MSG No. 133.467 $P4_2/n'b'c'$ [Type III, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `222.`

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

Table 2: Wyckoff site: `4b`, site symmetry: `222.`

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

Table 3: Wyckoff site: `4c`, site symmetry: `2.22`

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

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

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

Table 5: Wyckoff site: `8e`, site symmetry: `-1'`

No.	position	mapping
1	$[0, 0, 0]$	`[1,9]`
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[2,10]`

continued ...

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$\left[x, \frac{1}{4}, 0\right]$	[1,4]
2	$\left[\frac{1}{4}, x, \frac{1}{2}\right]$	[2,7]
3	$\left[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{2}\right]$	[3,8]
4	$\left[\frac{1}{2} - x, \frac{1}{4}, 0\right]$	[5,6]
5	$\left[-x, \frac{3}{4}, 0\right]$	[9,12]

Table 8

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

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

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

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

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

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

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

continued ...

Table 11

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

$[-x,\ -y,\ -z]$ [9]

$\left[y+\frac{1}{2},\ -x,\ \frac{1}{2}-z\right]$ [10]

$\left[-y,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$ [11]

$\left[-x,\ y+\frac{1}{2},\ z\right]$ [12]

4

$,\ z$

$\left[x+\frac{1}{2},\ -y,\ z\right]$