

MSG No. 189.223  $P\bar{6}'2'm$  [ Type III, hexagonal ]

Table 1: Wyckoff site: **1a**, site symmetry:  $-6'2'm$

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:  $-6'2'm$

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:  $3.m$

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:  $m'2'm$

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

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

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

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: ...m

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

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

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

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

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	$[-x, -x + y, \frac{1}{2}]$	[4,9]
5	$[x - y, -y, \frac{1}{2}]$	[5,7]
6	$[y, x, \frac{1}{2}]$	[6,8]

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