

MSG No. 175.137 $P6/m$ [Type I, hexagonal]

Table 1: Wyckoff site: 1a, 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: 1b, site symmetry: $6/m..$

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]$

Table 3: Wyckoff site: 2c, site symmetry: $-6..$

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[1, 3, 5, 8, 10, 12]$
2	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[2, 4, 6, 7, 9, 11]$

Table 4: Wyckoff site: 2d, site symmetry: $-6..$

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}]$	$[1, 3, 5, 8, 10, 12]$
2	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}]$	$[2, 4, 6, 7, 9, 11]$

Table 5: Wyckoff site: 2e, 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 6: Wyckoff site: 3f, site symmetry: $2/m..$

No.	position	mapping
1	$[\frac{1}{2}, 0, 0]$	$[1, 4, 7, 10]$
2	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[2, 5, 8, 11]$
3	$[0, \frac{1}{2}, 0]$	$[3, 6, 9, 12]$

Table 7: Wyckoff site: $3g$, site symmetry: $2/m$.

No.	position	mapping
1	$[\frac{1}{2}, 0, \frac{1}{2}]$	[1,4,7,10]
2	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[2,5,8,11]
3	$[0, \frac{1}{2}, \frac{1}{2}]$	[3,6,9,12]

Table 8: Wyckoff site: $4h$, site symmetry: 3 .

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	[1,3,5]
2	$[\frac{2}{3}, \frac{1}{3}, z]$	[2,4,6]
3	$[\frac{2}{3}, \frac{1}{3}, -z]$	[7,9,11]
4	$[\frac{1}{3}, \frac{2}{3}, -z]$	[8,10,12]

Table 9: Wyckoff site: $6i$, site symmetry: 2 .

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	[1,4]
2	$[\frac{1}{2}, \frac{1}{2}, z]$	[2,5]
3	$[0, \frac{1}{2}, z]$	[3,6]
4	$[\frac{1}{2}, 0, -z]$	[7,10]
5	$[\frac{1}{2}, \frac{1}{2}, -z]$	[8,11]
6	$[0, \frac{1}{2}, -z]$	[9,12]

Table 10: Wyckoff site: $6j$, site symmetry: m .

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

Table 11: Wyckoff site: $6k$, site symmetry: m .

No.	position	mapping
1	$[x, y, \frac{1}{2}]$	[1,10]

continued ...

Table 11

No.	position	mapping
2	$[x - y, x, \frac{1}{2}]$	[2,11]
3	$[-y, x - y, \frac{1}{2}]$	[3,12]
4	$[-x, -y, \frac{1}{2}]$	[4,7]
5	$[-x + y, -x, \frac{1}{2}]$	[5,8]
6	$[y, -x + y, \frac{1}{2}]$	[6,9]

Table 12: Wyckoff site: 121, site symmetry: 1

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