

MSG No. 175.139 $P6'/m$ [Type III, 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	$[\frac{1}{3}, \frac{2}{3}, 0]$	$[1, 2, 3, 4, 5, 6]$
2	$[\frac{2}{3}, \frac{1}{3}, 0]$	$[7, 8, 9, 10, 11, 12]$

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

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

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

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

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

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

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

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

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

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

Table 10: Wyckoff site: $6j$, site symmetry: 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	$[x-y, x, 0]$	[7,12]
5	$[-x, -y, 0]$	[8,10]
6	$[y, -x+y, 0]$	[9,11]

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

No.	position	mapping
1	$[x, y, \frac{1}{2}]$	[1,5]

continued ...

Table 11

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

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

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