MSG No. 126.378 $P4'/nn'c$ [Type III, tetragonal]

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

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: 4'2'2

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: 22'2'.

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[x,\ \frac{1}{4},\ \frac{1}{4}\right]$	`[1,11]`
2	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{1}{4}\right]$	`[2,12]`
3	$\left[\frac{1}{4},\ x,\ \frac{1}{4}\right]$	`[3,9]`

continued ...

Table 9

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

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

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

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

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