MSG No. 89.92 P_c422 [Type IV, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 422

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

Table 2: Wyckoff site: 2b, site symmetry: 42'2'

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

Table 3: Wyckoff site: 2c, site symmetry: 422

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[x,\ \frac{1}{2},\ \frac{1}{4}\right]$	`[1,12]`
2	$\left[\frac{1}{2},\ x,\ \frac{1}{4}\right]$	`[2,15]`
3	$\left[\frac{1}{2},\ -x,\ \frac{1}{4}\right]$	`[3,16]`

continued ...

Table 13

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

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

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

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

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

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

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$[-y,\ x,\ z]$	[2]
3	$[y,\ -x,\ z]$	[3]
4	$[x,\ -y,\ -z]$	[4]
5	$[-x,\ y,\ -z]$	[5]
6	$[-x,\ -y,\ z]$	[6]

continued ...

Table 16

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