SG No. 229 O_{h}^{9} $Im\bar{3}m$ [cubic]

* plus set: $+[0,\ 0,\ 0]$, $+\left[\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}\right]$

Table 1: Wyckoff site: `2a`, 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: `6b`, 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 3: Wyckoff site: `8c`, site symmetry: `.-3m`

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

Table 4: Wyckoff site: `12d`, 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 5: Wyckoff site: `12e`, 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]`

continued ...

Table 5

No.	position	mapping
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: `16f`, 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 7: Wyckoff site: `24g`, 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	$\left[0,\ x,\ \frac{1}{2}\right]$	`[13,16,38,39]`
8	$\left[0,\ -x,\ \frac{1}{2}\right]$	`[14,15,37,40]`
9	$\left[x,\ \frac{1}{2},\ 0\right]$	`[17,20,42,43]`
10	$\left[-x,\ \frac{1}{2},\ 0\right]$	`[18,19,41,44]`
11	$\left[\frac{1}{2},\ 0,\ -x\right]$	`[21,24,46,47]`
12	$\left[\frac{1}{2},\ 0,\ x\right]$	`[22,23,45,48]`

Table 8: Wyckoff site: `24h`, 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]`

continued ...

Table 8

No.	position	mapping
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 9: Wyckoff site: `48i`, site symmetry: `..2`

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

Table 10: Wyckoff site: `48j`, 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	$[y,\ 0,\ -z]$	`[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 11: Wyckoff site: `48k`, 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]`

continued ...

Table 11

No.	position	mapping
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 12: Wyckoff site: 96l, 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]
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]

continued ...

Table 12

No.	position	mapping
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]