

Table 1: Wyckoff site: **3a**, site symmetry: $.2.$

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

Table 2: Wyckoff site: **3b**, site symmetry: $.2.$

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

Table 3: Wyckoff site: **6c**, site symmetry: 1

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