MSG No. 126.383 $P4/n'n'c'$ [Type III, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `422`

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

Table 2: Wyckoff site: `2b`, site symmetry: `422`

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

Table 3: Wyckoff site: `4c`, site symmetry: `222.`

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

Table 4: Wyckoff site: `4d`, site symmetry: `-4'..`

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

Table 5: Wyckoff site: `4e`, site symmetry: `4..`

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

Table 6: Wyckoff site: `8f`, site symmetry: `-1'`

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

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

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

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

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

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

No.	position	mapping
1	$\left[x,\ \frac{1}{4},\ \frac{1}{4}\right]$	`[1,4]`
2	$\left[\frac{1}{4},\ x,\ \frac{1}{4}\right]$	`[2,7]`
3	$\left[\frac{1}{4},\ \frac{1}{2}-x,\ \frac{1}{4}\right]$	`[3,8]`

continued ...

Table 9

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

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

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

Table 11: Wyckoff site: 16k, site symmetry: 1

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