

MSG No. 187.212 $P\bar{6}'m2'$ [Type III, hexagonal]

Table 1: Wyckoff site: **1a**, site symmetry: $-6'm2'$

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: $-6'm2'$

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: **1c**, site symmetry: $-6'm2'$

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

Table 4: Wyckoff site: **1d**, site symmetry: $-6'm2'$

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

Table 5: Wyckoff site: **1e**, site symmetry: $-6'm2'$

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

Table 6: Wyckoff site: **1f**, site symmetry: $-6'm2'$

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

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

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

Table 8: Wyckoff site: 2h, site symmetry: 3m.

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

Table 9: Wyckoff site: 2i, site symmetry: 3m.

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

Table 10: Wyckoff site: 3j, site symmetry: m'm2'

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

Table 11: Wyckoff site: 3k, site symmetry: m'm2'

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

Table 12: Wyckoff site: 6l, site symmetry: m'..

No.	position	mapping
1	[x, y, 0]	[1,11]
2	[-y, x - y, 0]	[2,12]

continued ...

Table 12

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

Table 13: Wyckoff site: 6m, site symmetry: m' . .

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

Table 14: Wyckoff site: 6n, site symmetry: .m .

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

Table 15: Wyckoff site: 12o, site symmetry: 1

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

continued ...

Table 15

No.	position	mapping
12	$[-y, x - y, -z]$	[12]