MSG No. 98.158 $I4_1221'$ [Type II, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `2.221'`

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

Table 2: Wyckoff site: `4b`, site symmetry: `2.221'`

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

Table 3: Wyckoff site: `8c`, site symmetry: `2..1'`

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

Table 4: Wyckoff site: `8d`, site symmetry: `..21'`

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

Table 5: Wyckoff site: 8e, site symmetry: ..21'

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

Table 6: Wyckoff site: 8f, site symmetry: .2.1'

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

Table 7: Wyckoff site: 16g, site symmetry: 11'

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