MSG No. 181.177 $P6_42'2'$ [Type III, hexagonal]

Table 1: Wyckoff site: `3a`, site symmetry: `22'2'`

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

Table 2: Wyckoff site: `3b`, site symmetry: `22'2'`

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

Table 3: Wyckoff site: `3c`, site symmetry: `22'2'`

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

Table 4: Wyckoff site: `3d`, site symmetry: `22'2'`

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

Table 5: Wyckoff site: `6e`, site symmetry: `2..`

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

Table 6: Wyckoff site: `6f`, site symmetry: `2..`

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

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

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

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

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

Table 9: Wyckoff site: `6i`, site symmetry: `..2'`

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

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

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

Table 11: Wyckoff site: `12k`, site symmetry: `1`

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