MSG No. 127.388 $P4/mbm1'$ [Type II, tetragonal]

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

No.	position	mapping
1	$[0, 0, 0]$	[1,2,3,6,9,10,11,14,17,18,19,22,25,26,27,30]
2	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[4,5,7,8,12,13,15,16,20,21,23,24,28,29,31,32]

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

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	[1,2,3,6,9,10,11,14,17,18,19,22,25,26,27,30]
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[4,5,7,8,12,13,15,16,20,21,23,24,28,29,31,32]

Table 3: Wyckoff site: 2c, site symmetry: m.mm1'

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[1,6,7,8,9,14,15,16,17,22,23,24,25,30,31,32]
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[2,3,4,5,10,11,12,13,18,19,20,21,26,27,28,29]

Table 4: Wyckoff site: 2d, site symmetry: m.mm1'

No.	position	mapping
1	$\left[0, \frac{1}{2}, 0\right]$	[1,6,7,8,9,14,15,16,17,22,23,24,25,30,31,32]
2	$\left[\frac{1}{2}, 0, 0\right]$	[2,3,4,5,10,11,12,13,18,19,20,21,26,27,28,29]

Table 5: Wyckoff site: 4e, site symmetry: 4..1'

No.	position	mapping
1	$[0, 0, z]$	[1,2,3,6,17,18,19,22]
2	$\left[\frac{1}{2}, \frac{1}{2}, -z\right]$	[4,5,7,8,20,21,23,24]
3	$[0, 0, -z]$	[9,10,11,14,25,26,27,30]
4	$\left[\frac{1}{2}, \frac{1}{2}, z\right]$	[12,13,15,16,28,29,31,32]

Table 6: Wyckoff site: `4f`, site symmetry: `2.mm1'`

No.	position	mapping
1	$\left[0,\ \frac{1}{2},\ z\right]$	`[1,6,15,16,17,22,31,32]`
2	$\left[\frac{1}{2},\ 0,\ z\right]$	`[2,3,12,13,18,19,28,29]`
3	$\left[\frac{1}{2},\ 0,\ -z\right]$	`[4,5,10,11,20,21,26,27]`
4	$\left[0,\ \frac{1}{2},\ -z\right]$	`[7,8,9,14,23,24,25,30]`

Table 7: Wyckoff site: `4g`, site symmetry: `m.2m1'`

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ 0\right]$	`[1,7,14,16,17,23,30,32]`
2	$\left[\frac{1}{2}-x,\ x,\ 0\right]$	`[2,5,11,12,18,21,27,28]`
3	$\left[x+\frac{1}{2},\ -x,\ 0\right]$	`[3,4,10,13,19,20,26,29]`
4	$\left[-x,\ \frac{1}{2}-x,\ 0\right]$	`[6,8,9,15,22,24,25,31]`

Table 8: Wyckoff site: `4h`, site symmetry: `m.2m1'`

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[1,7,14,16,17,23,30,32]`
2	$\left[\frac{1}{2}-x,\ x,\ \frac{1}{2}\right]$	`[2,5,11,12,18,21,27,28]`
3	$\left[x+\frac{1}{2},\ -x,\ \frac{1}{2}\right]$	`[3,4,10,13,19,20,26,29]`
4	$\left[-x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[6,8,9,15,22,24,25,31]`

Table 9: Wyckoff site: `8i`, site symmetry: `m..1'`

No.	position	mapping
1	$[x,\ y,\ 0]$	`[1,14,17,30]`
2	$[-y,\ x,\ 0]$	`[2,11,18,27]`
3	$[y,\ -x,\ 0]$	`[3,10,19,26]`
4	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	`[4,13,20,29]`
5	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ 0\right]$	`[5,12,21,28]`
6	$[-x,\ -y,\ 0]$	`[6,9,22,25]`
7	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ 0\right]$	`[7,16,23,32]`
8	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ 0\right]$	`[8,15,24,31]`

Table 10: Wyckoff site: `8j`, site symmetry: `m..1'`

No.	position	mapping
1	$\left[x,\, y,\, \frac{1}{2}\right]$	`[1,14,17,30]`
2	$\left[-y,\, x,\, \frac{1}{2}\right]$	`[2,11,18,27]`
3	$\left[y,\, -x,\, \frac{1}{2}\right]$	`[3,10,19,26]`
4	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	`[4,13,20,29]`
5	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}\right]$	`[5,12,21,28]`
6	$\left[-x,\, -y,\, \frac{1}{2}\right]$	`[6,9,22,25]`
7	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}\right]$	`[7,16,23,32]`
8	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{1}{2}\right]$	`[8,15,24,31]`

Table 11: Wyckoff site: `8k`, site symmetry: `..m1'`

No.	position	mapping
1	$\left[x,\, x+\frac{1}{2},\, z\right]$	`[1,16,17,32]`
2	$\left[\frac{1}{2}-x,\, x,\, z\right]$	`[2,12,18,28]`
3	$\left[x+\frac{1}{2},\, -x,\, z\right]$	`[3,13,19,29]`
4	$\left[x+\frac{1}{2},\, -x,\, -z\right]$	`[4,10,20,26]`
5	$\left[\frac{1}{2}-x,\, x,\, -z\right]$	`[5,11,21,27]`
6	$\left[-x,\, \frac{1}{2}-x,\, z\right]$	`[6,15,22,31]`
7	$\left[x,\, x+\frac{1}{2},\, -z\right]$	`[7,14,23,30]`
8	$\left[-x,\, \frac{1}{2}-x,\, -z\right]$	`[8,9,24,25]`

Table 12: Wyckoff site: `16l`, site symmetry: `11'`

No.	position	mapping
1	$[x,\, y,\, z]$	`[1,17]`
2	$[-y,\, x,\, z]$	`[2,18]`
3	$[y,\, -x,\, z]$	`[3,19]`
4	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	`[4,20]`
5	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, -z\right]$	`[5,21]`
6	$[-x,\, -y,\, z]$	`[6,22]`
7	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, -z\right]$	`[7,23]`
8	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, -z\right]$	`[8,24]`
9	$[-x,\, -y,\, -z]$	`[9,25]`
10	$[y,\, -x,\, -z]$	`[10,26]`
11	$[-y,\, x,\, -z]$	`[11,27]`
12	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z\right]$	`[12,28]`
13	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z\right]$	`[13,29]`
14	$[x,\, y,\, -z]$	`[14,30]`
15	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, z\right]$	`[15,31]`
16	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z\right]$	`[16,32]`