

Table 1: Wyckoff site: 2a, site symmetry: 2.22

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

Table 2: Wyckoff site: 2b, site symmetry: 2.22

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

Table 3: Wyckoff site: 2c, site symmetry: 4..

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

Table 4: Wyckoff site: 4d, site symmetry: 2..

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

Table 5: Wyckoff site: 4e, site symmetry: ..2

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

Table 6: Wyckoff site: $4f$, site symmetry: $\dots 2$

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

Table 7: Wyckoff site: $8g$, site symmetry: 1

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