MSG No. 93.120 $P4_2221'$ [Type II, tetragonal]

Table 1: Wyckoff site: 2a, site symmetry: 222.1'

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

Table 2: Wyckoff site: 2b, site symmetry: 222.1'

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

Table 3: Wyckoff site: 2c, site symmetry: 222.1'

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

Table 4: Wyckoff site: 2d, site symmetry: 222.1'

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

Table 5: Wyckoff site: 2e, site symmetry: 2.221'

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

Table 6: Wyckoff site: 2f, site symmetry: 2.221'

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

Table 7: Wyckoff site: `4g`, site symmetry: `2..1'`

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

Table 8: Wyckoff site: `4h`, site symmetry: `2..1'`

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

Table 9: Wyckoff site: `4i`, site symmetry: `2..1'`

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

Table 10: Wyckoff site: `4j`, site symmetry: `.2.1'`

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

Table 11: Wyckoff site: `4k`, site symmetry: `.2.1'`

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

Table 12: Wyckoff site: `4l`, site symmetry: `.2.1'`

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

Table 13: Wyckoff site: `4m`, site symmetry: `.2.1'`

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

Table 14: Wyckoff site: `4n`, site symmetry: `..21'`

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

Table 15: Wyckoff site: `4o`, site symmetry: `..21'`

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

Table 16: Wyckoff site: `8p`, site symmetry: `11'`

No.	position	mapping
1	$[x,\ y,\ z]$	`[1,9]`
2	$\left[-y,\ x,\ z+\frac{1}{2}\right]$	`[2,10]`
3	$\left[y,\ -x,\ z+\frac{1}{2}\right]$	`[3,11]`
4	$[x,\ -y,\ -z]$	`[4,12]`

continued ...

Table 16

No.	position	mapping
5	$[-x,\, y,\, -z]$	`[5,13]`
6	$[-x,\, -y,\, z]$	`[6,14]`
7	$\left[y,\, x,\, \frac{1}{2} - z\right]$	`[7,15]`
8	$\left[-y,\, -x,\, \frac{1}{2} - z\right]$	`[8,16]`