

MSG No. 187.211 $P\bar{6}'m'2$ [Type III, hexagonal]

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

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: $-6'm'2$

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: $-6'm'2$

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: $-6'm'2$

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: $-6'm'2$

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: $-6'm'2$

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: $3\bar{m}'$.

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

Table 8: Wyckoff site: 2h, site symmetry: $3\bar{m}'$.

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

Table 9: Wyckoff site: 2i, site symmetry: $3\bar{m}'$.

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

Table 10: Wyckoff site: 3j, site symmetry: $\bar{m}'\bar{m}'2$

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

Table 11: Wyckoff site: 3k, site symmetry: $\bar{m}'\bar{m}'2$

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

Table 12: Wyckoff site: 6l, site symmetry: $\bar{m}'\dots$

No.	position	mapping
1	$[x, y, 0]$	$[1, 8]$
2	$[-y, x - y, 0]$	$[2, 9]$

continued ...

Table 12

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

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

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

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

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

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

continued ...

Table 15

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