

MSG No. 151.29 $P3_112$ [Type I, trigonal]

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

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

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

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

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 | $[x, x - y, -z]$ | [4] |
| 5 | $[-x + y, y, \frac{1}{3} - z]$ | [5] |
| 6 | $[-y, -x, \frac{2}{3} - z]$ | [6] |