MSG No. 205.36 $P_Ia\bar{3}$ [Type IV, cubic]

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

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[1,9,10,37,45,46]`
2	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[2,5,7,38,41,43]`
3	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[3,8,11,39,44,47]`
4	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[4,6,12,40,42,48]`
5	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	`[13,21,22,25,33,34]`
6	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[14,17,19,26,29,31]`
7	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	`[15,20,23,27,32,35]`
8	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[16,18,24,28,30,36]`

Table 2: Wyckoff site: `8b`, site symmetry: `.-3.`

No.	position	mapping
1	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[1,9,10,13,21,22]`
2	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[2,5,7,14,17,19]`
3	$[0, 0, 0]$	`[3,8,11,15,20,23]`
4	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[4,6,12,16,18,24]`
5	$\left[\frac{1}{2}, 0, 0\right]$	`[25,33,34,37,45,46]`
6	$\left[0, \frac{1}{2}, 0\right]$	`[26,29,31,38,41,43]`
7	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[27,32,35,39,44,47]`
8	$\left[0, 0, \frac{1}{2}\right]$	`[28,30,36,40,42,48]`

Table 3: Wyckoff site: `16c`, site symmetry: `.3.`

No.	position	mapping
1	$\left[x, \frac{1}{2}-x, x+\frac{1}{2}\right]$	`[1,9,10]`
2	$\left[x+\frac{1}{2}, x, \frac{1}{2}-x\right]$	`[2,5,7]`
3	$[-x, -x, -x]$	`[3,8,11]`
4	$\left[\frac{1}{2}-x, x+\frac{1}{2}, x\right]$	`[4,6,12]`
5	$\left[-x, x+\frac{1}{2}, \frac{1}{2}-x\right]$	`[13,21,22]`
6	$\left[\frac{1}{2}-x, -x, x+\frac{1}{2}\right]$	`[14,17,19]`
7	$[x, x, x]$	`[15,20,23]`
8	$\left[x+\frac{1}{2}, \frac{1}{2}-x, -x\right]$	`[16,18,24]`
9	$\left[x+\frac{1}{2}, -x, x\right]$	`[25,33,34]`
10	$\left[x, x+\frac{1}{2}, -x\right]$	`[26,29,31]`
11	$\left[\frac{1}{2}-x, \frac{1}{2}-x, \frac{1}{2}-x\right]$	`[27,32,35]`
12	$\left[-x, x, x+\frac{1}{2}\right]$	`[28,30,36]`
13	$\left[\frac{1}{2}-x, x, -x\right]$	`[37,45,46]`
14	$\left[-x, \frac{1}{2}-x, x\right]$	`[38,41,43]`
15	$\left[x+\frac{1}{2}, x+\frac{1}{2}, x+\frac{1}{2}\right]$	`[39,44,47]`

continued ...

Table 3

No.	position	mapping
16	$\left[x,\, -x,\, \frac{1}{2}-x\right]$	`[40,42,48]`

Table 4: Wyckoff site: `24d`, site symmetry: `2'..`

No.	position	mapping
1	$\left[x,\, \frac{1}{2},\, \frac{1}{4}\right]$	`[1,26]`
2	$\left[x+\frac{1}{2},\, 0,\, \frac{3}{4}\right]$	`[2,25]`
3	$\left[-x,\, 0,\, \frac{1}{4}\right]$	`[3,28]`
4	$\left[\frac{1}{2}-x,\, \frac{1}{2},\, \frac{3}{4}\right]$	`[4,27]`
5	$\left[\frac{1}{4},\, x,\, \frac{1}{2}\right]$	`[5,36]`
6	$\left[\frac{1}{2},\, \frac{1}{4},\, x\right]$	`[6,33]`
7	$\left[\frac{1}{2},\, \frac{3}{4},\, \frac{1}{2}-x\right]$	`[7,35]`
8	$\left[\frac{1}{4},\, -x,\, 0\right]$	`[8,34]`
9	$\left[0,\, \frac{3}{4},\, x+\frac{1}{2}\right]$	`[9,30]`
10	$\left[\frac{3}{4},\, \frac{1}{2}-x,\, \frac{1}{2}\right]$	`[10,32]`
11	$\left[0,\, \frac{1}{4},\, -x\right]$	`[11,31]`
12	$\left[\frac{3}{4},\, x+\frac{1}{2},\, 0\right]$	`[12,29]`
13	$\left[-x,\, \frac{1}{2},\, \frac{3}{4}\right]$	`[13,38]`
14	$\left[\frac{1}{2}-x,\, 0,\, \frac{1}{4}\right]$	`[14,37]`
15	$\left[x,\, 0,\, \frac{3}{4}\right]$	`[15,40]`
16	$\left[x+\frac{1}{2},\, \frac{1}{2},\, \frac{1}{4}\right]$	`[16,39]`
17	$\left[\frac{3}{4},\, -x,\, \frac{1}{2}\right]$	`[17,48]`
18	$\left[\frac{1}{2},\, \frac{3}{4},\, -x\right]$	`[18,45]`
19	$\left[\frac{1}{2},\, \frac{1}{4},\, x+\frac{1}{2}\right]$	`[19,47]`
20	$\left[\frac{3}{4},\, x,\, 0\right]$	`[20,46]`
21	$\left[0,\, \frac{1}{4},\, \frac{1}{2}-x\right]$	`[21,42]`
22	$\left[\frac{1}{4},\, x+\frac{1}{2},\, \frac{1}{2}\right]$	`[22,44]`
23	$\left[0,\, \frac{3}{4},\, x\right]$	`[23,43]`
24	$\left[\frac{1}{4},\, \frac{1}{2}-x,\, 0\right]$	`[24,41]`

