SG No. 222 O_{h}^{2} $Pn\bar{3}n$ [cubic]

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

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

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

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

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

Table 4: Wyckoff site: 12d, site symmetry: -4..

No.	position	mapping
1	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	[1,4,41,44]
2	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[2,3,42,43]
3	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	[5,8,37,40]
4	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[6,7,38,39]
5	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[9,12,46,47]
6	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[10,11,45,48]
7	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	[13,16,29,32]
8	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[14,15,30,31]

continued ...

Table 4

No.	position	mapping
9	$\left[0,\ \frac{1}{4},\ \frac{3}{4}\right]$	`[17,20,25,28]`
10	$\left[\frac{1}{2},\ \frac{1}{4},\ \frac{3}{4}\right]$	`[18,19,26,27]`
11	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}\right]$	`[21,24,34,35]`
12	$\left[\frac{1}{4},\ \frac{3}{4},\ 0\right]$	`[22,23,33,36]`

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

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

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

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

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

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

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

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

continued ...

Table 8

No.	position	mapping
16	$\left[\frac{3}{4}, y+\frac{1}{2}, y+\frac{1}{2}\right]$	[28,43]
17	$\left[-y, \frac{3}{4}, -y\right]$	[29,39]
18	$\left[-y, \frac{3}{4}, y+\frac{1}{2}\right]$	[30,37]
19	$\left[y+\frac{1}{2}, \frac{3}{4}, -y\right]$	[31,40]
20	$\left[y+\frac{1}{2}, \frac{3}{4}, y+\frac{1}{2}\right]$	[32,38]
21	$\left[-y, -y, \frac{3}{4}\right]$	[33,45]
22	$\left[y+\frac{1}{2}, -y, \frac{3}{4}\right]$	[34,47]
23	$\left[-y, y+\frac{1}{2}, \frac{3}{4}\right]$	[35,46]
24	$\left[y+\frac{1}{2}, y+\frac{1}{2}, \frac{3}{4}\right]$	[36,48]

Table 9: Wyckoff site: 48i, 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	$\left[y, x, \frac{1}{2}-z\right]$	[13]
14	$\left[\frac{1}{2}-y, \frac{1}{2}-x, \frac{1}{2}-z\right]$	[14]
15	$\left[y, \frac{1}{2}-x, z\right]$	[15]
16	$\left[\frac{1}{2}-y, x, z\right]$	[16]
17	$\left[x, z, \frac{1}{2}-y\right]$	[17]
18	$\left[\frac{1}{2}-x, z, y\right]$	[18]
19	$\left[\frac{1}{2}-x, \frac{1}{2}-z, \frac{1}{2}-y\right]$	[19]
20	$\left[x, \frac{1}{2}-z, y\right]$	[20]
21	$\left[z, y, \frac{1}{2}-x\right]$	[21]
22	$\left[z, \frac{1}{2}-y, x\right]$	[22]
23	$\left[\frac{1}{2}-z, y, x\right]$	[23]
24	$\left[\frac{1}{2}-z, \frac{1}{2}-y, \frac{1}{2}-x\right]$	[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]

continued ...

Table 9

No.	position	mapping
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	$\left[-y,\,-x,\,z+\frac{1}{2}\right]$	[37]
38	$\left[y+\frac{1}{2},\,x+\frac{1}{2},\,z+\frac{1}{2}\right]$	[38]
39	$\left[-y,\,x+\frac{1}{2},\,-z\right]$	[39]
40	$\left[y+\frac{1}{2},\,-x,\,-z\right]$	[40]
41	$\left[-x,\,-z,\,y+\frac{1}{2}\right]$	[41]
42	$\left[x+\frac{1}{2},\,-z,\,-y\right]$	[42]
43	$\left[x+\frac{1}{2},\,z+\frac{1}{2},\,y+\frac{1}{2}\right]$	[43]
44	$\left[-x,\,z+\frac{1}{2},\,-y\right]$	[44]
45	$\left[-z,\,-y,\,x+\frac{1}{2}\right]$	[45]
46	$\left[-z,\,y+\frac{1}{2},\,-x\right]$	[46]
47	$\left[z+\frac{1}{2},\,-y,\,-x\right]$	[47]
48	$\left[z+\frac{1}{2},\,y+\frac{1}{2},\,x+\frac{1}{2}\right]$	[48]