

MPG No. 23.5.86 $6'/m'$ [Type III, hexagonal]

Table 1: Wyckoff site: 1o, site symmetry: $6'/m'$

| 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: $6'..$

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

Table 3: Wyckoff site: 6b, site symmetry: $m'..$

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

Table 4: Wyckoff site: 12c, 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, -y, z] | [8] |
| 5 | [y, -x + y, z] | [9] |
| 6 | [x - y, x, z] | [7] |
| 7 | [-x, -y, -z] | [4] |
| 8 | [y, -x + y, -z] | [5] |
| 9 | [x - y, x, -z] | [6] |
| 10 | [x, y, -z] | [11] |
| 11 | [-y, x - y, -z] | [12] |
| 12 | [-x + y, -x, -z] | [10] |