Table 5: Wyckoff site: `48e`, 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	$[z,\, x,\, y]$	`[5]`
6	$[y,\, z,\, x]$	`[6]`
7	$\left[-y,\, z+\frac{1}{2},\, \frac{1}{2}-x\right]$	`[7]`
8	$\left[\frac{1}{2}-z,\, -x,\, y+\frac{1}{2}\right]$	`[8]`
9	$\left[\frac{1}{2}-y,\, -z,\, x+\frac{1}{2}\right]$	`[9]`

continued ...

Table 5

No.	position	mapping
10	$\left[z+\frac{1}{2},\ \frac{1}{2}-x,\ -y\right]$	[10]
11	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ -x\right]$	[11]
12	$\left[-z,\ x+\frac{1}{2},\ \frac{1}{2}-y\right]$	[12]
13	$[-x,\ -y,\ -z]$	[13]
14	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z\right]$	[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]
17	$[-z,\ -x,\ -y]$	[17]
18	$[-y,\ -z,\ -x]$	[18]
19	$\left[y,\ \frac{1}{2}-z,\ x+\frac{1}{2}\right]$	[19]
20	$\left[z+\frac{1}{2},\ x,\ \frac{1}{2}-y\right]$	[20]
21	$\left[y+\frac{1}{2},\ z,\ \frac{1}{2}-x\right]$	[21]
22	$\left[\frac{1}{2}-z,\ x+\frac{1}{2},\ y\right]$	[22]
23	$\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ x\right]$	[23]
24	$\left[z,\ \frac{1}{2}-x,\ y+\frac{1}{2}\right]$	[24]
25	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[25]
26	$\left[x,\ -y,\ \frac{1}{2}-z\right]$	[26]
27	$\left[\frac{1}{2}-x,\ y,\ -z\right]$	[27]
28	$\left[-x,\ \frac{1}{2}-y,\ z\right]$	[28]
29	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ y+\frac{1}{2}\right]$	[29]
30	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$	[30]
31	$\left[\frac{1}{2}-y,\ z,\ -x\right]$	[31]
32	$\left[-z,\ \frac{1}{2}-x,\ y\right]$	[32]
33	$\left[-y,\ \frac{1}{2}-z,\ x\right]$	[33]
34	$\left[z,\ -x,\ \frac{1}{2}-y\right]$	[34]
35	$\left[y,\ -z,\ \frac{1}{2}-x\right]$	[35]
36	$\left[\frac{1}{2}-z,\ x,\ -y\right]$	[36]
37	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[37]
38	$\left[-x,\ y,\ z+\frac{1}{2}\right]$	[38]
39	$\left[x+\frac{1}{2},\ -y,\ z\right]$	[39]
40	$\left[x,\ y+\frac{1}{2},\ -z\right]$	[40]
41	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ \frac{1}{2}-y\right]$	[41]
42	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[42]
43	$\left[y+\frac{1}{2},\ -z,\ x\right]$	[43]
44	$\left[z,\ x+\frac{1}{2},\ -y\right]$	[44]
45	$\left[y,\ z+\frac{1}{2},\ -x\right]$	[45]
46	$\left[-z,\ x,\ y+\frac{1}{2}\right]$	[46]
47	$\left[-y,\ z,\ x+\frac{1}{2}\right]$	[47]
48	$\left[z+\frac{1}{2},\ -x,\ y\right]$	[48]