MSG No. 120.323 $I\bar{4}'c'2$ [Type III, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `2.22`

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

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

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

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

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

Table 4: Wyckoff site: `4d`, site symmetry: `2.22`

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

Table 5: Wyckoff site: `8e`, site symmetry: `..2`

No.	position	mapping
1	$\left[x,\ x,\ \frac{1}{4}\right]$	`[1,3]`
2	$\left[-x,\ -x,\ \frac{1}{4}\right]$	`[2,4]`

continued ...

Table 5

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

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

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

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

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

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

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

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{1}{2}-x,\, x,\, 0\right]$	[6,15]
7	$\left[-x,\, x+\frac{1}{2},\, \frac{1}{2}\right]$	[7,14]
8	$\left[x,\, \frac{1}{2}-x,\, \frac{1}{2}\right]$	[8,13]

Table 9: Wyckoff site: 16i, site symmetry: 1

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