

Table 1: Wyckoff site: 4a, site symmetry: 432

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$
2	$[0, \frac{1}{2}, \frac{1}{2}]$	$[25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48]$
3	$[\frac{1}{2}, 0, \frac{1}{2}]$	$[49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72]$
4	$[\frac{1}{2}, \frac{1}{2}, 0]$	$[73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96]$

Table 2: Wyckoff site: 4b, site symmetry: 432

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$
2	$[\frac{1}{2}, 0, 0]$	$[25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48]$
3	$[0, \frac{1}{2}, 0]$	$[49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72]$
4	$[0, 0, \frac{1}{2}]$	$[73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96]$

Table 3: Wyckoff site: 8c, site symmetry: 23 .

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	$[1, 17, 18, 32, 46, 47, 57, 67, 72, 82, 92, 93]$
2	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	$[2, 7, 15, 27, 28, 35, 60, 62, 64, 77, 78, 85]$
3	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	$[3, 4, 11, 26, 31, 39, 53, 54, 61, 84, 86, 88]$
4	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	$[5, 6, 13, 36, 38, 40, 51, 52, 59, 74, 79, 87]$
5	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	$[8, 22, 23, 25, 41, 42, 58, 68, 69, 81, 91, 96]$
6	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	$[9, 19, 24, 34, 44, 45, 49, 65, 66, 80, 94, 95]$
7	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	$[10, 20, 21, 33, 43, 48, 56, 70, 71, 73, 89, 90]$
8	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	$[12, 14, 16, 29, 30, 37, 50, 55, 63, 75, 76, 83]$

Table 4: Wyckoff site: 24d, site symmetry: 2.22

No.	position	mapping
1	$[0, \frac{1}{4}, \frac{1}{4}]$	$[1, 13, 32, 38]$
2	$[0, \frac{3}{4}, \frac{1}{4}]$	$[2, 10, 27, 33]$
3	$[0, \frac{1}{4}, \frac{3}{4}]$	$[3, 9, 26, 34]$
4	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[4, 18, 88, 93]$
5	$[\frac{3}{4}, \frac{1}{4}, 0]$	$[5, 19, 87, 95]$
6	$[\frac{3}{4}, 0, \frac{1}{4}]$	$[6, 20, 59, 70]$
7	$[\frac{1}{4}, 0, \frac{1}{4}]$	$[7, 17, 60, 72]$
8	$[0, \frac{3}{4}, \frac{3}{4}]$	$[8, 14, 25, 37]$
9	$[\frac{1}{4}, 0, \frac{3}{4}]$	$[11, 22, 54, 68]$

continued ...

Table 4

No.	position	mapping
10	$[\frac{3}{4}, 0, \frac{3}{4}]$	[12, 24, 55, 65]
11	$[\frac{1}{4}, \frac{3}{4}, 0]$	[15, 23, 77, 91]
12	$[\frac{3}{4}, \frac{3}{4}, 0]$	[16, 21, 76, 90]
13	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	[28, 42, 64, 69]
14	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$	[29, 43, 63, 71]
15	$[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}]$	[30, 44, 83, 94]
16	$[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}]$	[31, 41, 84, 96]
17	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$	[35, 46, 78, 92]
18	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$	[36, 48, 79, 89]
19	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$	[39, 47, 53, 67]
20	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	[40, 45, 52, 66]
21	$[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[49, 61, 80, 86]
22	$[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[50, 58, 75, 81]
23	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[51, 57, 74, 82]
24	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[56, 62, 73, 85]

