MSG No. 61.439 P_Cbca [Type IV, orthorhombic]

Table 1: Wyckoff site: `4a`, site symmetry: `2'/m'..`

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

Table 2: Wyckoff site: `4b`, site symmetry: `2'/m'..`

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff site: `16g`, site symmetry: `1`

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