MSG No. 137.508 $P4_2/nmc1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: -4m21'

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[1,6,7,8,10,11,12,13,17,22,23,24,26,27,28,29]
2	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[2,3,4,5,9,14,15,16,18,19,20,21,25,30,31,32]

Table 2: Wyckoff site: 2b, site symmetry: -4m21'

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[1,6,7,8,10,11,12,13,17,22,23,24,26,27,28,29]
2	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[2,3,4,5,9,14,15,16,18,19,20,21,25,30,31,32]

Table 3: Wyckoff site: 4c, site symmetry: 2mm.1'

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, z\right]$	[1,6,12,13,17,22,28,29]
2	$\left[\frac{1}{4}, \frac{3}{4}, z+\frac{1}{2}\right]$	[2,3,15,16,18,19,31,32]
3	$\left[\frac{1}{4}, \frac{3}{4}, -z\right]$	[4,5,9,14,20,21,25,30]
4	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}-z\right]$	[7,8,10,11,23,24,26,27]

Table 4: Wyckoff site: 4d, site symmetry: 2mm.1'

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, z\right]$	[1,6,12,13,17,22,28,29]
2	$\left[\frac{1}{4}, \frac{1}{4}, z+\frac{1}{2}\right]$	[2,3,15,16,18,19,31,32]
3	$\left[\frac{3}{4}, \frac{3}{4}, -z\right]$	[4,5,9,14,20,21,25,30]
4	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}-z\right]$	[7,8,10,11,23,24,26,27]

Table 5: Wyckoff site: 8e, site symmetry: -11'

No.	position	mapping
1	$[0, 0, 0]$	[1,9,17,25]
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[2,10,18,26]
3	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[3,11,19,27]
4	$\left[\frac{1}{2}, 0, 0\right]$	[4,12,20,28]
5	$\left[0, \frac{1}{2}, 0\right]$	[5,13,21,29]
6	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[6,14,22,30]

continued ...

Table 5

No.	position	mapping
7	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[7,15,23,31]`
8	$\left[0, 0, \frac{1}{2}\right]$	`[8,16,24,32]`

Table 6: Wyckoff site: `8f`, site symmetry: `..21'`

No.	position	mapping
1	$\left[x, -x, \frac{1}{4}\right]$	`[1,8,17,24]`
2	$\left[x+\frac{1}{2}, x, \frac{3}{4}\right]$	`[2,4,18,20]`
3	$\left[-x, \frac{1}{2}-x, \frac{3}{4}\right]$	`[3,5,19,21]`
4	$\left[\frac{1}{2}-x, x+\frac{1}{2}, \frac{1}{4}\right]$	`[6,7,22,23]`
5	$\left[-x, x, \frac{3}{4}\right]$	`[9,16,25,32]`
6	$\left[\frac{1}{2}-x, -x, \frac{1}{4}\right]$	`[10,12,26,28]`
7	$\left[x, x+\frac{1}{2}, \frac{1}{4}\right]$	`[11,13,27,29]`
8	$\left[x+\frac{1}{2}, \frac{1}{2}-x, \frac{3}{4}\right]$	`[14,15,30,31]`

Table 7: Wyckoff site: `8g`, site symmetry: `.m.1'`

No.	position	mapping
1	$\left[\frac{1}{4}, y, z\right]$	`[1,12,17,28]`
2	$\left[\frac{1}{2}-y, \frac{1}{4}, z+\frac{1}{2}\right]$	`[2,15,18,31]`
3	$\left[y, \frac{1}{4}, z+\frac{1}{2}\right]$	`[3,16,19,32]`
4	$\left[\frac{3}{4}, -y, -z\right]$	`[4,9,20,25]`
5	$\left[\frac{3}{4}, y+\frac{1}{2}, -z\right]$	`[5,14,21,30]`
6	$\left[\frac{1}{4}, \frac{1}{2}-y, z\right]$	`[6,13,22,29]`
7	$\left[y+\frac{1}{2}, \frac{3}{4}, \frac{1}{2}-z\right]$	`[7,10,23,26]`
8	$\left[-y, \frac{3}{4}, \frac{1}{2}-z\right]$	`[8,11,24,27]`

Table 8: Wyckoff site: `16h`, site symmetry: `11'`

No.	position	mapping
1	$[x, y, z]$	`[1,17]`
2	$\left[\frac{1}{2}-y, x, z+\frac{1}{2}\right]$	`[2,18]`
3	$\left[y, \frac{1}{2}-x, z+\frac{1}{2}\right]$	`[3,19]`
4	$\left[x+\frac{1}{2}, -y, -z\right]$	`[4,20]`
5	$\left[-x, y+\frac{1}{2}, -z\right]$	`[5,21]`
6	$\left[\frac{1}{2}-x, \frac{1}{2}-y, z\right]$	`[6,22]`
7	$\left[y+\frac{1}{2}, x+\frac{1}{2}, \frac{1}{2}-z\right]$	`[7,23]`
8	$\left[-y, -x, \frac{1}{2}-z\right]$	`[8,24]`
9	$[-x, -y, -z]$	`[9,25]`

continued ...

Table 8

No.	position	mapping
10	$\left[y+\frac{1}{2},\,-x,\,\frac{1}{2}-z\right]$	[10,26]
11	$\left[-y,\,x+\frac{1}{2},\,\frac{1}{2}-z\right]$	[11,27]
12	$\left[\frac{1}{2}-x,\,y,\,z\right]$	[12,28]
13	$\left[x,\,\frac{1}{2}-y,\,z\right]$	[13,29]
14	$\left[x+\frac{1}{2},\,y+\frac{1}{2},\,-z\right]$	[14,30]
15	$\left[\frac{1}{2}-y,\,\frac{1}{2}-x,\,z+\frac{1}{2}\right]$	[15,31]
16	$\left[y,\,x,\,z+\frac{1}{2}\right]$	[16,32]