Table 5: Wyckoff site: **24e**, site symmetry: $4..$

No.	position	mapping
1	$[x, 0, 0]$	[1, 2, 3, 8]
2	$[0, 0, -x]$	[4, 16, 19, 23]
3	$[0, 0, x]$	[5, 15, 18, 21]
4	$[0, x, 0]$	[6, 11, 17, 24]
5	$[0, -x, 0]$	[7, 12, 20, 22]
6	$[-x, 0, 0]$	[9, 10, 13, 14]
7	$[x, \frac{1}{2}, \frac{1}{2}]$	[25, 26, 27, 32]
8	$[0, \frac{1}{2}, \frac{1}{2} - x]$	[28, 40, 43, 47]
9	$[0, \frac{1}{2}, x + \frac{1}{2}]$	[29, 39, 42, 45]
10	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[30, 35, 41, 48]
11	$[0, \frac{1}{2} - x, \frac{1}{2}]$	[31, 36, 44, 46]
12	$[-x, \frac{1}{2}, \frac{1}{2}]$	[33, 34, 37, 38]
13	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	[49, 50, 51, 56]
14	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[52, 64, 67, 71]
15	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[53, 63, 66, 69]
16	$[\frac{1}{2}, x, \frac{1}{2}]$	[54, 59, 65, 72]
17	$[\frac{1}{2}, -x, \frac{1}{2}]$	[55, 60, 68, 70]
18	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[57, 58, 61, 62]
19	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[73, 74, 75, 80]
20	$[\frac{1}{2}, \frac{1}{2}, -x]$	[76, 88, 91, 95]
21	$[\frac{1}{2}, \frac{1}{2}, x]$	[77, 87, 90, 93]
22	$[\frac{1}{2}, x + \frac{1}{2}, 0]$	[78, 83, 89, 96]
23	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	[79, 84, 92, 94]
24	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[81, 82, 85, 86]

Table 6: Wyckoff site: **32f**, site symmetry: $\bar{3}$.

No.	position	mapping
1	$[x, x, x]$	$[1, 17, 18]$
2	$[x, -x, x]$	$[2, 7, 15]$
3	$[x, x, -x]$	$[3, 4, 11]$
4	$[-x, x, x]$	$[5, 6, 13]$
5	$[x, -x, -x]$	$[8, 22, 23]$
6	$[-x, x, -x]$	$[9, 19, 24]$
7	$[-x, -x, x]$	$[10, 20, 21]$
8	$[-x, -x, -x]$	$[12, 14, 16]$
9	$[x, x + \frac{1}{2}, x + \frac{1}{2}]$	$[25, 41, 42]$
10	$[x, \frac{1}{2} - x, x + \frac{1}{2}]$	$[26, 31, 39]$
11	$[x, x + \frac{1}{2}, \frac{1}{2} - x]$	$[27, 28, 35]$
12	$[-x, x + \frac{1}{2}, x + \frac{1}{2}]$	$[29, 30, 37]$
13	$[x, \frac{1}{2} - x, \frac{1}{2} - x]$	$[32, 46, 47]$
14	$[-x, x + \frac{1}{2}, \frac{1}{2} - x]$	$[33, 43, 48]$
15	$[-x, \frac{1}{2} - x, x + \frac{1}{2}]$	$[34, 44, 45]$
16	$[-x, \frac{1}{2} - x, \frac{1}{2} - x]$	$[36, 38, 40]$
17	$[x + \frac{1}{2}, x, x + \frac{1}{2}]$	$[49, 65, 66]$
18	$[x + \frac{1}{2}, -x, x + \frac{1}{2}]$	$[50, 55, 63]$
19	$[x + \frac{1}{2}, x, \frac{1}{2} - x]$	$[51, 52, 59]$
20	$[\frac{1}{2} - x, x, x + \frac{1}{2}]$	$[53, 54, 61]$
21	$[x + \frac{1}{2}, -x, \frac{1}{2} - x]$	$[56, 70, 71]$
22	$[\frac{1}{2} - x, x, \frac{1}{2} - x]$	$[57, 67, 72]$
23	$[\frac{1}{2} - x, -x, x + \frac{1}{2}]$	$[58, 68, 69]$
24	$[\frac{1}{2} - x, -x, \frac{1}{2} - x]$	$[60, 62, 64]$
25	$[x + \frac{1}{2}, x + \frac{1}{2}, x]$	$[73, 89, 90]$
26	$[x + \frac{1}{2}, \frac{1}{2} - x, x]$	$[74, 79, 87]$
27	$[x + \frac{1}{2}, x + \frac{1}{2}, -x]$	$[75, 76, 83]$
28	$[\frac{1}{2} - x, x + \frac{1}{2}, x]$	$[77, 78, 85]$
29	$[x + \frac{1}{2}, \frac{1}{2} - x, -x]$	$[80, 94, 95]$
30	$[\frac{1}{2} - x, x + \frac{1}{2}, -x]$	$[81, 91, 96]$
31	$[\frac{1}{2} - x, \frac{1}{2} - x, x]$	$[82, 92, 93]$
32	$[\frac{1}{2} - x, \frac{1}{2} - x, -x]$	$[84, 86, 88]$

Table 7: Wyckoff site: **48g**, site symmetry: $\bar{6}$.

