SG No. 226 O_{h}^{6} $Fm\bar{3}c$ [cubic]

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

Table 1: Wyckoff site: `8a`, 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: `8b`, 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 3: Wyckoff site: `24c`, site symmetry: `-4m.2`

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

Table 4: Wyckoff site: `24d`, site symmetry: `4/m..`

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

Table 5: Wyckoff site: `48e`, site symmetry: `mm2..`

No.	position	mapping
1	$[x,\ 0,\ 0]$	`[1,4,26,27]`

continued ...

Table 5

No.	position	mapping
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 6: Wyckoff site: `48f`, site symmetry: `4..`

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

Table 7: Wyckoff site: `64g`, 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]`

continued ...

Table 7

No.	position	mapping
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 8: Wyckoff site: 96h, site symmetry: ..2

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

Table 9: Wyckoff site: 96i, 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]

continued ...

Table 9

No.	position	mapping
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]
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 10: Wyckoff site: 192j, 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]

continued ...

Table 10

No.	position	mapping
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]
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]