MSG No. 189.221 $P\bar{6}2m$ [Type I, hexagonal]

Table 1: Wyckoff site: `1a`, site symmetry: `-62m`

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: `-62m`

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

Table 3: Wyckoff site: `2c`, site symmetry: `-6..`

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

Table 4: Wyckoff site: `2d`, site symmetry: `-6..`

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

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: `m2m`

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

Table 7: Wyckoff site: 3g, site symmetry: m2m

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

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

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

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

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

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

No.	position	mapping
1	$\left[x, y, \frac{1}{2}\right]$	[1,8]

continued ...

Table 11

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

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