No.	position	mapping
1	$[0, y, y]$	$[1, 13]$
2	$[0, -y, y]$	$[2, 10]$
3	$[0, y, -y]$	$[3, 9]$
4	$[y, y, 0]$	$[4, 18]$
5	$[-y, y, 0]$	$[5, 19]$
6	$[-y, 0, y]$	$[6, 20]$
7	$[y, 0, y]$	$[7, 17]$

continued ...

Table 7

No.	position	mapping
8	$[0, -y, -y]$	$[8, 14]$
9	$[y, 0, -y]$	$[11, 22]$
10	$[-y, 0, -y]$	$[12, 24]$
11	$[y, -y, 0]$	$[15, 23]$
12	$[-y, -y, 0]$	$[16, 21]$
13	$[0, y + \frac{1}{2}, y + \frac{1}{2}]$	$[25, 37]$
14	$[0, \frac{1}{2} - y, y + \frac{1}{2}]$	$[26, 34]$
15	$[0, y + \frac{1}{2}, \frac{1}{2} - y]$	$[27, 33]$
16	$[y, y + \frac{1}{2}, \frac{1}{2}]$	$[28, 42]$
17	$[-y, y + \frac{1}{2}, \frac{1}{2}]$	$[29, 43]$
18	$[-y, \frac{1}{2}, y + \frac{1}{2}]$	$[30, 44]$
19	$[y, \frac{1}{2}, y + \frac{1}{2}]$	$[31, 41]$
20	$[0, \frac{1}{2} - y, \frac{1}{2} - y]$	$[32, 38]$
21	$[y, \frac{1}{2}, \frac{1}{2} - y]$	$[35, 46]$
22	$[-y, \frac{1}{2}, \frac{1}{2} - y]$	$[36, 48]$
23	$[y, \frac{1}{2} - y, \frac{1}{2}]$	$[39, 47]$
24	$[-y, \frac{1}{2} - y, \frac{1}{2}]$	$[40, 45]$
25	$[\frac{1}{2}, y, y + \frac{1}{2}]$	$[49, 61]$
26	$[\frac{1}{2}, -y, y + \frac{1}{2}]$	$[50, 58]$
27	$[\frac{1}{2}, y, \frac{1}{2} - y]$	$[51, 57]$
28	$[y + \frac{1}{2}, y, \frac{1}{2}]$	$[52, 66]$
29	$[\frac{1}{2} - y, y, \frac{1}{2}]$	$[53, 67]$
30	$[\frac{1}{2} - y, 0, y + \frac{1}{2}]$	$[54, 68]$
31	$[y + \frac{1}{2}, 0, y + \frac{1}{2}]$	$[55, 65]$
32	$[\frac{1}{2}, -y, \frac{1}{2} - y]$	$[56, 62]$
33	$[y + \frac{1}{2}, 0, \frac{1}{2} - y]$	$[59, 70]$
34	$[\frac{1}{2} - y, 0, \frac{1}{2} - y]$	$[60, 72]$
35	$[y + \frac{1}{2}, -y, \frac{1}{2}]$	$[63, 71]$
36	$[\frac{1}{2} - y, -y, \frac{1}{2}]$	$[64, 69]$
37	$[\frac{1}{2}, y + \frac{1}{2}, y]$	$[73, 85]$
38	$[\frac{1}{2}, \frac{1}{2} - y, y]$	$[74, 82]$
39	$[\frac{1}{2}, y + \frac{1}{2}, -y]$	$[75, 81]$
40	$[y + \frac{1}{2}, y + \frac{1}{2}, 0]$	$[76, 90]$
41	$[\frac{1}{2} - y, y + \frac{1}{2}, 0]$	$[77, 91]$
42	$[\frac{1}{2} - y, \frac{1}{2}, y]$	$[78, 92]$
43	$[y + \frac{1}{2}, \frac{1}{2}, y]$	$[79, 89]$
44	$[\frac{1}{2}, \frac{1}{2} - y, -y]$	$[80, 86]$
45	$[y + \frac{1}{2}, \frac{1}{2}, -y]$	$[83, 94]$
46	$[\frac{1}{2} - y, \frac{1}{2}, -y]$	$[84, 96]$
47	$[y + \frac{1}{2}, \frac{1}{2} - y, 0]$	$[87, 95]$
48	$[\frac{1}{2} - y, \frac{1}{2} - y, 0]$	$[88, 93]$

