

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

Table 1: Wyckoff site: 1o, site symmetry: m-3m

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: .3m

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: $\mathbf{m..}$

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: $\dots\mathbf{m}$

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]