MSG No. 135.483 $P4_2/mbc$ [Type I, tetragonal]

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

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

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

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: 2.22

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

Table 5: Wyckoff site: 8e, site symmetry: 2..

No.	position	mapping
1	$[0, 0, z]$	[1,6]
2	$\left[0, 0, z + \frac{1}{2}\right]$	[2,3]

continued …

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Table 5

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

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

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

Table 7: Wyckoff site: 8g, site symmetry: ..2

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

Table 8: Wyckoff site: 8h, site symmetry: m..

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

continued ...

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Table 8

No.	position	mapping
6	$[-x,\ -y,\ 0]$	[6,9]
7	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[7,16]
8	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[8,15]

Table 9: Wyckoff site: 16i, 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	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[4]
5	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ -z\right]$	[5]
6	$[-x,\ -y,\ z]$	[6]
7	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[7]
8	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[8]
9	$[-x,\ -y,\ -z]$	[9]
10	$\left[y,\ -x,\ \frac{1}{2}-z\right]$	[10]
11	$\left[-y,\ x,\ \frac{1}{2}-z\right]$	[11]
12	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z\right]$	[12]
13	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$	[13]
14	$[x,\ y,\ -z]$	[14]
15	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	[15]
16	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[16]