Table 8: Wyckoff site: 48h, site symmetry: $\dots 2$

No.	position	mapping
1	$[\frac{1}{2}, y, y]$	[1, 13]
2	$[\frac{1}{2}, -y, y]$	[2, 10]
3	$[\frac{1}{2}, y, -y]$	[3, 9]
4	$[y, y, \frac{1}{2}]$	[4, 18]
5	$[-y, y, \frac{1}{2}]$	[5, 19]
6	$[-y, \frac{1}{2}, y]$	[6, 20]
7	$[y, \frac{1}{2}, y]$	[7, 17]
8	$[\frac{1}{2}, -y, -y]$	[8, 14]
9	$[y, \frac{1}{2}, -y]$	[11, 22]
10	$[-y, \frac{1}{2}, -y]$	[12, 24]
11	$[y, -y, \frac{1}{2}]$	[15, 23]
12	$[-y, -y, \frac{1}{2}]$	[16, 21]
13	$[\frac{1}{2}, y + \frac{1}{2}, y + \frac{1}{2}]$	[25, 37]
14	$[\frac{1}{2}, \frac{1}{2} - y, y + \frac{1}{2}]$	[26, 34]
15	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - y]$	[27, 33]
16	$[y, y + \frac{1}{2}, 0]$	[28, 42]
17	$[-y, y + \frac{1}{2}, 0]$	[29, 43]
18	$[-y, 0, y + \frac{1}{2}]$	[30, 44]
19	$[y, 0, y + \frac{1}{2}]$	[31, 41]
20	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - y]$	[32, 38]
21	$[y, 0, \frac{1}{2} - y]$	[35, 46]
22	$[-y, 0, \frac{1}{2} - y]$	[36, 48]
23	$[y, \frac{1}{2} - y, 0]$	[39, 47]
24	$[-y, \frac{1}{2} - y, 0]$	[40, 45]
25	$[0, y, y + \frac{1}{2}]$	[49, 61]
26	$[0, -y, y + \frac{1}{2}]$	[50, 58]
27	$[0, y, \frac{1}{2} - y]$	[51, 57]
28	$[y + \frac{1}{2}, y, 0]$	[52, 66]
29	$[\frac{1}{2} - y, y, 0]$	[53, 67]
30	$[\frac{1}{2} - y, \frac{1}{2}, y + \frac{1}{2}]$	[54, 68]
31	$[y + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}]$	[55, 65]
32	$[0, -y, \frac{1}{2} - y]$	[56, 62]
33	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - y]$	[59, 70]
34	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - y]$	[60, 72]
35	$[y + \frac{1}{2}, -y, 0]$	[63, 71]
36	$[\frac{1}{2} - y, -y, 0]$	[64, 69]
37	$[0, y + \frac{1}{2}, y]$	[73, 85]
38	$[0, \frac{1}{2} - y, y]$	[74, 82]
39	$[0, y + \frac{1}{2}, -y]$	[75, 81]
40	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[76, 90]
41	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{2}]$	[77, 91]
42	$[\frac{1}{2} - y, 0, y]$	[78, 92]
43	$[y + \frac{1}{2}, 0, y]$	[79, 89]
44	$[0, \frac{1}{2} - y, -y]$	[80, 86]
45	$[y + \frac{1}{2}, 0, -y]$	[83, 94]
46	$[\frac{1}{2} - y, 0, -y]$	[84, 96]

continued ...

