MSG No. 128.401 $P4/m'nc$ [Type III, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `4/m'..`

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

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

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

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

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

Table 4: Wyckoff site: `4d`, site symmetry: `2.2'2'`

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

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

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

Table 6: Wyckoff site: `8f`, site symmetry: `2..`

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

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

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

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

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

Table 9: Wyckoff site: `16i`, site symmetry: `1`

No.	position	mapping
1	$[x,\ y,\ z]$	`[1]`
2	$[-y,\ x,\ z]$	`[2]`
3	$[y,\ -x,\ z]$	`[3]`

continued ...

Table 9

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