MSG No. 48.258 $Pnnn1'$ [Type II, orthorhombic]

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

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: -11'

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

Table 6: Wyckoff site: `4f`, site symmetry: `-11'`

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

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

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

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

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

Table 9: Wyckoff site: `4i`, site symmetry: `.2.1'`

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

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

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

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

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

Table 12: Wyckoff site: 4l, site symmetry: ..21'

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

Table 13: Wyckoff site: 8m, site symmetry: 11'

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