MSG No. 162.77 $P\bar{3}1m'$ [Type III, trigonal]

Table 1: Wyckoff site: `1a`, site symmetry: `-3.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: `-3.m'`

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: `3.2'`

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: `3.2'`

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: `..2'/m'`

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

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

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

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

Table 10: Wyckoff site: `6j`, site symmetry: `..2'`

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

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

No.	position	mapping
1	$[x, 0, z]$	`[1,11]`

continued ...

Table 11

No.	position	mapping
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 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	$[-x,\, -y,\, -z]$	[4]
5	$[y,\, -x+y,\, -z]$	[5]
6	$[x-y,\, x,\, -z]$	[6]
7	$[x,\, x-y,\, -z]$	[7]
8	$[-x+y,\, y,\, -z]$	[8]
9	$[-y,\, -x,\, -z]$	[9]
10	$[-x,\, -x+y,\, z]$	[10]
11	$[x-y,\, -y,\, z]$	[11]
12	$[y,\, x,\, z]$	[12]