SG No. 221 O_{h}^{1} $Pm\bar{3}m$ [cubic]

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

Table 1: Wyckoff site: `1a`, site symmetry: `m-3m`

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,`
		`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: `1b`, site symmetry: `m-3m`

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[1,2,3,4,5,6,7,8,9,10,11,12,13,14,15,16,17,18,19,20,21,22,23,24,`
		`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 3: Wyckoff site: `3c`, site symmetry: `4/mm.m`

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

Table 4: Wyckoff site: `3d`, site symmetry: `4/mm.m`

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

Table 5: Wyckoff site: `6e`, site symmetry: `4m.m`

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

Table 6: Wyckoff site: `6f`, site symmetry: `4m.m`

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

Table 7: Wyckoff site: `8g`, site symmetry: `.3m`

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

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	$\left[\frac{1}{2},\ x,\ 0\right]$	`[13,16,38,39]`
8	$\left[\frac{1}{2},\ -x,\ 0\right]$	`[14,15,37,40]`
9	$\left[x,\ 0,\ \frac{1}{2}\right]$	`[17,20,42,43]`
10	$\left[-x,\ 0,\ \frac{1}{2}\right]$	`[18,19,41,44]`
11	$\left[0,\ \frac{1}{2},\ -x\right]$	`[21,24,46,47]`
12	$\left[0,\ \frac{1}{2},\ x\right]$	`[22,23,45,48]`

Table 9: Wyckoff site: `12i`, site symmetry: `m.m2`

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

Table 10: Wyckoff site: `12j`, site symmetry: `m.m2`

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

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]`

continued ...

Table 11

No.	position	mapping
10	$[-y,\ z,\ 0]$	`[10,35]`
11	$[y,\ -z,\ 0]$	`[11,34]`
12	$[-y,\ -z,\ 0]$	`[12,33]`
13	$[y,\ 0,\ -z]$	`[13,40]`
14	$[-y,\ 0,\ -z]$	`[14,39]`
15	$[y,\ 0,\ z]$	`[15,38]`
16	$[-y,\ 0,\ z]$	`[16,37]`
17	$[0,\ z,\ -y]$	`[17,44]`
18	$[0,\ z,\ y]$	`[18,43]`
19	$[0,\ -z,\ -y]$	`[19,42]`
20	$[0,\ -z,\ y]$	`[20,41]`
21	$[z,\ y,\ 0]$	`[21,48]`
22	$[z,\ -y,\ 0]$	`[22,47]`
23	$[-z,\ y,\ 0]$	`[23,46]`
24	$[-z,\ -y,\ 0]$	`[24,45]`

Table 12: Wyckoff site: `24l`, site symmetry: `m..`

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

Table 13: Wyckoff site: `24m`, site symmetry: `..m`

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

Table 14: Wyckoff site: `48n`, 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	$[y, x, -z]$	`[13]`
14	$[-y, -x, -z]$	`[14]`
15	$[y, -x, z]$	`[15]`

continued ...

Table 14

No.	position	mapping
16	$[-y,\ x,\ z]$	[16]
17	$[x,\ z,\ -y]$	[17]
18	$[-x,\ z,\ y]$	[18]
19	$[-x,\ -z,\ -y]$	[19]
20	$[x,\ -z,\ y]$	[20]
21	$[z,\ y,\ -x]$	[21]
22	$[z,\ -y,\ x]$	[22]
23	$[-z,\ y,\ x]$	[23]
24	$[-z,\ -y,\ -x]$	[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	$[-y,\ -x,\ z]$	[37]
38	$[y,\ x,\ z]$	[38]
39	$[-y,\ x,\ -z]$	[39]
40	$[y,\ -x,\ -z]$	[40]
41	$[-x,\ -z,\ y]$	[41]
42	$[x,\ -z,\ -y]$	[42]
43	$[x,\ z,\ y]$	[43]
44	$[-x,\ z,\ -y]$	[44]
45	$[-z,\ -y,\ x]$	[45]
46	$[-z,\ y,\ -x]$	[46]
47	$[z,\ -y,\ -x]$	[47]
48	$[z,\ y,\ x]$	[48]