SG No. 224 O_{h}^4 $Pn\bar{3}m$ [cubic]

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

Table 1: Wyckoff site: 2a, site symmetry: -43m

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

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

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

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

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

Table 4: Wyckoff site: 6d, site symmetry: -42.m

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

Table 5: Wyckoff site: 8e, site symmetry: .3m

No.	position	mapping
1	$[x, x, x]$	[1,5,9,38,43,48]

Table 5

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

Table 6: Wyckoff site: `12f`, site symmetry: `2.22`

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

Table 7: Wyckoff site: `12g`, site symmetry: `2.mm`

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

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

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

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

No.	position	mapping
1	$\left[\frac{1}{2}, y, y + \frac{1}{2}\right]$	[1,18]
2	$\left[0, \frac{1}{2} - y, y + \frac{1}{2}\right]$	[2,20]
3	$[0, y, -y]$	[3,17]
4	$\left[\frac{1}{2}, \frac{1}{2} - y, -y\right]$	[4,19]
5	$\left[y + \frac{1}{2}, \frac{1}{2}, y\right]$	[5,15]
6	$\left[y + \frac{1}{2}, 0, \frac{1}{2} - y\right]$	[6,13]
7	$[-y, 0, y]$	[7,16]
8	$\left[-y, \frac{1}{2}, \frac{1}{2} - y\right]$	[8,14]
9	$\left[y, y + \frac{1}{2}, \frac{1}{2}\right]$	[9,21]
10	$\left[\frac{1}{2} - y, y + \frac{1}{2}, 0\right]$	[10,23]
11	$[y, -y, 0]$	[11,22]
12	$\left[\frac{1}{2} - y, -y, \frac{1}{2}\right]$	[12,24]
13	$\left[\frac{1}{2}, -y, \frac{1}{2} - y\right]$	[25,42]
14	$\left[0, y + \frac{1}{2}, \frac{1}{2} - y\right]$	[26,44]
15	$[0, -y, y]$	[27,41]

continued …

Table 9

No.	position	mapping
16	$\left[\frac{1}{2}, y + \frac{1}{2}, y\right]$	[28,43]
17	$\left[\frac{1}{2} - y, \frac{1}{2}, -y\right]$	[29,39]
18	$\left[\frac{1}{2} - y, 0, y + \frac{1}{2}\right]$	[30,37]
19	$[y, 0, -y]$	[31,40]
20	$\left[y, \frac{1}{2}, y + \frac{1}{2}\right]$	[32,38]
21	$\left[-y, \frac{1}{2} - y, \frac{1}{2}\right]$	[33,45]
22	$\left[y + \frac{1}{2}, \frac{1}{2} - y, 0\right]$	[34,47]
23	$[-y, y, 0]$	[35,46]
24	$\left[y + \frac{1}{2}, y, \frac{1}{2}\right]$	[36,48]

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

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

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

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

Table 12: Wyckoff site: `48l`, site symmetry: `1`

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

continued …

Table 12

No.	position	mapping
16	$\left[-y,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[16]
17	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, -y\right]$	[17]
18	$\left[-x,\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[18]
19	$[-x,\, -z,\, -y]$	[19]
20	$\left[x+\frac{1}{2},\, -z,\, y+\frac{1}{2}\right]$	[20]
21	$\left[z+\frac{1}{2},\, y+\frac{1}{2},\, -x\right]$	[21]
22	$\left[z+\frac{1}{2},\, -y,\, x+\frac{1}{2}\right]$	[22]
23	$\left[-z,\, y+\frac{1}{2},\, x+\frac{1}{2}\right]$	[23]
24	$[-z,\, -y,\, -x]$	[24]
25	$[-x,\, -y,\, -z]$	[25]
26	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, -z\right]$	[26]
27	$\left[x+\frac{1}{2},\, -y,\, z+\frac{1}{2}\right]$	[27]
28	$\left[-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[28]
29	$[-z,\, -x,\, -y]$	[29]
30	$\left[-z,\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[30]
31	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, -y\right]$	[31]
32	$\left[z+\frac{1}{2},\, -x,\, y+\frac{1}{2}\right]$	[32]
33	$[-y,\, -z,\, -x]$	[33]
34	$\left[y+\frac{1}{2},\, -z,\, x+\frac{1}{2}\right]$	[34]
35	$\left[-y,\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[35]
36	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, -x\right]$	[36]
37	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, z\right]$	[37]
38	$[y,\, x,\, z]$	[38]
39	$\left[\frac{1}{2}-y,\, x,\, \frac{1}{2}-z\right]$	[39]
40	$\left[y,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[40]
41	$\left[\frac{1}{2}-x,\, \frac{1}{2}-z,\, y\right]$	[41]
42	$\left[x,\, \frac{1}{2}-z,\, \frac{1}{2}-y\right]$	[42]
43	$[x,\, z,\, y]$	[43]
44	$\left[\frac{1}{2}-x,\, z,\, \frac{1}{2}-y\right]$	[44]
45	$\left[\frac{1}{2}-z,\, \frac{1}{2}-y,\, x\right]$	[45]
46	$\left[\frac{1}{2}-z,\, y,\, \frac{1}{2}-x\right]$	[46]
47	$\left[z,\, \frac{1}{2}-y,\, \frac{1}{2}-x\right]$	[47]
48	$[z,\, y,\, x]$	[48]