SG No. 227 O_{h}^{7} $Fd\bar{3}m$ [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: `-43m`

No.	position	mapping
1	$\left[\frac{1}{8},\,\frac{1}{8},\,\frac{1}{8}\right]$	`[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	$\left[\frac{7}{8},\,\frac{3}{8},\,\frac{3}{8}\right]$	`[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: `8b`, site symmetry: `-43m`

No.	position	mapping
1	$\left[\frac{3}{8},\,\frac{3}{8},\,\frac{3}{8}\right]$	`[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	$\left[\frac{1}{8},\,\frac{5}{8},\,\frac{1}{8}\right]$	`[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 3: Wyckoff site: `16c`, site symmetry: `.-3m`

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

Table 4: Wyckoff site: `16d`, 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	$\left[\frac{1}{4},\,\frac{3}{4},\,0\right]$	`[2,7,12,13,17,21,26,31,36,37,41,45]`
3	$\left[\frac{3}{4},\,0,\,\frac{1}{4}\right]$	`[3,8,10,15,20,22,27,32,34,39,44,46]`
4	$\left[0,\,\frac{1}{4},\,\frac{3}{4}\right]$	`[4,6,11,16,18,23,28,30,35,40,42,47]`

Table 5: Wyckoff site: `32e`, site symmetry: `.3m`

No.	position	mapping
1	$[x,\,x,\,x]$	`[1,5,9,38,43,48]`
2	$\left[\frac{3}{4}-x,\,\frac{1}{4}-x,\,x+\frac{1}{2}\right]$	`[2,7,12,37,41,45]`
3	$\left[\frac{1}{4}-x,\,x+\frac{1}{2},\,\frac{3}{4}-x\right]$	`[3,8,10,39,44,46]`
4	$\left[x+\frac{1}{2},\,\frac{3}{4}-x,\,\frac{1}{4}-x\right]$	`[4,6,11,40,42,47]`
5	$\left[x+\frac{3}{4},\,x+\frac{1}{4},\,\frac{1}{2}-x\right]$	`[13,17,21,26,31,36]`

continued ...

Table 5

No.	position	mapping
6	$[-x,\ -x,\ -x]$	`[14,19,24,25,29,33]`
7	$\left[x+\frac{1}{4},\ \frac{1}{2}-x,\ x+\frac{3}{4}\right]$	`[15,20,22,27,32,34]`
8	$\left[\frac{1}{2}-x,\ x+\frac{3}{4},\ x+\frac{1}{4}\right]$	`[16,18,23,28,30,35]`

Table 6: Wyckoff site: `48f`, site symmetry: `2.mm`

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

Table 7: Wyckoff site: `96g`, site symmetry: `..m`

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

continued ...

Table 7

No.	position	mapping
20	$\left[x+\frac{1}{4},\ \frac{1}{2}-z,\ x+\frac{3}{4}\right]$	[20,34]
21	$\left[z+\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{2}-x\right]$	[21,31]
22	$\left[z+\frac{1}{4},\ \frac{1}{2}-x,\ x+\frac{3}{4}\right]$	[22,32]
23	$\left[\frac{1}{2}-z,\ x+\frac{3}{4},\ x+\frac{1}{4}\right]$	[23,30]
24	$[-z,\ -x,\ -x]$	[24,29]

Table 8: Wyckoff site: 96h, site symmetry: ..2

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

Table 9: Wyckoff site: 192i, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$\left[\frac{3}{4}-x,\ \frac{1}{4}-y,\ z+\frac{1}{2}\right]$	[2]
3	$\left[\frac{1}{4}-x,\ y+\frac{1}{2},\ \frac{3}{4}-z\right]$	[3]
4	$\left[x+\frac{1}{2},\ \frac{3}{4}-y,\ \frac{1}{4}-z\right]$	[4]
5	$[z,\ x,\ y]$	[5]

continued ...

Table 9

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