MSG No. 90.101 P_C42_12 [Type IV, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 4'2'2

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: 42'2'

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

Table 4: Wyckoff site: 2d, site symmetry: 42'2'

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

Table 5: Wyckoff site: 4e, site symmetry: 2.22

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

Table 6: Wyckoff site: `4f`, site symmetry: `2.22`

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

Table 7: Wyckoff site: `4g`, site symmetry: `4'..`

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

Table 8: Wyckoff site: `4h`, site symmetry: `4..`

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[1,15]`
2	$\left[-x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[2,13]`
3	$\left[x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[3,12]`

continued ...

Table 13

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

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

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

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

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

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

No.	position	mapping
1	$[x,\,y,\,z]$	[1]
2	$\left[\frac{1}{2}-y,\,x+\frac{1}{2},\,z\right]$	[2]
3	$\left[y+\frac{1}{2},\,\frac{1}{2}-x,\,z\right]$	[3]
4	$\left[x+\frac{1}{2},\,\frac{1}{2}-y,\,-z\right]$	[4]
5	$\left[\frac{1}{2}-x,\,y+\frac{1}{2},\,-z\right]$	[5]
6	$[-x,\,-y,\,z]$	[6]

continued ...

Table 16

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