MSG No. 163.80 $P\bar{3}1c1'$ [Type II, trigonal]

Table 1: Wyckoff site: 2a, site symmetry: 3.21'

No.	position	mapping
1	$\left[0,\ 0,\ \frac{1}{4}\right]$	[1,2,3,4,5,6,13,14,15,16,17,18]
2	$\left[0,\ 0,\ \frac{3}{4}\right]$	[7,8,9,10,11,12,19,20,21,22,23,24]

Table 2: Wyckoff site: 2b, site symmetry: -3..1'

No.	position	mapping
1	$[0,\ 0,\ 0]$	[1,2,3,7,8,9,13,14,15,19,20,21]
2	$\left[0,\ 0,\ \frac{1}{2}\right]$	[4,5,6,10,11,12,16,17,18,22,23,24]

Table 3: Wyckoff site: 2c, site symmetry: 3.21'

No.	position	mapping
1	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{4}\right]$	[1,2,3,4,5,6,13,14,15,16,17,18]
2	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{3}{4}\right]$	[7,8,9,10,11,12,19,20,21,22,23,24]

Table 4: Wyckoff site: 2d, site symmetry: 3.21'

No.	position	mapping
1	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{4}\right]$	[1,2,3,4,5,6,13,14,15,16,17,18]
2	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{3}{4}\right]$	[7,8,9,10,11,12,19,20,21,22,23,24]

Table 5: Wyckoff site: 4e, site symmetry: 3..1'

No.	position	mapping
1	$[0,\ 0,\ z]$	[1,2,3,13,14,15]
2	$\left[0,\ 0,\ \frac{1}{2}-z\right]$	[4,5,6,16,17,18]
3	$[0,\ 0,\ -z]$	[7,8,9,19,20,21]
4	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	[10,11,12,22,23,24]

Table 6: Wyckoff site: `4f`, site symmetry: `3..1'`

No.	position	mapping
1	$\left[\frac{1}{3},\ \frac{2}{3},\ z\right]$	`[1,2,3,13,14,15]`
2	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{2}-z\right]$	`[4,5,6,16,17,18]`
3	$\left[\frac{2}{3},\ \frac{1}{3},\ -z\right]$	`[7,8,9,19,20,21]`
4	$\left[\frac{2}{3},\ \frac{1}{3},\ z+\frac{1}{2}\right]$	`[10,11,12,22,23,24]`

Table 7: Wyckoff site: `6g`, site symmetry: `-11'`

No.	position	mapping
1	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[1,7,13,19]`
2	$\left[0,\ \frac{1}{2},\ 0\right]$	`[2,8,14,20]`
3	$\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$	`[3,9,15,21]`
4	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[4,10,16,22]`
5	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[5,11,17,23]`
6	$\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[6,12,18,24]`

Table 8: Wyckoff site: `6h`, site symmetry: `..21'`

No.	position	mapping
1	$\left[x,\ -x,\ \frac{1}{4}\right]$	`[1,6,13,18]`
2	$\left[x,\ 2x,\ \frac{1}{4}\right]$	`[2,4,14,16]`
3	$\left[-2x,\ -x,\ \frac{1}{4}\right]$	`[3,5,15,17]`
4	$\left[-x,\ x,\ \frac{3}{4}\right]$	`[7,12,19,24]`
5	$\left[-x,\ -2x,\ \frac{3}{4}\right]$	`[8,10,20,22]`
6	$\left[2x,\ x,\ \frac{3}{4}\right]$	`[9,11,21,23]`

Table 9: Wyckoff site: `12i`, site symmetry: `11'`

No.	position	mapping
1	$[x,\ y,\ z]$	`[1,13]`
2	$[-y,\ x-y,\ z]$	`[2,14]`
3	$[-x+y,\ -x,\ z]$	`[3,15]`
4	$\left[x,\ x-y,\ \frac{1}{2}-z\right]$	`[4,16]`
5	$\left[-x+y,\ y,\ \frac{1}{2}-z\right]$	`[5,17]`
6	$\left[-y,\ -x,\ \frac{1}{2}-z\right]$	`[6,18]`
7	$[-x,\ -y,\ -z]$	`[7,19]`
8	$[y,\ -x+y,\ -z]$	`[8,20]`
9	$[x-y,\ x,\ -z]$	`[9,21]`
10	$\left[-x,\ -x+y,\ z+\frac{1}{2}\right]$	`[10,22]`
11	$\left[x-y,\ -y,\ z+\frac{1}{2}\right]$	`[11,23]`

continued ...

Table 9

No.	position	mapping
12	$\left[y,\, x,\, z+\frac{1}{2}\right]$	`[12,24]`