MSG No. 54.338 $Pcca1'$ [Type II, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: -11'

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

Table 2: Wyckoff site: 4b, site symmetry: -11'

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

Table 3: Wyckoff site: 4c, site symmetry: .2.1'

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

Table 4: Wyckoff site: 4d, site symmetry: ..21'

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

Table 5: Wyckoff site: 4e, site symmetry: ..21'

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

continued ...

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Table 5

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

Table 6: Wyckoff site: 8f, 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	$\left[-x,\, y,\, \frac{1}{2}-z\right]$	[3,11]
4	$\left[\frac{1}{2}-x,\, -y,\, z\right]$	[4,12]
5	$[-x,\, -y,\, -z]$	[5,13]
6	$\left[\frac{1}{2}-x,\, y,\, z+\frac{1}{2}\right]$	[6,14]
7	$\left[x,\, -y,\, z+\frac{1}{2}\right]$	[7,15]
8	$\left[x+\frac{1}{2},\, y,\, -z\right]$	[8,16]