MSG No. 54.351 P_Ccca [Type IV, orthorhombic]

Table 1: Wyckoff site: 4a, site symmetry: 2'22'

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

Table 2: Wyckoff site: 4b, site symmetry: 2'22'

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

Table 3: Wyckoff site: 8c, site symmetry: -1

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

Table 4: Wyckoff site: 8d, site symmetry: -1'

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

Table 5: Wyckoff site: `8e`, site symmetry: `.2.`

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

Table 6: Wyckoff site: `8f`, site symmetry: `2'..`

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

Table 7: Wyckoff site: `8g`, site symmetry: `..2'`

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

Table 8: Wyckoff site: `8h`, site symmetry: `..2`

No.	position	mapping
1	$\left[\frac{3}{4}, 0, z\right]$	[1,4]
2	$\left[\frac{1}{4}, 0, \frac{1}{2} - z\right]$	[2,3]
3	$\left[\frac{1}{4}, 0, -z\right]$	[5,8]

continued ...

Table 8

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

Table 9: Wyckoff site: 16i, site symmetry: 1

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