

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: $2'/\text{m..}$

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: $2'..\cdot$

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: $\text{m}..\cdot$

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: $\text{m}..\cdot$

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]