MSG No. 135.491 $P4_2/m'b'c'$ [Type III, tetragonal]

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

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

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

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

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	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[2,3,10,11]`
3	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[4,5,12,13]`
4	$\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[7,8,15,16]`

Table 4: Wyckoff site: `4d`, site symmetry: `2.22`

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

Table 5: Wyckoff site: `8e`, site symmetry: `2..`

No.	position	mapping
1	$[0,\ 0,\ z]$	`[1,6]`
2	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	`[2,3]`

continued ...

Table 5

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

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

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

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

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

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

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

continued ...

Table 8

No.	position	mapping
6	$[-x,\ -y,\ 0]$	`[6,9]`
7	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[7,16]`
8	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[8,15]`

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

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