MSG No. 126.380 $P4'/n'n'c$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff site: `8g`, 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	$\left[\frac{1}{4},\ \frac{3}{4},\ -z\right]$	`[5,6]`
4	$\left[\frac{1}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	`[7,8]`
5	$\left[\frac{3}{4},\ \frac{1}{4},\ z\right]$	`[9,10]`
6	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	`[11,12]`
7	$\left[\frac{3}{4},\ \frac{1}{4},\ -z\right]$	`[13,16]`
8	$\left[\frac{3}{4},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	`[14,15]`

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

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

Table 9: Wyckoff site: `8i`, 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	$\left[\frac{3}{4},\ -x,\ \frac{3}{4}\right]$	`[5,7]`

continued ...

Table 9

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

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

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

Table 11: Wyckoff site: 16k, 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	$\left[y+\frac{1}{2},\, -x,\, -z\right]$	[5]
6	$\left[-y,\, x+\frac{1}{2},\, -z\right]$	[6]
7	$\left[-y,\, -x,\, z+\frac{1}{2}\right]$	[7]
8	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[8]
9	$\left[\frac{1}{2}-y,\, x,\, z\right]$	[9]
10	$\left[y,\, \frac{1}{2}-x,\, z\right]$	[10]
11	$\left[y,\, x,\, \frac{1}{2}-z\right]$	[11]
12	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[12]
13	$[-x,\, -y,\, -z]$	[13]
14	$\left[-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[14]
15	$\left[x+\frac{1}{2},\, -y,\, z+\frac{1}{2}\right]$	[15]
16	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, -z\right]$	[16]