MSG No. 49.266 $Pccm1'$ [Type II, orthorhombic]

Table 1: Wyckoff site: 2a, site symmetry: ..2/m1'

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

Table 2: Wyckoff site: 2b, site symmetry: ..2/m1'

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

Table 3: Wyckoff site: 2c, site symmetry: ..2/m1'

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

Table 4: Wyckoff site: 2d, site symmetry: ..2/m1'

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

Table 5: Wyckoff site: 2e, site symmetry: 2221'

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

Table 6: Wyckoff site: 2f, site symmetry: 2221'

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

Table 7: Wyckoff site: 2g, site symmetry: 2221'

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

Table 8: Wyckoff site: 2h, site symmetry: 2221'

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

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

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

Table 10: Wyckoff site: 4j, site symmetry: 2..1'

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

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

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

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

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

Table 13: Wyckoff site: 4m, site symmetry: ..21'

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

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

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

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

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

Table 16: Wyckoff site: 4p, site symmetry: ..21'

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

Table 17: Wyckoff site: `4q`, site symmetry: `..m1'`

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

Table 18: Wyckoff site: `8r`, site symmetry: `11'`

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