

SG No. 228 $O_h^8 Fd\bar{3}c$ [cubic]

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

Table 1: Wyckoff site: 16a, site symmetry: $23.$

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

Table 2: Wyckoff site: 32b, site symmetry: $.32$

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

Table 3: Wyckoff site: 32c, site symmetry: $.-3.$

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

Table 4: Wyckoff site: 48d, site symmetry: $-4..$

No.	position	mapping
1	$[\frac{7}{8}, \frac{1}{8}, \frac{1}{8}]$	$[1, 4, 41, 44]$
2	$[\frac{3}{8}, \frac{5}{8}, \frac{5}{8}]$	$[2, 3, 42, 43]$
3	$[\frac{1}{8}, \frac{7}{8}, \frac{1}{8}]$	$[5, 8, 37, 40]$

continued ...

Table 4

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

Table 5: Wyckoff site: 64e, site symmetry: .3.

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

Table 6: Wyckoff site: 96f, site symmetry: 2..

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

continued ...

Table 6

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

Table 7: Wyckoff site: $96g$, site symmetry: $\dots 2$

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

Table 8: Wyckoff site: 192h, site symmetry: 1

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

continued ...

Table 8

No.	position	mapping
47	$[z, \frac{1}{4} - y, \frac{3}{4} - x]$	[47]
48	$[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}]$	[48]