

MSG No. 146.12 R_I3 [Type IV, trigonal]

Table 1: Wyckoff site: **6a**, site symmetry: 3..

| No. | position | mapping |
|-----|---|--------------|
| 1 | $[0, 0, z]$ | [1, 2, 3] |
| 2 | $[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{3}]$ | [4, 5, 6] |
| 3 | $[\frac{1}{3}, \frac{2}{3}, z + \frac{2}{3}]$ | [7, 8, 9] |
| 4 | $[0, 0, z + \frac{1}{2}]$ | [10, 11, 12] |
| 5 | $[\frac{2}{3}, \frac{1}{3}, z + \frac{5}{6}]$ | [13, 14, 15] |
| 6 | $[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{6}]$ | [16, 17, 18] |

Table 2: Wyckoff site: **18b**, site symmetry: 1

| No. | position | mapping |
|-----|--|---------|
| 1 | $[x, y, z]$ | [1] |
| 2 | $[-y, x - y, z]$ | [2] |
| 3 | $[-x + y, -x, z]$ | [3] |
| 4 | $[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$ | [4] |
| 5 | $[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{1}{3}]$ | [5] |
| 6 | $[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{1}{3}]$ | [6] |
| 7 | $[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$ | [7] |
| 8 | $[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{2}{3}]$ | [8] |
| 9 | $[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{2}{3}]$ | [9] |
| 10 | $[x, y, z + \frac{1}{2}]$ | [10] |
| 11 | $[-y, x - y, z + \frac{1}{2}]$ | [11] |
| 12 | $[-x + y, -x, z + \frac{1}{2}]$ | [12] |
| 13 | $[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{5}{6}]$ | [13] |
| 14 | $[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{5}{6}]$ | [14] |
| 15 | $[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{5}{6}]$ | [15] |
| 16 | $[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{1}{6}]$ | [16] |
| 17 | $[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{1}{6}]$ | [17] |
| 18 | $[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{1}{6}]$ | [18] |