MSG No. 121.329 $I\bar{4}'2'm$ [Type III, tetragonal]

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

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: `-4'2'm`

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	$\left[0,\ \frac{1}{2},\ 0\right]$	`[1,2,5,6]`
2	$\left[\frac{1}{2},\ 0,\ 0\right]$	`[3,4,7,8]`
3	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[9,10,13,14]`
4	$\left[0,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[11,12,15,16]`

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `2.mm`

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	$[x,\ 0,\ 0]$	`[1,5]`
2	$[-x,\ 0,\ 0]$	`[2,6]`
3	$[0,\ -x,\ 0]$	`[3,7]`
4	$[0,\ x,\ 0]$	`[4,8]`
5	$\left[x+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$	`[9,13]`
6	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[10,14]`
7	$\left[\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[11,15]`
8	$\left[\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[12,16]`

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

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

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

No.	position	mapping
1	$\left[0,\ \frac{1}{2},\ z\right]$	`[1,2]`
2	$\left[\frac{1}{2},\ 0,\ z\right]$	`[3,4]`
3	$\left[0,\ \frac{1}{2},\ -z\right]$	`[5,6]`
4	$\left[\frac{1}{2},\ 0,\ -z\right]$	`[7,8]`
5	$\left[\frac{1}{2},\ 0,\ z+\frac{1}{2}\right]$	`[9,10]`
6	$\left[0,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	`[11,12]`
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 9: Wyckoff site: `8i`, site symmetry: `..m`

No.	position	mapping
1	$[x,\ x,\ z]$	`[1,4]`
2	$[-x,\ -x,\ z]$	`[2,3]`
3	$[x,\ -x,\ -z]$	`[5,7]`

continued ...

Table 9

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

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	$[x,\ -y,\ -z]$	`[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	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	`[10]`
11	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	`[11]`
12	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	`[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	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	`[15]`
16	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	`[16]`