MSG No. 133.461 $P4_2/n'bc$ [Type III, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `22'2'.`

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

Table 2: Wyckoff site: `4b`, site symmetry: `22'2'.`

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

Table 3: Wyckoff site: `4c`, site symmetry: `2.2'2'`

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

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

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

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

No.	position	mapping
1	$[0, 0, 0]$	`[1,13]`
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[2,14]`

continued ...

Table 5

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

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

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

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

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

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

No.	position	mapping
1	$\left[x, \frac{1}{4}, 0\right]$	[1,9]
2	$\left[\frac{1}{4}, x, \frac{1}{2}\right]$	[2,11]
3	$\left[\frac{1}{4}, \frac{1}{2}-x, \frac{1}{2}\right]$	[3,12]
4	$\left[\frac{1}{2}-x, \frac{1}{4}, 0\right]$	[4,10]
5	$\left[-x, \frac{3}{4}, 0\right]$	[5,13]

continued ...

Table 8

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

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

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

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

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

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	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	[4]
5	$\left[-x,\ y+\frac{1}{2},\ z\right]$	[5]
6	$\left[x+\frac{1}{2},\ -y,\ z\right]$	[6]
7	$\left[-y,\ -x,\ z+\frac{1}{2}\right]$	[7]
8	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[8]

continued ...

Table 11

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