

MSG No. 173.130 $P6_31'$ [Type II, hexagonal]

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

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

Table 2: Wyckoff site: 2b, site symmetry: $3..1'$

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

Table 3: Wyckoff site: 6c, site symmetry: $11'$

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