

PG No. 23  $C_{6h}$   $6/m$  [ 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, 4, 5, 6]
2	[0, 0, $-z$ ]	[7, 8, 9, 10, 11, 12]

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

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

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	[ $-x$ , $-y$ , $z$ ]	[4]
5	[ $y$ , $-x + y$ , $z$ ]	[5]
6	[ $x - y$ , $x$ , $z$ ]	[6]
7	[ $-x$ , $-y$ , $-z$ ]	[7]
8	[ $y$ , $-x + y$ , $-z$ ]	[8]
9	[ $x - y$ , $x$ , $-z$ ]	[9]
10	[ $x$ , $y$ , $-z$ ]	[10]
11	[ $-y$ , $x - y$ , $-z$ ]	[11]
12	[ $-x + y$ , $-x$ , $-z$ ]	[12]