MSG No. 60.432 P_Ibcn [Type IV, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `2'22'`

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

Table 2: Wyckoff site: `4b`, site symmetry: `2'22'`

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

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

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

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

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

Table 5: Wyckoff site: `8e`, site symmetry: `-1'`

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	`[1,13]`
2	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{3}{4}\right]$	`[2,14]`

continued ...

Table 5

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

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

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

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

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

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

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

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	[6,15]
7	$\left[0, 0, z+\frac{1}{2}\right]$	[7,14]
8	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}-z\right]$	[8,13]

Table 9: Wyckoff site: 8i, site symmetry: ..2'

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

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

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

Table 11: Wyckoff site: 16k, 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	$\left[-x, y, \frac{1}{2}-z\right]$	[3]
4	$\left[\frac{1}{2}-x, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[4]
5	$[-x, -y, -z]$	[5]
6	$\left[\frac{1}{2}-x, y+\frac{1}{2}, z\right]$	[6]
7	$\left[x, -y, z+\frac{1}{2}\right]$	[7]
8	$\left[x+\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[8]

continued ...

Table 11

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