MSG No. 125.367 $P4'/nbm'$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff site: `4g`, site symmetry: `4'..`

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

Table 8: Wyckoff site: `4h`, site symmetry: `2.m'm'`

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

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

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

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

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

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

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

Table 12: Wyckoff site: `8l`, site symmetry: `.2.`

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

Table 13: Wyckoff site: `8m`, site symmetry: `..m'`

No.	position	mapping
1	$[x,\ -x,\ z]$	`[1,15]`
2	$\left[x,\ x+\frac{1}{2},\ -z\right]$	`[2,14]`
3	$\left[\frac{1}{2}-x,\ -x,\ -z\right]$	`[3,13]`

continued ...

Table 13

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

Table 14: Wyckoff site: 16n, site symmetry: 1

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