MSG No. 119.317 $I\bar{4}'m'2$ [Type III, tetragonal]

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

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

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

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

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

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

Table 4: Wyckoff site: 2d, site symmetry: -4'm'2

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

Table 5: Wyckoff site: 4e, site symmetry: 2m'm'.

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

Table 6: Wyckoff site: `4f`, site symmetry: `2m'm'`.

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `.m'`.

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

continued ...

Table 9

No.	position	mapping
8	$\left[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z\right]$	[12,13]

Table 10: Wyckoff site: 16j, site symmetry: 1

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