MSG No. 88.85 $I4_1'/a'$ [Type III, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `-4..`

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

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

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

Table 3: Wyckoff site: `8c`, site symmetry: `-1'`

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

Table 4: Wyckoff site: `8d`, site symmetry: `-1'`

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

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

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

Table 6: Wyckoff site: `16f`, site symmetry: `1`

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