

MPG No. 23.3.84 $6'/m$ [Type III, hexagonal]

Table 1: Wyckoff site: **1o**, site symmetry: $6'/\mathbf{m}$

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: $\mathbf{m}..$

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

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