MSG No. 180.168 $P6_222'$ [Type II, hexagonal]

Table 1: Wyckoff site: 3a, site symmetry: 2221'

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

Table 2: Wyckoff site: 3b, site symmetry: 2221'

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

Table 3: Wyckoff site: 3c, site symmetry: 2221'

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

Table 4: Wyckoff site: 3d, site symmetry: 2221'

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

Table 5: Wyckoff site: 6e, site symmetry: 2..1'

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

Table 6: Wyckoff site: `6f`, site symmetry: `2..1'`

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

Table 7: Wyckoff site: `6g`, site symmetry: `.2.1'`

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

Table 8: Wyckoff site: `6h`, site symmetry: `.2.1'`

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

Table 9: Wyckoff site: `6i`, site symmetry: `..21'`

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

Table 10: Wyckoff site: `6j`, site symmetry: `..21'`

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

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

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