

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 11: Wyckoff site: $8k$, site symmetry: -1

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

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

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

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

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

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

| No. | position | mapping |
|-----|-------------------------------------|---------|
| 1 | $[x, y, \frac{1}{4}]$ | [1,16] |
| 2 | $[x, \frac{1}{2} - y, \frac{1}{4}]$ | [2,15] |
| 3 | $[\frac{1}{2} - x, y, \frac{1}{4}]$ | [3,14] |

continued ...

Table 14

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

Table 15: Wyckoff site: 16o, site symmetry: 1

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