MSG No. 21.39 $C2221'$ [Type II, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: 2221'

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

Table 2: Wyckoff site: 2b, site symmetry: 2221'

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

Table 3: Wyckoff site: 2c, site symmetry: 2221'

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

Table 4: Wyckoff site: 2d, site symmetry: 2221'

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

Table 5: Wyckoff site: 4e, site symmetry: 2..1'

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

Table 6: Wyckoff site: `4f`, site symmetry: `2..1'`

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

Table 7: Wyckoff site: `4g`, site symmetry: `.2.1'`

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

Table 8: Wyckoff site: `4h`, site symmetry: `.2.1'`

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

Table 9: Wyckoff site: `4i`, site symmetry: `..21'`

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

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

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

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

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

Table 12: Wyckoff site: 8l, site symmetry: 11'

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