MSG No. 97.154 $I42'2'$ [Type III, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `42'2'`

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: `42'2'`

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: `4c`, site symmetry: `22'2'.`

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

Table 4: Wyckoff site: `4d`, site symmetry: `2.2'2'`

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[x,\ 0,\ \frac{1}{2}\right]$	`[1,5]`
2	$\left[0,\ x,\ \frac{1}{2}\right]$	`[2,7]`
3	$\left[0,\ -x,\ \frac{1}{2}\right]$	`[3,8]`

continued ...

Table 9

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

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

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

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

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