MSG No. 87.76 $I4/m1'$ [Type II, tetragonal]

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

No.	position	mapping
1	$[0, 0, 0]$	`[1,2,3,4,5,6,7,8,17,18,19,20,21,22,23,24]`
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[9,10,11,12,13,14,15,16,25,26,27,28,29,30,31,32]`

Table 2: Wyckoff site: `2b`, site symmetry: `4/m..1'`

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	`[1,2,3,4,5,6,7,8,17,18,19,20,21,22,23,24]`
2	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[9,10,11,12,13,14,15,16,25,26,27,28,29,30,31,32]`

Table 3: Wyckoff site: `4c`, site symmetry: `2/m..1'`

No.	position	mapping
1	$\left[0, \frac{1}{2}, 0\right]$	`[1,4,5,8,17,20,21,24]`
2	$\left[\frac{1}{2}, 0, 0\right]$	`[2,3,6,7,18,19,22,23]`
3	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[9,12,13,16,25,28,29,32]`
4	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[10,11,14,15,26,27,30,31]`

Table 4: Wyckoff site: `4d`, site symmetry: `-4..1'`

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	`[1,4,14,15,17,20,30,31]`
2	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	`[2,3,13,16,18,19,29,32]`
3	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	`[5,8,10,11,21,24,26,27]`
4	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	`[6,7,9,12,22,23,25,28]`

Table 5: Wyckoff site: `4e`, site symmetry: `4..1'`

No.	position	mapping
1	$[0, 0, z]$	`[1,2,3,4,17,18,19,20]`
2	$[0, 0, -z]$	`[5,6,7,8,21,22,23,24]`
3	$\left[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}\right]$	`[9,10,11,12,25,26,27,28]`
4	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z\right]$	`[13,14,15,16,29,30,31,32]`

Table 6: Wyckoff site: `8f`, site symmetry: `-11'`

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

Table 7: Wyckoff site: `8g`, site symmetry: `2..1'`

No.	position	mapping
1	$\left[0, \frac{1}{2}, z\right]$	`[1,4,17,20]`
2	$\left[\frac{1}{2}, 0, z\right]$	`[2,3,18,19]`
3	$\left[0, \frac{1}{2}, -z\right]$	`[5,8,21,24]`
4	$\left[\frac{1}{2}, 0, -z\right]$	`[6,7,22,23]`
5	$\left[\frac{1}{2}, 0, z+\frac{1}{2}\right]$	`[9,12,25,28]`
6	$\left[0, \frac{1}{2}, z+\frac{1}{2}\right]$	`[10,11,26,27]`
7	$\left[\frac{1}{2}, 0, \frac{1}{2}-z\right]$	`[13,16,29,32]`
8	$\left[0, \frac{1}{2}, \frac{1}{2}-z\right]$	`[14,15,30,31]`

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

No.	position	mapping
1	$[x, y, 0]$	`[1,8,17,24]`
2	$[-y, x, 0]$	`[2,7,18,23]`
3	$[y, -x, 0]$	`[3,6,19,22]`
4	$[-x, -y, 0]$	`[4,5,20,21]`
5	$\left[x+\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}\right]$	`[9,16,25,32]`
6	$\left[\frac{1}{2}-y, x+\frac{1}{2}, \frac{1}{2}\right]$	`[10,15,26,31]`
7	$\left[y+\frac{1}{2}, \frac{1}{2}-x, \frac{1}{2}\right]$	`[11,14,27,30]`
8	$\left[\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}\right]$	`[12,13,28,29]`

Table 9: Wyckoff site: `16i`, site symmetry: `11'`

No.	position	mapping
1	$[x, y, z]$	`[1,17]`
2	$[-y, x, z]$	`[2,18]`
3	$[y, -x, z]$	`[3,19]`

continued ...

Table 9

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