MSG No. 57.387 $P_{b}bcm$ [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `m'2'm`

No.	position	mapping
1	$\left[0,\ y,\ \frac{1}{4}\right]$	`[1,8,11,14]`
2	$\left[0,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	`[2,7,12,13]`

continued ...

Table 5

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

continued ...

Table 12

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