MSG No. 48.263 $P_{C}nnn$ [Type IV, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `222`

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

Table 2: Wyckoff site: `4b`, site symmetry: `222`

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[1,5,12,16]`
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[2,6,11,15]`

continued ...

Table 5

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

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

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

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

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

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

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

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

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

Table 10: Wyckoff site: `8j`, site symmetry: `..2`

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

Table 11: Wyckoff site: `8k`, site symmetry: `..2'`

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

Table 12: Wyckoff site: `8l`, site symmetry: `..m'`

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,16]`
2	$\left[x,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[2,15]`
3	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}\right]$	`[3,14]`

continued ...

Table 12

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

Table 13: Wyckoff site: 16m, site symmetry: 1

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