MSG No. 21.43 C_a222 [Type IV, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `222`

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

Table 2: Wyckoff site: `4b`, site symmetry: `22'2'`

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

Table 3: Wyckoff site: `4c`, site symmetry: `2'22'`

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

Table 4: Wyckoff site: `4d`, site symmetry: `222`

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

Table 5: Wyckoff site: `4e`, site symmetry: `2'2'2`

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

continued ...

Table 5

No.	position	mapping
3	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	`[3,6,9,16]`
4	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	`[4,5,10,15]`

Table 6: Wyckoff site: `4f`, site symmetry: `22'2'`

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

Table 7: Wyckoff site: `4g`, site symmetry: `2'22'`

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

Table 8: Wyckoff site: `4h`, site symmetry: `2'2'2`

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

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

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

continued ...

Table 9

No.	position	mapping
8	$\left[-x,\ \frac{1}{2},\ 0\right]$	`[15,16]`

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

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

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

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

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

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

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

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

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

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

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

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

Table 16: Wyckoff site: `8p`, site symmetry: `.2'.`

No.	position	mapping
1	$\left[\frac{1}{4},\ y,\ \frac{1}{2}\right]$	`[1,11]`
2	$\left[\frac{1}{4},\ -y,\ \frac{1}{2}\right]$	`[2,12]`
3	$\left[\frac{3}{4},\ y,\ \frac{1}{2}\right]$	`[3,9]`

continued ...

Table 16

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

Table 17: Wyckoff site: 8q, site symmetry: ..2

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

Table 18: Wyckoff site: 8r, site symmetry: ..2'

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

Table 19: Wyckoff site: 8s, site symmetry: ..2'

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

continued ...

Table 19

No.	position	mapping
7	$\left[\frac{1}{2},\ \frac{3}{4},\ -z\right]$	[7,10]
8	$\left[\frac{1}{2},\ \frac{1}{4},\ z\right]$	[8,9]

Table 20: Wyckoff site: 8t, site symmetry: ..2

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

Table 21: Wyckoff site: 16u, site symmetry: 1

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