MSG No. 134.478 $P4'_2/n'nm'$ [Type III, tetragonal]

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

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

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

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff site: `4g`, site symmetry: `2.m'm'`

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

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

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

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$[x, -x, z]$	[1,15]
2	$\left[\frac{1}{2} - x, x + \frac{1}{2}, z\right]$	[2,16]
3	$[-x, x, -z]$	[3,13]

continued ...

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Table 13

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

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

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