MSG No. 127.394 $P4'/m'bm'$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 4'/m'..

No.	position	mapping
1	$[0, 0, 0]$	[1,2,5,6,9,10,13,14]
2	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[3,4,7,8,11,12,15,16]

Table 2: Wyckoff site: 2b, site symmetry: 4'/m'..

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	[1,2,5,6,9,10,13,14]
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[3,4,7,8,11,12,15,16]

Table 3: Wyckoff site: 2c, site symmetry: m'.m'm'

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[1,2,3,4,13,14,15,16]
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[5,6,7,8,9,10,11,12]

Table 4: Wyckoff site: 2d, site symmetry: m'.m'm'

No.	position	mapping
1	$\left[0, \frac{1}{2}, 0\right]$	[1,2,3,4,13,14,15,16]
2	$\left[\frac{1}{2}, 0, 0\right]$	[5,6,7,8,9,10,11,12]

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

No.	position	mapping
1	$[0, 0, z]$	[1,2,9,10]
2	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	[3,4,11,12]
3	$[0, 0, -z]$	[5,6,13,14]
4	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	[7,8,15,16]

Table 6: Wyckoff site: `4f`, site symmetry: `2.m'm'`

No.	position	mapping
1	$\left[0,\ \frac{1}{2},\ z\right]$	`[1,2,15,16]`
2	$\left[0,\ \frac{1}{2},\ -z\right]$	`[3,4,13,14]`
3	$\left[\frac{1}{2},\ 0,\ -z\right]$	`[5,6,11,12]`
4	$\left[\frac{1}{2},\ 0,\ z\right]$	`[7,8,9,10]`

Table 7: Wyckoff site: `4g`, site symmetry: `m'.2m'`

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ 0\right]$	`[1,3,14,16]`
2	$\left[-x,\ \frac{1}{2}-x,\ 0\right]$	`[2,4,13,15]`
3	$\left[x+\frac{1}{2},\ -x,\ 0\right]$	`[5,8,10,11]`
4	$\left[\frac{1}{2}-x,\ x,\ 0\right]$	`[6,7,9,12]`

Table 8: Wyckoff site: `4h`, site symmetry: `m'.2m'`

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[1,3,14,16]`
2	$\left[-x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[2,4,13,15]`
3	$\left[x+\frac{1}{2},\ -x,\ \frac{1}{2}\right]$	`[5,8,10,11]`
4	$\left[\frac{1}{2}-x,\ x,\ \frac{1}{2}\right]$	`[6,7,9,12]`

Table 9: Wyckoff site: `8i`, site symmetry: `m'..`

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,14]`
2	$[-x,\ -y,\ 0]$	`[2,13]`
3	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ 0\right]$	`[3,16]`
4	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ 0\right]$	`[4,15]`
5	$[y,\ -x,\ 0]$	`[5,10]`
6	$[-y,\ x,\ 0]$	`[6,9]`
7	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ 0\right]$	`[7,12]`
8	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	`[8,11]`

Table 10: Wyckoff site: `8j`, site symmetry: `m'..`

No.	position	mapping
1	$\left[x,\ y,\ \frac{1}{2}\right]$	`[1,14]`
2	$\left[-x,\ -y,\ \frac{1}{2}\right]$	`[2,13]`
3	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[3,16]`
4	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[4,15]`
5	$\left[y,\ -x,\ \frac{1}{2}\right]$	`[5,10]`
6	$\left[-y,\ x,\ \frac{1}{2}\right]$	`[6,9]`
7	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	`[7,12]`
8	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[8,11]`

Table 11: Wyckoff site: `8k`, site symmetry: `..m'`

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ z\right]$	`[1,16]`
2	$\left[-x,\ \frac{1}{2}-x,\ z\right]$	`[2,15]`
3	$\left[x,\ x+\frac{1}{2},\ -z\right]$	`[3,14]`
4	$\left[-x,\ \frac{1}{2}-x,\ -z\right]$	`[4,13]`
5	$\left[x+\frac{1}{2},\ -x,\ -z\right]$	`[5,11]`
6	$\left[\frac{1}{2}-x,\ x,\ -z\right]$	`[6,12]`
7	$\left[\frac{1}{2}-x,\ x,\ z\right]$	`[7,9]`
8	$\left[x+\frac{1}{2},\ -x,\ z\right]$	`[8,10]`

Table 12: Wyckoff site: `16l`, site symmetry: `1`

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