

Table 1: Wyckoff site: 4a, site symmetry: $\dots 2/m$

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

Table 2: Wyckoff site: 4b, site symmetry: $\dots 2/m'$

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

Table 3: Wyckoff site: 4c, site symmetry: $\dots 2/m$

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

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

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

Table 5: Wyckoff site: 8e, site symmetry: $\dots 2$

| No. | position | mapping |
|-----|----------------------------------|----------|
| 1 | $[0, 0, z]$ | $[1, 4]$ |
| 2 | $[\frac{1}{2}, \frac{1}{2}, -z]$ | $[2, 3]$ |

continued ...

Table 5

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

Table 6: Wyckoff site: **8f**, site symmetry: $\bar{3}2$

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

Table 7: Wyckoff site: **8g**, site symmetry: $\bar{3}m$

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

Table 8: Wyckoff site: **8h**, site symmetry: $\bar{3}m'$

| No. | position | mapping |
|-----|---|-----------|
| 1 | $[x, y, \frac{1}{4}]$ | $[1, 16]$ |
| 2 | $[x + \frac{1}{2}, \frac{1}{2} - y, \frac{3}{4}]$ | $[2, 15]$ |
| 3 | $[\frac{1}{2} - x, y + \frac{1}{2}, \frac{3}{4}]$ | $[3, 14]$ |
| 4 | $[-x, -y, \frac{1}{4}]$ | $[4, 13]$ |
| 5 | $[-x, -y, \frac{3}{4}]$ | $[5, 12]$ |

continued ...

Table 8

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

Table 9: Wyckoff site: 16i, site symmetry: 1

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