Table 8

No.	position	mapping
47	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[87,95]
48	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{2}]$	[88,93]

Table 9: Wyckoff site: 48i, site symmetry: 2. .

No.	position	mapping
1	$[x, \frac{1}{4}, \frac{1}{4}]$	[1,32]
2	$[x, \frac{3}{4}, \frac{1}{4}]$	[2,27]
3	$[x, \frac{1}{4}, \frac{3}{4}]$	[3,26]
4	$[\frac{1}{4}, \frac{1}{4}, -x]$	[4,88]
5	$[\frac{3}{4}, \frac{1}{4}, x]$	[5,87]
6	$[\frac{3}{4}, x, \frac{1}{4}]$	[6,59]
7	$[\frac{1}{4}, -x, \frac{1}{4}]$	[7,60]
8	$[x, \frac{3}{4}, \frac{3}{4}]$	[8,25]
9	$[-x, \frac{1}{4}, \frac{3}{4}]$	[9,34]
10	$[-x, \frac{3}{4}, \frac{1}{4}]$	[10,33]
11	$[\frac{1}{4}, x, \frac{3}{4}]$	[11,54]
12	$[\frac{3}{4}, -x, \frac{3}{4}]$	[12,55]
13	$[-x, \frac{1}{4}, \frac{1}{4}]$	[13,38]
14	$[-x, \frac{3}{4}, \frac{3}{4}]$	[14,37]
15	$[\frac{1}{4}, \frac{3}{4}, x]$	[15,77]
16	$[\frac{3}{4}, \frac{3}{4}, -x]$	[16,76]
17	$[\frac{1}{4}, x, \frac{1}{4}]$	[17,72]
18	$[\frac{1}{4}, \frac{1}{4}, x]$	[18,93]
19	$[\frac{3}{4}, \frac{1}{4}, -x]$	[19,95]
20	$[\frac{3}{4}, -x, \frac{1}{4}]$	[20,70]
21	$[\frac{3}{4}, \frac{3}{4}, x]$	[21,90]
22	$[\frac{1}{4}, -x, \frac{3}{4}]$	[22,68]
23	$[\frac{1}{4}, \frac{3}{4}, -x]$	[23,91]
24	$[\frac{3}{4}, x, \frac{3}{4}]$	[24,65]
25	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[28,64]
26	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[29,63]
27	$[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[30,83]
28	$[\frac{1}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[31,84]
29	$[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[35,78]
30	$[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[36,79]
31	$[\frac{1}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[39,53]
32	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[40,52]
33	$[\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[41,96]
34	$[\frac{1}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[42,69]
35	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[43,71]
36	$[\frac{3}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[44,94]
37	$[\frac{3}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[45,66]
38	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[46,92]

continued ...

Table 9

No.	position	mapping
39	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[47, 67]
40	$[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[48, 89]
41	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[49, 80]
42	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[50, 75]
43	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[51, 74]
44	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[56, 73]
45	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[57, 82]
46	$[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$	[58, 81]
47	$[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$	[61, 86]
48	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]$	[62, 85]

Table 10: Wyckoff site: 96j, site symmetry: 1

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

continued ...

