

MSG No. 175.141  $P6'/m'$  [ 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]	[1,2,3,10,11,12]
2	[ $\frac{2}{3}$ , $\frac{1}{3}$ , 0]	[4,5,6,7,8,9]

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

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

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]	[1,4,8,11]
2	[0, $\frac{1}{2}$ , 0]	[2,5,9,12]
3	[ $\frac{1}{2}$ , $\frac{1}{2}$ , 0]	[3,6,7,10]

Table 7: Wyckoff site: 3g, site symmetry:  $2'/\mathbf{m}'\dots$ 

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

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

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

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

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	$[\frac{1}{2}, 0, -z]$	[4,11]
5	$[0, \frac{1}{2}, -z]$	[5,12]
6	$[\frac{1}{2}, \frac{1}{2}, -z]$	[6,10]

Table 10: Wyckoff site: 6j, site symmetry:  $\mathbf{m}'\dots$ 

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

Table 11: Wyckoff site: 6k, site symmetry:  $\mathbf{m}'\dots$ 

No.	position	mapping
1	$[x, y, \frac{1}{2}]$	[1,11]

*continued ...*

Table 11

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

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	$[-x, -y, -z]$	[4]
5	$[y, -x + y, -z]$	[5]
6	$[x - y, x, -z]$	[6]
7	$[x - y, x, z]$	[7]
8	$[-x, -y, z]$	[8]
9	$[y, -x + y, z]$	[9]
10	$[-x + y, -x, -z]$	[10]
11	$[x, y, -z]$	[11]
12	$[-y, x - y, -z]$	[12]