

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

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

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

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

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 | $[x - y, -y, -z]$ | $[7]$ |
| 8 | $[y, x, \frac{2}{3} - z]$ | $[8]$ |
| 9 | $[-x, -x + y, \frac{1}{3} - z]$ | $[9]$ |
| 10 | $[x, x - y, \frac{5}{6} - z]$ | $[10]$ |
| 11 | $[-x + y, y, \frac{1}{2} - z]$ | $[11]$ |
| 12 | $[-y, -x, \frac{1}{6} - z]$ | $[12]$ |