Table 10

No.	position	mapping
31	$[y, \frac{1}{2} - x, z + \frac{1}{2}]$	[31]
32	$[x, \frac{1}{2} - y, \frac{1}{2} - z]$	[32]
33	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[33]
34	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[34]
35	$[y, x + \frac{1}{2}, \frac{1}{2} - z]$	[35]
36	$[-y, \frac{1}{2} - x, \frac{1}{2} - z]$	[36]
37	$[-x, z + \frac{1}{2}, y + \frac{1}{2}]$	[37]
38	$[-x, \frac{1}{2} - z, \frac{1}{2} - y]$	[38]
39	$[z, \frac{1}{2} - y, x + \frac{1}{2}]$	[39]
40	$[-z, \frac{1}{2} - y, \frac{1}{2} - x]$	[40]
41	$[z, x + \frac{1}{2}, y + \frac{1}{2}]$	[41]
42	$[y, z + \frac{1}{2}, x + \frac{1}{2}]$	[42]
43	$[-y, z + \frac{1}{2}, \frac{1}{2} - x]$	[43]
44	$[-z, \frac{1}{2} - x, y + \frac{1}{2}]$	[44]
45	$[-y, \frac{1}{2} - z, x + \frac{1}{2}]$	[45]
46	$[z, \frac{1}{2} - x, \frac{1}{2} - y]$	[46]
47	$[y, \frac{1}{2} - z, \frac{1}{2} - x]$	[47]
48	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[48]
49	$[x + \frac{1}{2}, y, z + \frac{1}{2}]$	[49]
50	$[x + \frac{1}{2}, -z, y + \frac{1}{2}]$	[50]
51	$[x + \frac{1}{2}, z, \frac{1}{2} - y]$	[51]
52	$[z + \frac{1}{2}, y, \frac{1}{2} - x]$	[52]
53	$[\frac{1}{2} - z, y, x + \frac{1}{2}]$	[53]
54	$[\frac{1}{2} - y, x, z + \frac{1}{2}]$	[54]
55	$[y + \frac{1}{2}, -x, z + \frac{1}{2}]$	[55]
56	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[56]
57	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[57]
58	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[58]
59	$[y + \frac{1}{2}, x, \frac{1}{2} - z]$	[59]
60	$[\frac{1}{2} - y, -x, \frac{1}{2} - z]$	[60]
61	$[\frac{1}{2} - x, z, y + \frac{1}{2}]$	[61]
62	$[\frac{1}{2} - x, -z, \frac{1}{2} - y]$	[62]
63	$[z + \frac{1}{2}, -y, x + \frac{1}{2}]$	[63]
64	$[\frac{1}{2} - z, -y, \frac{1}{2} - x]$	[64]
65	$[z + \frac{1}{2}, x, y + \frac{1}{2}]$	[65]
66	$[y + \frac{1}{2}, z, x + \frac{1}{2}]$	[66]
67	$[\frac{1}{2} - y, z, \frac{1}{2} - x]$	[67]
68	$[\frac{1}{2} - z, -x, y + \frac{1}{2}]$	[68]
69	$[\frac{1}{2} - y, -z, x + \frac{1}{2}]$	[69]
70	$[z + \frac{1}{2}, -x, \frac{1}{2} - y]$	[70]
71	$[y + \frac{1}{2}, -z, \frac{1}{2} - x]$	[71]
72	$[\frac{1}{2} - z, x, \frac{1}{2} - y]$	[72]
73	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[73]
74	$[x + \frac{1}{2}, \frac{1}{2} - z, y]$	[74]
75	$[x + \frac{1}{2}, z + \frac{1}{2}, -y]$	[75]
76	$[z + \frac{1}{2}, y + \frac{1}{2}, -x]$	[76]
77	$[\frac{1}{2} - z, y + \frac{1}{2}, x]$	[77]

continued ...

Table 10

No.	position	mapping
78	$[\frac{1}{2} - y, x + \frac{1}{2}, z]$	[78]
79	$[y + \frac{1}{2}, \frac{1}{2} - x, z]$	[79]
80	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[80]
81	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[81]
82	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[82]
83	$[y + \frac{1}{2}, x + \frac{1}{2}, -z]$	[83]
84	$[\frac{1}{2} - y, \frac{1}{2} - x, -z]$	[84]
85	$[\frac{1}{2} - x, z + \frac{1}{2}, y]$	[85]
86	$[\frac{1}{2} - x, \frac{1}{2} - z, -y]$	[86]
87	$[z + \frac{1}{2}, \frac{1}{2} - y, x]$	[87]
88	$[\frac{1}{2} - z, \frac{1}{2} - y, -x]$	[88]
89	$[z + \frac{1}{2}, x + \frac{1}{2}, y]$	[89]
90	$[y + \frac{1}{2}, z + \frac{1}{2}, x]$	[90]
91	$[\frac{1}{2} - y, z + \frac{1}{2}, -x]$	[91]
92	$[\frac{1}{2} - z, \frac{1}{2} - x, y]$	[92]
93	$[\frac{1}{2} - y, \frac{1}{2} - z, x]$	[93]
94	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[94]
95	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[95]
96	$[\frac{1}{2} - z, x + \frac{1}{2}, -y]$	[96]