

Table 1: Wyckoff site: 2a, site symmetry: $-4'm2'$

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

Table 2: Wyckoff site: 2b, site symmetry: $-4'm2'$

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

Table 3: Wyckoff site: 2c, site symmetry: $4mm$

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

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

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

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

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

Table 6: Wyckoff site: 4f, site symmetry: $2mm$.

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

Table 7: Wyckoff site: 8g, site symmetry: $..2'$

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

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

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

Table 9: Wyckoff site: 8i, site symmetry: $.m$.

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

continued ...

Table 9

| No. | position | mapping |
|-----|-------------------------|---------|
| 8 | $[-y, \frac{3}{4}, -z]$ | [12,15] |

Table 10: Wyckoff site: 8j, site symmetry: $\bar{3}m$

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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