MSG No. 135.487 $P4'_2/mbc'$ [Type III, tetragonal]

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

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

Table 2: Wyckoff site: `4b`, site symmetry: `-4'..`

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

Table 3: Wyckoff site: `4c`, site symmetry: `2/m..`

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

Table 4: Wyckoff site: `4d`, site symmetry: `2.2'2'`

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

Table 5: Wyckoff site: `8e`, site symmetry: `2..`

No.	position	mapping
1	$[0,\ 0,\ z]$	`[1,4]`
2	$\left[\frac{1}{2},\ \frac{1}{2},\ -z\right]$	`[2,3]`

continued ...

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: 2..

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

Table 7: Wyckoff site: 8g, site symmetry: ..2'

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

Table 8: Wyckoff site: 8h, site symmetry: m..

No.	position	mapping
1	$[x,\ y,\ 0]$	[1,8]
2	$[x+\frac{1}{2},\ \frac{1}{2}-y,\ 0]$	[2,7]
3	$[\frac{1}{2}-x,\ y+\frac{1}{2},\ 0]$	[3,6]
4	$[-x,\ -y,\ 0]$	[4,5]
5	$[-y,\ x,\ \frac{1}{2}]$	[9,14]

continued ...

Table 8

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

Table 9: Wyckoff site: `16i`, site symmetry: `1`

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