MSG No. 164.85 $P\bar{3}m1$ [Type I, trigonal]

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

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: `-3m.`

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: `3m.`

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

Table 4: Wyckoff site: `2d`, site symmetry: `3m.`

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

Table 5: Wyckoff site: `3e`, site symmetry: `.2/m.`

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

Table 6: Wyckoff site: `3f`, site symmetry: `.2/m.`

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

Table 7: Wyckoff site: `6g`, site symmetry: `.2.`

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

Table 8: Wyckoff site: `6h`, site symmetry: `.2.`

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

Table 9: Wyckoff site: `6i`, 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	$[2x,\ x,\ -z]$	`[4,9]`
5	$[-x,\ x,\ -z]$	`[5,7]`
6	$[-x,\ -2x,\ -z]$	`[6,8]`

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

continued ...

Table 10

No.	position	mapping
10	$[-x+y,\ y,\ z]$	`[10]`
11	$[-y,\ -x,\ z]$	`[11]`
12	$[x,\ x-y,\ z]$	`[12]`