MSG No. 136.503 $P4_2/m'n'm'$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff site: `4g`, site symmetry: `m'.m'2`

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

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

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

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

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

Table 10: Wyckoff site: 8j, site symmetry: ..m'

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

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

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