

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: $-42'm'$

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

Table 3: Wyckoff site: 2c, 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 4: Wyckoff site: 2d, site symmetry: $-42'm'$

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

Table 5: Wyckoff site: 4e, site symmetry: $22'2'$

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

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

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

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

| No. | position | mapping |
|-----|---------------------------|----------------|
| 1 | $[0, 0, z]$ | [1, 2, 15, 16] |
| 2 | $[0, 0, -z]$ | [3, 4, 13, 14] |
| 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: $2.m'm'$

| No. | position | mapping |
|-----|---|----------------|
| 1 | $[\frac{1}{2}, \frac{1}{2}, z]$ | [1, 2, 15, 16] |
| 2 | $[\frac{1}{2}, \frac{1}{2}, -z]$ | [3, 4, 13, 14] |
| 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: $m'.2m'$

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

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

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

Table 11: Wyckoff site: $8k$, site symmetry: $2..$

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

Table 12: Wyckoff site: $8l$, site symmetry: $.2'$.

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

Table 13: Wyckoff site: $8m$, site symmetry: $.2'$.

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

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

| No. | position | mapping |
|-----|---------------|---------|
| 1 | $[x, y, 0]$ | [1,14] |
| 2 | $[-x, -y, 0]$ | [2,13] |
| 3 | $[y, x, 0]$ | [3,16] |

continued ...

Table 14

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

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

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

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

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