

Table 1: Wyckoff site: 2a, site symmetry: $m'm'm'$.

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

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

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

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

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

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

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

Table 5: Wyckoff site: 2e, site symmetry: $-4m'2'$

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

Table 6: Wyckoff site: 2f, site symmetry: $-4m'2'$

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

Table 7: Wyckoff site: 4g, site symmetry: $2m'm'$.

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

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

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

Table 9: Wyckoff site: 4i, site symmetry: $2m'm'$.

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

Table 10: Wyckoff site: 4j, site symmetry: $m'2m'$.

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

Table 11: Wyckoff site: 4k, site symmetry: $m'2m'$.

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

Table 12: Wyckoff site: $4l$, site symmetry: $m'2m'$.

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

Table 13: Wyckoff site: $4m$, site symmetry: $m'2m'$.

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

Table 14: Wyckoff site: $8n$, site symmetry: $. . 2'$

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

Table 15: Wyckoff site: $8o$, site symmetry: $.m'$.

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

Table 16: Wyckoff site: $8p$, site symmetry: $.m'$.

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

Table 17: Wyckoff site: $8q$, site symmetry: m' .

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

Table 18: Wyckoff site: $16r$, 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 | $[y, -x, \frac{1}{2} - z]$ | [5] |
| 6 | $[-y, x, \frac{1}{2} - z]$ | [6] |
| 7 | $[-y, -x, z + \frac{1}{2}]$ | [7] |
| 8 | $[y, x, z + \frac{1}{2}]$ | [8] |
| 9 | $[-y, x, z + \frac{1}{2}]$ | [9] |
| 10 | $[y, -x, z + \frac{1}{2}]$ | [10] |
| 11 | $[y, x, \frac{1}{2} - z]$ | [11] |
| 12 | $[-y, -x, \frac{1}{2} - z]$ | [12] |
| 13 | $[-x, -y, -z]$ | [13] |
| 14 | $[-x, y, z]$ | [14] |
| 15 | $[x, -y, z]$ | [15] |
| 16 | $[x, y, -z]$ | [16] |