MSG No. 134.479 $P4_2/n'n'm'$ [Type III, tetragonal]

Table 1: Wyckoff site: `2a`, site symmetry: `-4'2m'`

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

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

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

Table 3: Wyckoff site: `4c`, site symmetry: `222.`

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

continued ...

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Table 13

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

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

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