MSG No. 162.78 $P_c\bar{3}1m$ [Type IV, trigonal]

Table 1: Wyckoff site: `2a`, site symmetry: `-3.m`

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

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

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

Table 3: Wyckoff site: `4c`, 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]`
3	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{2}\right]$	`[13,14,15,16,17,18]`
4	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{2}\right]$	`[19,20,21,22,23,24]`

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

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

Table 5: Wyckoff site: `4e`, 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]`
3	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[13,14,15,22,23,24]`
4	$\left[0,\ 0,\ \frac{1}{2}-z\right]$	`[16,17,18,19,20,21]`

Table 6: Wyckoff site: `6f`, 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]`
4	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[13,17,19,23]`
5	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[14,18,20,24]`
6	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[15,16,21,22]`

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

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

Table 8: Wyckoff site: `8h`, 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]`
5	$\left[\frac{1}{3}, \frac{2}{3}, z+\frac{1}{2}\right]$	`[13,14,15]`
6	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{2}-z\right]$	`[16,17,18]`
7	$\left[\frac{2}{3}, \frac{1}{3}, \frac{1}{2}-z\right]$	`[19,20,21]`
8	$\left[\frac{2}{3}, \frac{1}{3}, z+\frac{1}{2}\right]$	`[22,23,24]`

Table 9: Wyckoff site: `12i`, 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]`
7	$\left[x, -x, \frac{1}{2}\right]$	`[13,18]`

continued ...

Table 9

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

Table 10: Wyckoff site: 12j, site symmetry: ..2'

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

Table 11: Wyckoff site: 12k, site symmetry: ..m

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

Table 12: Wyckoff site: `24l`, 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]`
13	$\left[x,\ y,\ z+\frac{1}{2}\right]$	`[13]`
14	$\left[-y,\ x-y,\ z+\frac{1}{2}\right]$	`[14]`
15	$\left[-x+y,\ -x,\ z+\frac{1}{2}\right]$	`[15]`
16	$\left[x,\ x-y,\ \frac{1}{2}-z\right]$	`[16]`
17	$\left[-x+y,\ y,\ \frac{1}{2}-z\right]$	`[17]`
18	$\left[-y,\ -x,\ \frac{1}{2}-z\right]$	`[18]`
19	$\left[-x,\ -y,\ \frac{1}{2}-z\right]$	`[19]`
20	$\left[y,\ -x+y,\ \frac{1}{2}-z\right]$	`[20]`
21	$\left[x-y,\ x,\ \frac{1}{2}-z\right]$	`[21]`
22	$\left[-x,\ -x+y,\ z+\frac{1}{2}\right]$	`[22]`
23	$\left[x-y,\ -y,\ z+\frac{1}{2}\right]$	`[23]`
24	$\left[y,\ x,\ z+\frac{1}{2}\right]$	`[24]`