MSG No. 137.515 $P4_2/n'm'c'$ [Type III, tetragonal]

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

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

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

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

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

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

Table 4: Wyckoff site: `4d`, site symmetry: `2m'm'.`

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

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]`
3	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[3,11]`
4	$\left[\frac{1}{2}, 0, 0\right]$	`[4,12]`
5	$\left[0, \frac{1}{2}, 0\right]$	`[5,13]`
6	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[6,14]`

continued ...

Table 5

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

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

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

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

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

Table 8: Wyckoff site: `16h`, 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	$\left[-x, y + \frac{1}{2}, -z\right]$	[5]
6	$\left[\frac{1}{2} - x, \frac{1}{2} - y, z\right]$	[6]
7	$\left[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z\right]$	[7]
8	$\left[-y, -x, \frac{1}{2} - z\right]$	[8]
9	$[-x, -y, -z]$	[9]

Table 8

No.	position	mapping
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	$\left[\frac{1}{2} - x, \, y, \, z\right]$	[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	$\left[\frac{1}{2} - y, \, \frac{1}{2} - x, \, z + \frac{1}{2}\right]$	[15]
16	$\left[y, \, x, \, z + \frac{1}{2}\right]$	[16]

No.	position	mapping
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	$\left[\frac{1}{2} - x, \, y, \, z\right]$	

$\left[x, \, \frac{1}{2}\right.$ 3 $\left.\right]$

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

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