MSG No. 48.262 P_cnnn [Type IV, orthorhombic]

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry: 222

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

Table 4: Wyckoff site: 4d, site symmetry: 222

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

Table 5: Wyckoff site: 8e, site symmetry: -1

No.	position	mapping
1	$[0, 0, 0]$	[1,5]
2	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[2,6]

continued …

Table 5

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

Table 6: Wyckoff site: 8f, site symmetry: -1'

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

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

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

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

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

continued ...

Table 8

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

Table 9: Wyckoff site: 8i, site symmetry: .2'.

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

Table 10: Wyckoff site: 8j, site symmetry: .2.

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

Table 11: Wyckoff site: 8k, site symmetry: ..2

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

Table 12: Wyckoff site: 8l, site symmetry: ..2

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

Table 13: Wyckoff site: 16m, 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	$\left[\frac{1}{2} - x,\, y,\, \frac{1}{2} - z\right]$	[3]
4	$\left[\frac{1}{2} - x,\, \frac{1}{2} - y,\, z\right]$	[4]
5	$[-x,\, -y,\, -z]$	[5]
6	$\left[-x,\, y + \frac{1}{2},\, z + \frac{1}{2}\right]$	[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	$\left[x,\, y,\, z + \frac{1}{2}\right]$	[9]
10	$\left[x,\, \frac{1}{2} - y,\, -z\right]$	[10]
11	$\left[\frac{1}{2} - x,\, y,\, -z\right]$	[11]
12	$\left[\frac{1}{2} - x,\, \frac{1}{2} - y,\, z + \frac{1}{2}\right]$	[12]
13	$\left[-x,\, -y,\, \frac{1}{2} - z\right]$	[13]
14	$\left[-x,\, y + \frac{1}{2},\, z\right]$	[14]
15	$\left[x + \frac{1}{2},\, -y,\, z\right]$	[15]
16	$\left[x + \frac{1}{2},\, y + \frac{1}{2},\, \frac{1}{2} - z\right]$	[16]