

Table 1: Wyckoff site: 2a, site symmetry: 3.2

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

Table 2: Wyckoff site: 2b, site symmetry: 3.2'

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

Table 3: Wyckoff site: 2c, site symmetry: 3.2

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

Table 4: Wyckoff site: 2d, site symmetry: 3.2'

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

Table 5: Wyckoff site: 2e, site symmetry: 3.2

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

Table 6: Wyckoff site: 2f, site symmetry: 3.2'

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

Table 7: Wyckoff site: 4g, site symmetry: 3..

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

Table 8: Wyckoff site: 4h, site symmetry: 3..

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

Table 9: Wyckoff site: 4i, site symmetry: 3..

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

Table 10: Wyckoff site: 6j, site symmetry: ..2

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

Table 11: Wyckoff site: 6k, site symmetry: ..2'

| No. | position | mapping |
|-----|------------------------|-----------|
| 1 | $[x, -x, \frac{1}{4}]$ | $[1, 12]$ |
| 2 | $[x, 2x, \frac{1}{4}]$ | $[2, 10]$ |

continued ...

Table 11

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

Table 12: Wyckoff site: 121, site symmetry: 1

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