SG No. 223 O_{h}^{3} $Pm\bar{3}n$ [cubic]

* plus set: + [0, 0, 0]

Table 1: Wyckoff site: 2a, site symmetry: m-3.

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

Table 2: Wyckoff site: 6b, site symmetry: mmm..

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

Table 3: Wyckoff site: 6c, site symmetry: -4m.2

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

Table 4: Wyckoff site: 6d, site symmetry: -4m.2

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

Table 5: Wyckoff site: `8e`, site symmetry: `.32`

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

Table 6: Wyckoff site: `12f`, site symmetry: `mm2..`

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

Table 7: Wyckoff site: `12g`, site symmetry: `mm2..`

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

Table 8: Wyckoff site: `12h`, site symmetry: `mm2..`

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

Table 9: Wyckoff site: `16i`, site symmetry: `.3.`

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

Table 10: Wyckoff site: `24j`, site symmetry: `..2`

No.	position	mapping
1	$\left[\frac{1}{4},\ y,\ y+\frac{1}{2}\right]$	`[1,18]`
2	$\left[\frac{3}{4},\ -y,\ y+\frac{1}{2}\right]$	`[2,20]`
3	$\left[\frac{3}{4},\ y,\ \frac{1}{2}-y\right]$	`[3,17]`
4	$\left[\frac{1}{4},\ -y,\ \frac{1}{2}-y\right]$	`[4,19]`
5	$\left[y+\frac{1}{2},\ \frac{1}{4},\ y\right]$	`[5,15]`

continued ...

Table 10

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

Table 11: Wyckoff site: 24k, site symmetry: m..

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

continued ...

Table 11

No.	position	mapping
22	$\left[z+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[22,47]
23	$\left[\frac{1}{2}-z,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[23,46]
24	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[24,45]

Table 12: Wyckoff site: 4l, site symmetry: 1

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

continued ...

Table 12

No.	position	mapping
38	$\left[y+\frac{1}{2}, x+\frac{1}{2}, z+\frac{1}{2}\right]$	[38]
39	$\left[\frac{1}{2}-y, x+\frac{1}{2}, \frac{1}{2}-z\right]$	[39]
40	$\left[y+\frac{1}{2}, \frac{1}{2}-x, \frac{1}{2}-z\right]$	[40]
41	$\left[\frac{1}{2}-x, \frac{1}{2}-z, y+\frac{1}{2}\right]$	[41]
42	$\left[x+\frac{1}{2}, \frac{1}{2}-z, \frac{1}{2}-y\right]$	[42]
43	$\left[x+\frac{1}{2}, z+\frac{1}{2}, y+\frac{1}{2}\right]$	[43]
44	$\left[\frac{1}{2}-x, z+\frac{1}{2}, \frac{1}{2}-y\right]$	[44]
45	$\left[\frac{1}{2}-z, \frac{1}{2}-y, x+\frac{1}{2}\right]$	[45]
46	$\left[\frac{1}{2}-z, y+\frac{1}{2}, \frac{1}{2}-x\right]$	[46]
47	$\left[z+\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}-x\right]$	[47]
48	$\left[z+\frac{1}{2}, y+\frac{1}{2}, x+\frac{1}{2}\right]$	[48]