MSG No. 124.356 $P4'/m'c'c$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 4'22'

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

Table 2: Wyckoff site: 2b, site symmetry: 4'/m'..

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

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

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

Table 4: Wyckoff site: 2d, site symmetry: 4'/m'..

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

Table 5: Wyckoff site: 4e, site symmetry: 2/m'..

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,16]`
2	$\left[x,\ -y,\ \frac{1}{2}\right]$	`[2,15]`
3	$\left[-x,\ y,\ \frac{1}{2}\right]$	`[3,14]`

continued ...

Table 13

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

Table 14: Wyckoff site: 16n, site symmetry: 1

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