MSG No. 91.110 P_I4_122 [Type IV, tetragonal]

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

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

Table 2: Wyckoff site: `4b`, site symmetry: `2.22`

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

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

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

Table 4: Wyckoff site: `8d`, site symmetry: `..2'`

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

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

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

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

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

Table 7: Wyckoff site: `16g`, site symmetry: `1`

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