MSG No. 84.56 P_c4_2/m [Type IV, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 4'/m..

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

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

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

Table 3: Wyckoff site: 2c, site symmetry: 4'/m..

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Table 12: Wyckoff site: `16l`, 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	$\left[y,\ -x,\ \frac{1}{2}-z\right]$	`[6]`
7	$\left[-y,\ x,\ \frac{1}{2}-z\right]$	`[7]`
8	$[x,\ y,\ -z]$	`[8]`
9	$\left[x,\ y,\ z+\frac{1}{2}\right]$	`[9]`
10	$[-y,\ x,\ z]$	`[10]`
11	$[y,\ -x,\ z]$	`[11]`
12	$\left[-x,\ -y,\ z+\frac{1}{2}\right]$	`[12]`
13	$\left[-x,\ -y,\ \frac{1}{2}-z\right]$	`[13]`
14	$[y,\ -x,\ -z]$	`[14]`
15	$[-y,\ x,\ -z]$	`[15]`
16	$\left[x,\ y,\ \frac{1}{2}-z\right]$	`[16]`