

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

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, 2, 19, 20, 27, 28, 41, 42]
2	[ $-x$ , 0, 0]	[3, 4, 17, 18, 25, 26, 43, 44]
3	[0, $x$ , 0]	[9, 11, 14, 16, 34, 36, 37, 39]
4	[0, $-x$ , 0]	[10, 12, 13, 15, 33, 35, 38, 40]
5	[0, 0, $x$ ]	[5, 8, 22, 23, 30, 31, 45, 48]
6	[0, 0, $-x$ ]	[6, 7, 21, 24, 29, 32, 46, 47]

Table 3: Wyckoff site: 8b, site symmetry:  $.3m$ 

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

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

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

*continued ...*

Table 4

No.	position	mapping
10	$[-y, y, 0]$	$[7, 22, 30, 47]$
11	$[y, -y, 0]$	$[6, 23, 31, 46]$
12	$[-y, -y, 0]$	$[8, 21, 29, 48]$

Table 5: Wyckoff site: **24d**, site symmetry:  $m'..$ 

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

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

No.	position	mapping
1	$[x, x, z]$	$[1, 37]$
2	$[-x, -x, z]$	$[4, 40]$
3	$[-x, x, -z]$	$[3, 39]$
4	$[x, -x, -z]$	$[2, 38]$
5	$[z, x, x]$	$[9, 45]$
6	$[z, -x, -x]$	$[10, 46]$
7	$[-z, -x, x]$	$[12, 48]$

*continued ...*

Table 6

No.	position	mapping
8	$[-z, x, -x]$	[11,47]
9	$[x, z, x]$	[5,41]
10	$[-x, z, -x]$	[7,43]
11	$[x, -z, -x]$	[6,42]
12	$[-x, -z, x]$	[8,44]
13	$[x, x, -z]$	[16,28]
14	$[-x, -x, -z]$	[13,25]
15	$[x, -x, z]$	[15,27]
16	$[-x, x, z]$	[14,26]
17	$[x, z, -x]$	[20,32]
18	$[-x, z, x]$	[18,30]
19	$[-x, -z, -x]$	[17,29]
20	$[x, -z, x]$	[19,31]
21	$[z, x, -x]$	[24,36]
22	$[z, -x, x]$	[23,35]
23	$[-z, x, x]$	[22,34]
24	$[-z, -x, -x]$	[21,33]

Table 7: Wyckoff site: **48f**, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[-x, -y, z]$	[4]
3	$[-x, y, -z]$	[3]
4	$[x, -y, -z]$	[2]
5	$[z, x, y]$	[9]
6	$[z, -x, -y]$	[10]
7	$[-z, -x, y]$	[12]
8	$[-z, x, -y]$	[11]
9	$[y, z, x]$	[5]
10	$[-y, z, -x]$	[7]
11	$[y, -z, -x]$	[6]
12	$[-y, -z, x]$	[8]
13	$[y, x, -z]$	[16]
14	$[-y, -x, -z]$	[13]
15	$[y, -x, z]$	[15]
16	$[-y, x, z]$	[14]
17	$[x, z, -y]$	[20]
18	$[-x, z, y]$	[18]
19	$[-x, -z, -y]$	[17]
20	$[x, -z, y]$	[19]
21	$[z, y, -x]$	[24]
22	$[z, -y, x]$	[23]
23	$[-z, y, x]$	[22]

*continued ...*

Table 7

No.	position	mapping
24	$[-z, -y, -x]$	[21]
25	$[-x, -y, -z]$	[25]
26	$[x, y, -z]$	[28]
27	$[x, -y, z]$	[27]
28	$[-x, y, z]$	[26]
29	$[-z, -x, -y]$	[33]
30	$[-z, x, y]$	[34]
31	$[z, x, -y]$	[36]
32	$[z, -x, y]$	[35]
33	$[-y, -z, -x]$	[29]
34	$[y, -z, x]$	[31]
35	$[-y, z, x]$	[30]
36	$[y, z, -x]$	[32]
37	$[-y, -x, z]$	[40]
38	$[y, x, z]$	[37]
39	$[-y, x, -z]$	[39]
40	$[y, -x, -z]$	[38]
41	$[-x, -z, y]$	[44]
42	$[x, -z, -y]$	[42]
43	$[x, z, y]$	[41]
44	$[-x, z, -y]$	[43]
45	$[-z, -y, x]$	[48]
46	$[-z, y, -x]$	[47]
47	$[z, -y, -x]$	[46]
48	$[z, y, x]$	[45]