MSG No. 54.347 P_bcca [Type IV, orthorhombic]

Table 1: Wyckoff site: `8a`, site symmetry: `-1`

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

Table 2: Wyckoff site: `8b`, site symmetry: `-1'`

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

Table 3: Wyckoff site: `8c`, site symmetry: `.2.`

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

Table 4: Wyckoff site: 8d, site symmetry: ..2

No.	position	mapping
1	$\left[\frac{1}{4}, 0, z\right]$	[1,4]
2	$\left[\frac{3}{4}, 0, \frac{1}{2} - z\right]$	[2,3]
3	$\left[\frac{3}{4}, 0, -z\right]$	[5,8]
4	$\left[\frac{1}{4}, 0, z + \frac{1}{2}\right]$	[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 5: Wyckoff site: 8e, site symmetry: ..2'

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

Table 6: Wyckoff site: 16f, 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	$\left[x, y + \frac{1}{2}, z\right]$	[9]
10	$\left[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z\right]$	[10]
11	$\left[-x, y + \frac{1}{2}, \frac{1}{2} - z\right]$	[11]
12	$\left[\frac{1}{2} - x, \frac{1}{2} - y, z\right]$	[12]
13	$\left[-x, \frac{1}{2} - y, -z\right]$	[13]
14	$\left[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}\right]$	[14]
15	$\left[x, \frac{1}{2} - y, z + \frac{1}{2}\right]$	[15]
16	$\left[x + \frac{1}{2}, y + \frac{1}{2}, -z\right]$	[16]