MSG No. 124.352 $P4/mcc1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 4221'

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

Table 2: Wyckoff site: 2b, 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	$\left[0,\ 0,\ \frac{1}{2}\right]$	[4,5,7,8,12,13,15,16,20,21,23,24,28,29,31,32]

Table 3: Wyckoff site: 2c, site symmetry: 4221'

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

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

No.	position	mapping
1	$\left[\frac{1}{2},\ \frac{1}{2},\ 0\right]$	[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 5: Wyckoff site: 4e, site symmetry: 2/m..1'

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

Table 6: Wyckoff site: `4f`, site symmetry: `222.1'`

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

Table 7: Wyckoff site: `4g`, site symmetry: `4..1'`

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

Table 8: Wyckoff site: `4h`, site symmetry: `4..1'`

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

Table 9: Wyckoff site: `8i`, site symmetry: `2..1'`

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

Table 10: Wyckoff site: `8j`, site symmetry: `..21'`

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

Table 11: Wyckoff site: `8k`, site symmetry: `.2.1'`

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

Table 12: Wyckoff site: `8l`, site symmetry: `.2.1'`

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

Table 13: Wyckoff site: `8m`, 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]`

continued ...

Table 13

No.	position	mapping
4	$\left[x,\, -y,\, \frac{1}{2}\right]$	[4,13,20,29]
5	$\left[-x,\, y,\, \frac{1}{2}\right]$	[5,12,21,28]
6	$[-x,\, -y,\, 0]$	[6,9,22,25]
7	$\left[y,\, x,\, \frac{1}{2}\right]$	[7,16,23,32]
8	$\left[-y,\, -x,\, \frac{1}{2}\right]$	[8,15,24,31]

Table 14: Wyckoff site: 16n, 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	$\left[x,\, -y,\, \frac{1}{2}-z\right]$	[4,20]
5	$\left[-x,\, y,\, \frac{1}{2}-z\right]$	[5,21]
6	$[-x,\, -y,\, z]$	[6,22]
7	$\left[y,\, x,\, \frac{1}{2}-z\right]$	[7,23]
8	$\left[-y,\, -x,\, \frac{1}{2}-z\right]$	[8,24]
9	$[-x,\, -y,\, -z]$	[9,25]
10	$[y,\, -x,\, -z]$	[10,26]
11	$[-y,\, x,\, -z]$	[11,27]
12	$\left[-x,\, y,\, z+\frac{1}{2}\right]$	[12,28]
13	$\left[x,\, -y,\, z+\frac{1}{2}\right]$	[13,29]
14	$[x,\, y,\, -z]$	[14,30]
15	$\left[-y,\, -x,\, z+\frac{1}{2}\right]$	[15,31]
16	$\left[y,\, x,\, z+\frac{1}{2}\right]$	[16,32]