff site: 12k, site symmetry: $\dots 2'$

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

Table 12: Wyckoff site: 12l, site symmetry: $\dots 2'$

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

Table 13: Wyckoff site: 24m, 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 | $[z, x, y]$ | [5] |
| 6 | $[y, z, x]$ | [6] |
| 7 | $[-y, z, -x]$ | [7] |
| 8 | $[-z, -x, y]$ | [8] |
| 9 | $[-y, -z, x]$ | [9] |

continued ...

Table 13

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