MSG No. 62.451 $P_{b}nma$ [Type IV, orthorhombic]

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[0,\ y,\ 0]$	`[1,11]`
2	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[2,12]`

continued ...

Table 5

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

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

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

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

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

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

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

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[6,12]
7	$\left[x,\ \frac{1}{2},\ z\right]$	[7,9]
8	$\left[x+\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	[8,10]

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

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