MSG No. 126.381 $P4/nn'c'$ [Type III, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 42'2'

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

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

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

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

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

Table 4: Wyckoff site: 4d, 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	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[9,10,15,16]
4	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[11,12,13,14]

Table 5: Wyckoff site: 4e, 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	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - z\right]$	[9,10,11,12]
4	$\left[\frac{3}{4}, \frac{3}{4}, z + \frac{1}{2}\right]$	[13,14,15,16]

Table 6: Wyckoff site: `8f`, 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	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[9,13]
6	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[10,14]
7	$\left[0, 0, \frac{1}{2}\right]$	[11,15]
8	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[12,16]

Table 7: Wyckoff site: `8g`, 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	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - z\right]$	[9,10]
6	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - z\right]$	[11,12]
7	$\left[\frac{3}{4}, \frac{1}{4}, z + \frac{1}{2}\right]$	[13,14]
8	$\left[\frac{1}{4}, \frac{3}{4}, z + \frac{1}{2}\right]$	[15,16]

Table 8: Wyckoff site: `8h`, site symmetry: `..2'`

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

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

No.	position	mapping
1	$\left[x, \frac{1}{4}, \frac{1}{4}\right]$	[1,9]
2	$\left[\frac{1}{4}, x, \frac{1}{4}\right]$	[2,11]
3	$\left[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}\right]$	[3,12]

continued ...

2

Table 9

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

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

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

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