

MSG No. 189.225 $P\bar{6}2'm'$ [Type III, hexagonal]

Table 1: Wyckoff site: **1a**, site symmetry: $-62'm'$

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: $-62'm'$

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: $3.m'$

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

Table 6: Wyckoff site: **3f**, site symmetry: $m2'm'$

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: $m\bar{2}'m'$

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	$[\frac{1}{3}, \frac{2}{3}, -z]$	[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: .. m'

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

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

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

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

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	$[x - y, -y, \frac{1}{2}]$	[7,11]
5	$[y, x, \frac{1}{2}]$	[8,12]
6	$[-x, -x + y, \frac{1}{2}]$	[9,10]

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