

Table 1: Wyckoff site: $1o$, site symmetry: $6/mmm$

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

Table 2: Wyckoff site: $2a$, site symmetry: $6mm$

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

Table 3: Wyckoff site: $6b$, site symmetry: $m2m$

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

Table 4: Wyckoff site: $6c$, site symmetry: $mm2$

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

Table 5: Wyckoff site: $12d$, site symmetry: $. . m$

| No. | position | mapping |
|-----|---------------|-----------|
| 1 | $[x, 0, z]$ | $[1, 22]$ |
| 2 | $[0, x, z]$ | $[3, 24]$ |
| 3 | $[-x, -x, z]$ | $[5, 20]$ |

continued ...

Table 5

| No. | position | mapping |
|-----|----------------|------------|
| 4 | $[-x, 0, z]$ | $[4, 19]$ |
| 5 | $[0, -x, z]$ | $[6, 21]$ |
| 6 | $[x, x, z]$ | $[2, 23]$ |
| 7 | $[0, x, -z]$ | $[9, 18]$ |
| 8 | $[x, 0, -z]$ | $[7, 16]$ |
| 9 | $[-x, -x, -z]$ | $[11, 14]$ |
| 10 | $[0, -x, -z]$ | $[12, 15]$ |
| 11 | $[-x, 0, -z]$ | $[10, 13]$ |
| 12 | $[x, x, -z]$ | $[8, 17]$ |

Table 6: Wyckoff site: $12\mathbf{e}$, site symmetry: $\bar{6}m$.

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

Table 7: Wyckoff site: $12\mathbf{f}$, site symmetry: $m\bar{3}m$.

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

Table 8: Wyckoff site: $24g$, site symmetry: 1

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