MSG No. 53.331 $P_{b}mna$ [Type IV, orthorhombic]

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

No.	position	mapping
1	$[0,\ 0,\ 0]$	`[1,2,5,6]`
2	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[3,4,7,8]`
3	$\left[0,\ \frac{1}{2},\ 0\right]$	`[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: `2/m..`

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

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

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

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

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

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

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

continued ...

Table 5

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

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

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

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

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

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

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

continued ...

Table 8

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

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

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