MSG No. 55.364 P_Ibam [Type IV, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: `4c`, 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	$\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[9,12,13,16]`
4	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[10,11,14,15]`

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

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

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	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[3,15]
4	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[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	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[7,11]
8	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[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	$\left[\frac{1}{2}-x, \frac{1}{2}, \frac{3}{4}\right]$	[3,12]
4	$\left[-x, 0, \frac{1}{4}\right]$	[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	$\left[x+\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[7,16]
8	$\left[x, 0, \frac{3}{4}\right]$	[8,15]

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

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

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

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

continued ...

Table 8

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

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

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

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

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

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	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, -z\right]$	`[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]`

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	$\left[-x, y, \frac{1}{2}-z\right]$	[11]
12	$\left[\frac{1}{2}-x, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[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	$\left[x, -y, z+\frac{1}{2}\right]$	[15]
16	$\left[x+\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[16]