MSG No. 138.523 $P4'_2/ncm'$ [Type III, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `2.2'2'`

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

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

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

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

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

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

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

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

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

continued ...

Table 5

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

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

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

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

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

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

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

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

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

Table 10: Wyckoff site: `16j`, 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	$\left[-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[3]`
4	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	`[4]`
5	$[-x,\ -y,\ -z]$	`[5]`
6	$\left[\frac{1}{2}-x,\ y,\ z+\frac{1}{2}\right]$	`[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	$\left[\frac{1}{2}-y,\ x,\ z+\frac{1}{2}\right]$	`[9]`
10	$\left[y,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	`[10]`
11	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ -z\right]$	`[11]`
12	$[-y,\ -x,\ -z]$	`[12]`
13	$\left[y+\frac{1}{2},\ -x,\ \frac{1}{2}-z\right]$	`[13]`
14	$\left[-y,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[14]`
15	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z\right]$	`[15]`
16	$[y,\ x,\ z]$	`[16]`