SG No. 203 T_{h}^4 $Fd\bar{3}$ [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: `23.`

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]`
2	$\left[\frac{7}{8},\,\frac{7}{8},\,\frac{7}{8}\right]$	`[13,14,15,16,17,18,19,20,21,22,23,24]`

Table 2: Wyckoff site: `8b`, site symmetry: `23.`

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

Table 3: Wyckoff site: `16c`, site symmetry: `.-3.`

No.	position	mapping
1	$[0,\,0,\,0]$	`[1,5,9,13,17,21]`
2	$\left[\frac{3}{4},\,\frac{3}{4},\,0\right]$	`[2,7,12,14,19,24]`
3	$\left[\frac{3}{4},\,0,\,\frac{3}{4}\right]$	`[3,8,10,15,20,22]`
4	$\left[0,\,\frac{3}{4},\,\frac{3}{4}\right]$	`[4,6,11,16,18,23]`

Table 4: Wyckoff site: `16d`, site symmetry: `.-3.`

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

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

No.	position	mapping
1	$[x,\,x,\,x]$	`[1,5,9]`
2	$\left[\frac{3}{4}-x,\,\frac{3}{4}-x,\,x\right]$	`[2,7,12]`
3	$\left[\frac{3}{4}-x,\,x,\,\frac{3}{4}-x\right]$	`[3,8,10]`
4	$\left[x,\,\frac{3}{4}-x,\,\frac{3}{4}-x\right]$	`[4,6,11]`
5	$[-x,\,-x,\,-x]$	`[13,17,21]`

continued ...

Table 5

No.	position	mapping
6	$\left[x+\frac{1}{4},\, x+\frac{1}{4},\, -x\right]$	[14,19,24]
7	$\left[x+\frac{1}{4},\, -x,\, x+\frac{1}{4}\right]$	[15,20,22]
8	$\left[-x,\, x+\frac{1}{4},\, x+\frac{1}{4}\right]$	[16,18,23]

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

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

Table 7: Wyckoff site: 96g, site symmetry: 1

No.	position	mapping
1	$[x,\, y,\, z]$	[1]
2	$\left[\frac{3}{4}-x,\, \frac{3}{4}-y,\, z\right]$	[2]
3	$\left[\frac{3}{4}-x,\, y,\, \frac{3}{4}-z\right]$	[3]
4	$\left[x,\, \frac{3}{4}-y,\, \frac{3}{4}-z\right]$	[4]
5	$[z,\, x,\, y]$	[5]
6	$\left[z,\, \frac{3}{4}-x,\, \frac{3}{4}-y\right]$	[6]
7	$\left[\frac{3}{4}-z,\, \frac{3}{4}-x,\, y\right]$	[7]
8	$\left[\frac{3}{4}-z,\, x,\, \frac{3}{4}-y\right]$	[8]
9	$[y,\, z,\, x]$	[9]
10	$\left[\frac{3}{4}-y,\, z,\, \frac{3}{4}-x\right]$	[10]
11	$\left[y,\, \frac{3}{4}-z,\, \frac{3}{4}-x\right]$	[11]
12	$\left[\frac{3}{4}-y,\, \frac{3}{4}-z,\, x\right]$	[12]
13	$[-x,\, -y,\, -z]$	[13]
14	$\left[x+\frac{1}{4},\, y+\frac{1}{4},\, -z\right]$	[14]
15	$\left[x+\frac{1}{4},\, -y,\, z+\frac{1}{4}\right]$	[15]
16	$\left[-x,\, y+\frac{1}{4},\, z+\frac{1}{4}\right]$	[16]
17	$[-z,\, -x,\, -y]$	[17]
18	$\left[-z,\, x+\frac{1}{4},\, y+\frac{1}{4}\right]$	[18]
19	$\left[z+\frac{1}{4},\, x+\frac{1}{4},\, -y\right]$	[19]

continued ...

Table 7

No.	position	mapping
20	$\left[z+\frac{1}{4},\,-x,\,y+\frac{1}{4}\right]$	[20]
21	$[-y,\,-z,\,-x]$	[21]
22	$\left[y+\frac{1}{4},\,-z,\,x+\frac{1}{4}\right]$	[22]
23	$\left[-y,\,z+\frac{1}{4},\,x+\frac{1}{4}\right]$	[23]
24	$\left[y+\frac{1}{4},\,z+\frac{1}{4},\,-x\right]$	[24]