

Table 1: Wyckoff site: 6a, site symmetry: $2'..$

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

Table 2: Wyckoff site: 6b, site symmetry: $2'..$

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

Table 3: Wyckoff site: 12c, site symmetry: 1

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