MSG No. 85.64 P_c4/n [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `-4..`

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

Table 2: Wyckoff site: `4b`, site symmetry: `-4'..`

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

Table 3: Wyckoff site: `4c`, site symmetry: `4..`

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

Table 4: Wyckoff site: `8d`, site symmetry: `-1`

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

Table 5: Wyckoff site: `8e`, site symmetry: `-1'`

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

Table 6: Wyckoff site: `8f`, site symmetry: `2..`

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

Table 7: Wyckoff site: `16g`, site symmetry: `1`

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