MSG No. 89.88 $P4221'$ [Type II, tetragonal]

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

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

Table 2: Wyckoff site: `1b`, site symmetry: `4221'`

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

Table 3: Wyckoff site: `1c`, site symmetry: `4221'`

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

Table 4: Wyckoff site: `1d`, site symmetry: `4221'`

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

Table 5: Wyckoff site: `2e`, site symmetry: `222.1'`

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

Table 6: Wyckoff site: `2f`, site symmetry: `222.1'`

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

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

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

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

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

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	$\left[\frac{1}{2},\ 0,\ z\right]$	[2,3,10,11]
3	$\left[0,\ \frac{1}{2},\ -z\right]$	[4,5,12,13]
4	$\left[\frac{1}{2},\ 0,\ -z\right]$	[7,8,15,16]

Table 10: Wyckoff site: 4j, site symmetry: ..21'

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

Table 11: Wyckoff site: 4k, site symmetry: ..21'

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

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

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

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

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

Table 14: Wyckoff site: 4n, site symmetry: .2.1'

No.	position	mapping
1	$\left[x,\ 0,\ \frac{1}{2}\right]$	[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	$\left[-x,\ 0,\ \frac{1}{2}\right]$	[5,6,13,14]

Table 15: Wyckoff site: 4o, site symmetry: .2.1'

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

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

No.	position	mapping
1	$[x,\ y,\ z]$	[1,9]
2	$[-y,\ x,\ z]$	[2,10]
3	$[y,\ -x,\ z]$	[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	$[y, x, -z]$	`[7,15]`
8	$[-y, -x, -z]$	`[8,16]`