

MPG No. 22.1.79 $\bar{6}$ [Type I, hexagonal]

Table 1: Wyckoff site: **1o**, site symmetry: **-6**

| No. | position | mapping |
|-----|-----------|---------------|
| 1 | [0, 0, 0] | [1,2,3,4,5,6] |

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

| No. | position | mapping |
|-----|---------------|---------|
| 1 | [0, 0, z] | [1,2,3] |
| 2 | [0, 0, $-z$] | [4,5,6] |

Table 3: Wyckoff site: **3b**, site symmetry: **m..**

| No. | position | mapping |
|-----|------------------------|---------|
| 1 | [x , y , 0] | [1,5] |
| 2 | [$-y$, $x - y$, 0] | [2,6] |
| 3 | [$-x + y$, $-x$, 0] | [3,4] |

Table 4: Wyckoff site: **6c**, 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 , $-z$] | [5] |
| 5 | [$-y$, $x - y$, $-z$] | [6] |
| 6 | [$-x + y$, $-x$, $-z$] | [4] |