MSG No. 133.462 $P4'_2/nb'c$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[0, 0, 0]$	`[1,5]`
2	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[2,6]`

continued ...

Table 5

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

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

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

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

No.	position	mapping
1	$\left[\frac{3}{4},\ \frac{1}{4},\ z\right]$	`[1,2]`
2	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	`[3,4]`
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	$\left[\frac{1}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	`[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 8: Wyckoff site: `8h`, site symmetry: `.2'.`

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

continued ...

Table 8

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

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

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

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

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

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

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