

Table 1: Wyckoff site: 6a, site symmetry:  $\dots 2$

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

Table 2: Wyckoff site: 6b, site symmetry:  $\dots 2'$

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

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

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