

PG No. 19  $C_{3v}$   $3m$  (3m1 setting) [ trigonal ]

Table 1: Wyckoff site: **1a**, site symmetry: **3m**.

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

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

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

Table 3: 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   | [-y, -x, z]     | [4]     |
| 5   | [-x + y, y, z]  | [5]     |
| 6   | [x, x - y, z]   | [6]     |