MSG No. 211.56 $I432$ [Type I, cubic]

Table 1: Wyckoff site: 2a, site symmetry: 432

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

Table 2: Wyckoff site: 6b, site symmetry: 42.2

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

Table 3: Wyckoff site: 8c, site symmetry: .32

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

Table 4: Wyckoff site: 12d, site symmetry: 2.22

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	[1,8,37,38]
2	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[2,3,33,34]
3	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[4,16,42,45]
4	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[5,15,43,47]
5	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[6,11,44,46]
6	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	[7,12,41,48]
7	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	[9,10,26,27]
8	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	[13,14,25,32]
9	$\left[0, \frac{1}{4}, \frac{1}{2}\right]$	[17,24,31,36]

continued ...

Table 4

No.	position	mapping
10	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[18,21,28,40]
11	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[19,23,29,39]
12	$\left[0, \frac{3}{4}, \frac{1}{2}\right]$	[20,22,30,35]

Table 5: Wyckoff site: 12e, site symmetry: 4..

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

Table 6: Wyckoff site: 16f, site symmetry: .3.

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

Table 7: Wyckoff site: 24g, site symmetry: 2..

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

Table 8: Wyckoff site: 24h, site symmetry: ..2

No.	position	mapping
1	$[0,\ y,\ y]$	[1,13]
2	$[0,\ -y,\ y]$	[2,10]
3	$[0,\ y,\ -y]$	[3,9]
4	$[y,\ y,\ 0]$	[4,18]
5	$[-y,\ y,\ 0]$	[5,19]
6	$[-y,\ 0,\ y]$	[6,20]
7	$[y,\ 0,\ y]$	[7,17]
8	$[0,\ -y,\ -y]$	[8,14]
9	$[y,\ 0,\ -y]$	[11,22]
10	$[-y,\ 0,\ -y]$	[12,24]
11	$[y,\ -y,\ 0]$	[15,23]
12	$[-y,\ -y,\ 0]$	[16,21]
13	$\left[\frac{1}{2},\ y+\frac{1}{2},\ y+\frac{1}{2}\right]$	[25,37]
14	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ y+\frac{1}{2}\right]$	[26,34]
15	$\left[\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-y\right]$	[27,33]

continued ...

Table 8

No.	position	mapping
16	$\left[y+\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}\right]$	[28,42]
17	$\left[\frac{1}{2}-y, y+\frac{1}{2}, \frac{1}{2}\right]$	[29,43]
18	$\left[\frac{1}{2}-y, \frac{1}{2}, y+\frac{1}{2}\right]$	[30,44]
19	$\left[y+\frac{1}{2}, \frac{1}{2}, y+\frac{1}{2}\right]$	[31,41]
20	$\left[\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}-y\right]$	[32,38]
21	$\left[y+\frac{1}{2}, \frac{1}{2}, \frac{1}{2}-y\right]$	[35,46]
22	$\left[\frac{1}{2}-y, \frac{1}{2}, \frac{1}{2}-y\right]$	[36,48]
23	$\left[y+\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}\right]$	[39,47]
24	$\left[\frac{1}{2}-y, \frac{1}{2}-y, \frac{1}{2}\right]$	[40,45]

Table 9: Wyckoff site: 24i, site symmetry: ..2

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

Table 10: Wyckoff site: `48j`, site symmetry: `1`

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

continued ...

Table 10

No.	position	mapping
47	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[47]
48	$\left[\frac{1}{2}-z,\ x+\frac{1}{2},\ \frac{1}{2}-y\right]$	[48]