MSG No. 162.76 $P\bar{3}'1m'$ [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	$\left[\frac{1}{3},\ \frac{2}{3},\ 0\right]$	`[1,2,3,4,5,6]`
2	$\left[\frac{2}{3},\ \frac{1}{3},\ 0\right]$	`[7,8,9,10,11,12]`

Table 4: Wyckoff site: `2d`, site symmetry: `3.2`

No.	position	mapping
1	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{2}\right]$	`[1,2,3,4,5,6]`
2	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{2}\right]$	`[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: `..2/m'`

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

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

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

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	$\left[\frac{1}{3}, \frac{2}{3}, -z\right]$	`[4,5,6]`
3	$\left[\frac{2}{3}, \frac{1}{3}, -z\right]$	`[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	$[x, -x, 0]$	`[1,6]`
2	$[x, 2x, 0]$	`[2,4]`
3	$[-2x, -x, 0]$	`[3,5]`
4	$[-x, x, 0]$	`[7,12]`
5	$[-x, -2x, 0]$	`[8,10]`
6	$[2x, x, 0]$	`[9,11]`

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

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

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	$[x,\ x,\ -z]$	`[4,9]`
5	$[-x,\ 0,\ -z]$	`[5,7]`
6	$[0,\ -x,\ -z]$	`[6,8]`

Table 12: Wyckoff site: `12l`, 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	$[-x,\ -y,\ -z]$	`[7]`
8	$[y,\ -x+y,\ -z]$	`[8]`
9	$[x-y,\ x,\ -z]$	`[9]`
10	$[-x,\ -x+y,\ z]$	`[10]`
11	$[x-y,\ -y,\ z]$	`[11]`
12	$[y,\ x,\ z]$	`[12]`