

MPG No. 23.4.85 $6/m'$ [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, 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]	[3, 12]
3	[-x + y, -x, 0]	[5, 8]
4	[-x, -y, 0]	[4, 7]
5	[y, -x + y, 0]	[6, 9]
6	[x - y, x, 0]	[2, 11]

Table 4: Wyckoff site: 12c, site symmetry: 1

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