

MPG No. 20.3.73  $\bar{3}'m$  (-3'm1 setting) [ Type III, trigonal ]

Table 1: Wyckoff site: 1o, site symmetry: -3'm1

| No. | position  | mapping                      |
|-----|-----------|------------------------------|
| 1   | [0, 0, 0] | [1,2,3,4,5,6,7,8,9,10,11,12] |

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

| No. | position   | mapping          |
|-----|------------|------------------|
| 1   | [0, 0, z]  | [1,2,3,4,5,6]    |
| 2   | [0, 0, -z] | [7,8,9,10,11,12] |

Table 3: Wyckoff site: 6b, site symmetry: .2'.

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

Table 4: Wyckoff site: 6c, site symmetry: .m.

| No. | position      | mapping |
|-----|---------------|---------|
| 1   | [x, -x, z]    | [1,5]   |
| 2   | [x, 2x, z]    | [2,6]   |
| 3   | [-2x, -x, z]  | [3,4]   |
| 4   | [-x, x, -z]   | [8,10]  |
| 5   | [2x, x, -z]   | [7,12]  |
| 6   | [-x, -2x, -z] | [9,11]  |

Table 5: Wyckoff site: 12d, site symmetry: 1

| No. | position        | mapping |
|-----|-----------------|---------|
| 1   | [x, y, z]       | [1]     |
| 2   | [-y, x - y, z]  | [2]     |
| 3   | [-x + y, -x, z] | [3]     |

*continued ...*

Table 5

| No. | position           | mapping |
|-----|--------------------|---------|
| 4   | $[y, x, -z]$       | [8]     |
| 5   | $[x - y, -y, -z]$  | [7]     |
| 6   | $[-x, -x + y, -z]$ | [9]     |
| 7   | $[-x, -y, -z]$     | [10]    |
| 8   | $[y, -x + y, -z]$  | [11]    |
| 9   | $[x - y, x, -z]$   | [12]    |
| 10  | $[-y, -x, z]$      | [5]     |
| 11  | $[-x + y, y, z]$   | [4]     |
| 12  | $[x, x - y, z]$    | [6]     |