

# PG No. 32 $O_h$ $m\bar{3}m$ [ cubic ]

Table 1: Wyckoff site: 1o, site symmetry:  $m\bar{3}m$

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

Table 2: Wyckoff site: 6a, site symmetry:  $4m.m$

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

Table 3: Wyckoff site: 8b, site symmetry:  $\bar{3}m$

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

Table 4: Wyckoff site: 12c, site symmetry:  $m.m2$

No.	position	mapping
1	$[0, y, y]$	$[1, 18, 28, 43]$
2	$[0, -y, y]$	$[2, 20, 27, 41]$
3	$[0, y, -y]$	$[3, 17, 26, 44]$
4	$[0, -y, -y]$	$[4, 19, 25, 42]$
5	$[y, 0, y]$	$[5, 15, 32, 38]$
6	$[y, 0, -y]$	$[6, 13, 31, 40]$
7	$[-y, 0, y]$	$[7, 16, 30, 37]$
8	$[-y, 0, -y]$	$[8, 14, 29, 39]$
9	$[y, y, 0]$	$[9, 21, 36, 48]$

*continued ...*

Table 4

No.	position	mapping
10	$[-y, y, 0]$	$[10, 23, 35, 46]$
11	$[y, -y, 0]$	$[11, 22, 34, 47]$
12	$[-y, -y, 0]$	$[12, 24, 33, 45]$

Table 5: Wyckoff site: 24d, 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	$[z, 0, y]$	$[5, 32]$
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	$[y, 0, -z]$	$[13, 40]$
14	$[-y, 0, -z]$	$[14, 39]$
15	$[y, 0, z]$	$[15, 38]$
16	$[-y, 0, z]$	$[16, 37]$
17	$[0, z, -y]$	$[17, 44]$
18	$[0, z, y]$	$[18, 43]$
19	$[0, -z, -y]$	$[19, 42]$
20	$[0, -z, y]$	$[20, 41]$
21	$[z, y, 0]$	$[21, 48]$
22	$[z, -y, 0]$	$[22, 47]$
23	$[-z, y, 0]$	$[23, 46]$
24	$[-z, -y, 0]$	$[24, 45]$

Table 6: Wyckoff site: 24e, site symmetry:  $..m$ 

No.	position	mapping
1	$[x, x, z]$	$[1, 38]$
2	$[-x, -x, z]$	$[2, 37]$
3	$[-x, x, -z]$	$[3, 39]$
4	$[x, -x, -z]$	$[4, 40]$
5	$[z, x, x]$	$[5, 48]$
6	$[z, -x, -x]$	$[6, 47]$
7	$[-z, -x, x]$	$[7, 45]$

*continued ...*

Table 6

No.	position	mapping
8	$[-z, x, -x]$	[8,46]
9	$[x, z, x]$	[9,43]
10	$[-x, z, -x]$	[10,44]
11	$[x, -z, -x]$	[11,42]
12	$[-x, -z, x]$	[12,41]
13	$[x, x, -z]$	[13,26]
14	$[-x, -x, -z]$	[14,25]
15	$[x, -x, z]$	[15,27]
16	$[-x, x, z]$	[16,28]
17	$[x, z, -x]$	[17,36]
18	$[-x, z, x]$	[18,35]
19	$[-x, -z, -x]$	[19,33]
20	$[x, -z, x]$	[20,34]
21	$[z, x, -x]$	[21,31]
22	$[z, -x, x]$	[22,32]
23	$[-z, x, x]$	[23,30]
24	$[-z, -x, -x]$	[24,29]

Table 7: Wyckoff site: **48f**, 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	$[y, x, -z]$	[13]
14	$[-y, -x, -z]$	[14]
15	$[y, -x, z]$	[15]
16	$[-y, x, z]$	[16]
17	$[x, z, -y]$	[17]
18	$[-x, z, y]$	[18]
19	$[-x, -z, -y]$	[19]
20	$[x, -z, y]$	[20]
21	$[z, y, -x]$	[21]
22	$[z, -y, x]$	[22]
23	$[-z, y, x]$	[23]

*continued ...*

Table 7

No.	position	mapping
24	$[-z, -y, -x]$	[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	$[-y, -x, z]$	[37]
38	$[y, x, z]$	[38]
39	$[-y, x, -z]$	[39]
40	$[y, -x, -z]$	[40]
41	$[-x, -z, y]$	[41]
42	$[x, -z, -y]$	[42]
43	$[x, z, y]$	[43]
44	$[-x, z, -y]$	[44]
45	$[-z, -y, x]$	[45]
46	$[-z, y, -x]$	[46]
47	$[z, -y, -x]$	[47]
48	$[z, y, x]$	[48]