MSG No. 126.379 $P4'/nnc'$ [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	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[5,6,7,8]
3	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[9,10,11,12]
4	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[13,14,15,16]

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

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

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	$\left[\frac{3}{4}, \frac{3}{4}, -z\right]$	[5,8,13,14]
4	$\left[\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}\right]$	[6,7,15,16]

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

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

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

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

continued ...

Table 9

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

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	$\left[-x, \frac{1}{4}, \frac{3}{4}\right]$	[5,6]
4	$\left[x+\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[7,8]
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	$\left[\frac{1}{4}, -x, \frac{3}{4}\right]$	[13,15]
8	$\left[\frac{1}{4}, x+\frac{1}{2}, \frac{3}{4}\right]$	[14,16]

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	$[-x, -y, -z]$	[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	$\left[\frac{1}{2}-y, x, z\right]$	[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	$\left[y+\frac{1}{2}, -x, -z\right]$	[13]
14	$\left[-y, x+\frac{1}{2}, -z\right]$	[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]