MSG No. 93.125 P_C4_222 [Type IV, tetragonal]

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

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

Table 2: Wyckoff site: `4b`, site symmetry: `2.2'2'`

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

Table 3: Wyckoff site: `4c`, site symmetry: `2.22`

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

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

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

Table 5: Wyckoff site: `4e`, site symmetry: `222.`

No.	position	mapping
1	$[0,\ 0,\ 0]$	`[1,4,5,6]`
2	$\left[0,\ 0,\ \frac{1}{2}\right]$	`[2,3,7,8]`

continued ...

Table 5

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

Table 6: Wyckoff site: `4f`, site symmetry: `222.`

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

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

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

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

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

Table 9: Wyckoff site: `8i`, site symmetry: `2'..`

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

Table 10: Wyckoff site: `8j`, site symmetry: `..2`

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

Table 11: Wyckoff site: `8k`, site symmetry: `..2'`

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

Table 12: Wyckoff site: `8l`, site symmetry: `..2`

No.	position	mapping
1	$\left[x, x, \frac{1}{4}\right]$	`[1,7]`
2	$\left[-x, x, \frac{3}{4}\right]$	`[2,5]`
3	$\left[x, -x, \frac{3}{4}\right]$	`[3,4]`

continued ...

Table 12

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

Table 13: Wyckoff site: 8m, site symmetry: ..2'

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

Table 14: Wyckoff site: 8n, site symmetry: .2.

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

Table 15: Wyckoff site: 8o, site symmetry: .2.

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

continued ...

Table 15

No.	position	mapping
7	$\left[y+\frac{1}{2},\ \frac{1}{2},\ 0\right]$	`[11,15]`
8	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	`[12,14]`

Table 16: Wyckoff site: `16p`, site symmetry: `1`

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