

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]     |