SG No. 230 O_{h}^{10} $Ia\bar{3}d$ [cubic]

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

Table 1: Wyckoff site: `16a`, site symmetry: `.-3.`

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

Table 2: Wyckoff site: `16b`, site symmetry: `.32`

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

Table 3: Wyckoff site: `24c`, site symmetry: `2.22`

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

Table 4: Wyckoff site: `24d`, site symmetry: `-4..`

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

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

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

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

No.	position	mapping
1	$\left[x,\, 0,\, \frac{1}{4}\right]$	[1,4]
2	$\left[\frac{1}{2} - x,\, 0,\, \frac{3}{4}\right]$	[2,3]
3	$\left[\frac{1}{4},\, x,\, 0\right]$	[5,8]
4	$\left[\frac{3}{4},\, \frac{1}{2} - x,\, 0\right]$	[6,7]
5	$\left[0,\, \frac{1}{4},\, x\right]$	[9,12]

continued ...

2

Table 6

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

Table 7: Wyckoff site: 48g, site symmetry: ..2

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

continued …

3

Table 7

No.	position	mapping
22	$\left[y,\ y+\frac{1}{4},\ \frac{5}{8}\right]$	[34,46]
23	$\left[\frac{1}{2}-y,\ \frac{3}{4}-y,\ \frac{1}{8}\right]$	[35,47]
24	$\left[y+\frac{1}{2},\ \frac{1}{4}-y,\ \frac{3}{8}\right]$	[36,45]

Table 8: Wyckoff site: `96h`, site symmetry: `1`

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$\left[\frac{1}{2}-x,\ -y,\ z+\frac{1}{2}\right]$	[2]
3	$\left[-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[3]
4	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[4]
5	$[z,\ x,\ y]$	[5]
6	$\left[z+\frac{1}{2},\ \frac{1}{2}-x,\ -y\right]$	[6]
7	$\left[\frac{1}{2}-z,\ -x,\ y+\frac{1}{2}\right]$	[7]
8	$\left[-z,\ x+\frac{1}{2},\ \frac{1}{2}-y\right]$	[8]
9	$[y,\ z,\ x]$	[9]
10	$\left[-y,\ z+\frac{1}{2},\ \frac{1}{2}-x\right]$	[10]
11	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ -x\right]$	[11]
12	$\left[\frac{1}{2}-y,\ -z,\ x+\frac{1}{2}\right]$	[12]
13	$\left[y+\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{4}-z\right]$	[13]
14	$\left[\frac{3}{4}-y,\ \frac{3}{4}-x,\ \frac{3}{4}-z\right]$	[14]
15	$\left[y+\frac{1}{4},\ \frac{1}{4}-x,\ z+\frac{3}{4}\right]$	[15]
16	$\left[\frac{1}{4}-y,\ x+\frac{3}{4},\ z+\frac{1}{4}\right]$	[16]
17	$\left[x+\frac{3}{4},\ z+\frac{1}{4},\ \frac{1}{4}-y\right]$	[17]
18	$\left[\frac{1}{4}-x,\ z+\frac{3}{4},\ y+\frac{1}{4}\right]$	[18]
19	$\left[\frac{3}{4}-x,\ \frac{3}{4}-z,\ \frac{3}{4}-y\right]$	[19]
20	$\left[x+\frac{1}{4},\ \frac{1}{4}-z,\ y+\frac{3}{4}\right]$	[20]
21	$\left[z+\frac{3}{4},\ y+\frac{1}{4},\ \frac{1}{4}-x\right]$	[21]
22	$\left[z+\frac{1}{4},\ \frac{1}{4}-y,\ x+\frac{3}{4}\right]$	[22]
23	$\left[\frac{1}{4}-z,\ y+\frac{3}{4},\ x+\frac{1}{4}\right]$	[23]
24	$\left[\frac{3}{4}-z,\ \frac{3}{4}-y,\ \frac{3}{4}-x\right]$	[24]
25	$[-x,\ -y,\ -z]$	[25]
26	$\left[x+\frac{1}{2},\ y,\ \frac{1}{2}-z\right]$	[26]
27	$\left[x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[27]
28	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z\right]$	[28]
29	$[-z,\ -x,\ -y]$	[29]
30	$\left[\frac{1}{2}-z,\ x+\frac{1}{2},\ y\right]$	[30]
31	$\left[z+\frac{1}{2},\ x,\ \frac{1}{2}-y\right]$	[31]
32	$\left[z,\ \frac{1}{2}-x,\ y+\frac{1}{2}\right]$	[32]
33	$[-y,\ -z,\ -x]$	[33]
34	$\left[y,\ \frac{1}{2}-z,\ x+\frac{1}{2}\right]$	[34]
35	$\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ x\right]$	[35]
36	$\left[y+\frac{1}{2},\ z,\ \frac{1}{2}-x\right]$	[36]
37	$\left[\frac{1}{4}-y,\ \frac{3}{4}-x,\ z+\frac{3}{4}\right]$	[37]

continued ...

4

Table 8

No.	position	mapping
38	$\left[y + \frac{1}{4},\, x + \frac{1}{4},\, z + \frac{1}{4}\right]$	[38]
39	$\left[\frac{3}{4} - y,\, x + \frac{3}{4},\, \frac{1}{4} - z\right]$	[39]
40	$\left[y + \frac{3}{4},\, \frac{1}{4} - x,\, \frac{3}{4} - z\right]$	[40]
41	$\left[\frac{1}{4} - x,\, \frac{3}{4} - z,\, y + \frac{3}{4}\right]$	[41]
42	$\left[x + \frac{3}{4},\, \frac{1}{4} - z,\, \frac{3}{4} - y\right]$	[42]
43	$\left[x + \frac{1}{4},\, z + \frac{1}{4},\, y + \frac{1}{4}\right]$	[43]
44	$\left[\frac{3}{4} - x,\, z + \frac{3}{4},\, \frac{1}{4} - y\right]$	[44]
45	$\left[\frac{1}{4} - z,\, \frac{3}{4} - y,\, x + \frac{3}{4}\right]$	[45]
46	$\left[\frac{3}{4} - z,\, y + \frac{3}{4},\, \frac{1}{4} - x\right]$	[46]
47	$\left[z + \frac{3}{4},\, \frac{1}{4} - y,\, \frac{3}{4} - x\right]$	[47]
48	$\left[z + \frac{1}{4},\, y + \frac{1}{4},\, x + \frac{1}{4}\right]$	[48]