

Table 1: Wyckoff site: 8a, site symmetry: 23 .

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

Table 2: Wyckoff site: 8b, site symmetry: 23 .

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

Table 3: Wyckoff site: 24c, site symmetry: $22'2'..$

No.	position	mapping
1	$[0, \frac{1}{4}, \frac{1}{4}]$	$[1, 14, 51, 64]$
2	$[0, \frac{3}{4}, \frac{3}{4}]$	$[2, 13, 52, 63]$
3	$[0, \frac{1}{4}, \frac{3}{4}]$	$[3, 16, 49, 62]$
4	$[0, \frac{3}{4}, \frac{1}{4}]$	$[4, 15, 50, 61]$
5	$[\frac{1}{4}, 0, \frac{1}{4}]$	$[5, 36, 58, 80]$
6	$[\frac{1}{4}, \frac{1}{4}, 0]$	$[6, 45, 71, 79]$
7	$[\frac{3}{4}, \frac{1}{4}, 0]$	$[7, 47, 69, 78]$
8	$[\frac{3}{4}, 0, \frac{1}{4}]$	$[8, 34, 60, 77]$
9	$[\frac{3}{4}, \frac{3}{4}, 0]$	$[9, 42, 67, 83]$
10	$[\frac{1}{4}, 0, \frac{3}{4}]$	$[10, 32, 53, 84]$
11	$[\frac{1}{4}, \frac{3}{4}, 0]$	$[11, 43, 66, 81]$
12	$[\frac{3}{4}, 0, \frac{3}{4}]$	$[12, 29, 56, 82]$
13	$[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}]$	$[17, 48, 70, 92]$
14	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	$[18, 33, 59, 91]$
15	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$	$[19, 35, 57, 90]$

continued ...

Table 3

No.	position	mapping
16	$[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}]$	[20,46,72,89]
17	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	[21,30,55,95]
18	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$	[22,44,65,96]
19	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$	[23,31,54,93]
20	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$	[24,41,68,94]
21	$[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[25,38,75,88]
22	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[26,37,76,87]
23	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[27,40,73,86]
24	$[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[28,39,74,85]

Table 4: Wyckoff site: 24d, site symmetry: $22'2'..$

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

Table 5: Wyckoff site: **32e**, site symmetry: $\bar{3}$.

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

Table 6: Wyckoff site: **48f**, site symmetry: $2\bar{1}$.

No.	position	mapping
1	$[x, 0, 0]$	$[1, 2]$
2	$[-x, 0, 0]$	$[3, 4]$
3	$[0, x, 0]$	$[5, 12]$
4	$[0, 0, x]$	$[6, 9]$
5	$[0, 0, -x]$	$[7, 11]$
6	$[0, -x, 0]$	$[8, 10]$
7	$[x, \frac{1}{2}, \frac{1}{2}]$	$[13, 14]$

continued ...

Table 6

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

Table 7: Wyckoff site: $48g$, site symmetry: $2' \dots$

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

continued ...

Table 7

No.	position	mapping
47	$[\frac{1}{2}, \frac{1}{4}, -x]$	[47,79]
48	$[\frac{1}{4}, x + \frac{1}{2}, 0]$	[48,65]

Table 8: Wyckoff site: 48h, site symmetry: $2'..$

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

continued ...

Table 8

No.	position	mapping
39	$[\frac{1}{2} - x, \frac{3}{4}, 0]$	[39,76]
40	$[\frac{1}{2} - x, \frac{1}{4}, 0]$	[40,75]
41	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[41,96]
42	$[\frac{3}{4}, \frac{1}{2}, x]$	[42,69]
43	$[\frac{1}{4}, \frac{1}{2}, -x]$	[43,71]
44	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}]$	[44,94]
45	$[\frac{1}{4}, \frac{1}{2}, x]$	[45,66]
46	$[\frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}]$	[46,92]
47	$[\frac{3}{4}, \frac{1}{2}, -x]$	[47,67]
48	$[\frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}]$	[48,89]

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

No.	position	mapping
1	$[x, \frac{1}{4}, \frac{1}{4}]$	[1,14]
2	$[x, \frac{3}{4}, \frac{3}{4}]$	[2,13]
3	$[-x, \frac{1}{4}, \frac{3}{4}]$	[3,16]
4	$[-x, \frac{3}{4}, \frac{1}{4}]$	[4,15]
5	$[\frac{1}{4}, x, \frac{1}{4}]$	[5,36]
6	$[\frac{1}{4}, \frac{1}{4}, x]$	[6,45]
7	$[\frac{3}{4}, \frac{1}{4}, -x]$	[7,47]
8	$[\frac{3}{4}, -x, \frac{1}{4}]$	[8,34]
9	$[\frac{3}{4}, \frac{3}{4}, x]$	[9,42]
10	$[\frac{1}{4}, -x, \frac{3}{4}]$	[10,32]
11	$[\frac{1}{4}, \frac{3}{4}, -x]$	[11,43]
12	$[\frac{3}{4}, x, \frac{3}{4}]$	[12,29]
13	$[\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[17,48]
14	$[\frac{1}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[18,33]
15	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[19,35]
16	$[\frac{3}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[20,46]
17	$[\frac{3}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[21,30]
18	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[22,44]
19	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[23,31]
20	$[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[24,41]
21	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[25,38]
22	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[26,37]
23	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[27,40]
24	$[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$	[28,39]
25	$[x, \frac{1}{4}, \frac{3}{4}]$	[49,62]
26	$[x, \frac{3}{4}, \frac{1}{4}]$	[50,61]
27	$[-x, \frac{1}{4}, \frac{1}{4}]$	[51,64]
28	$[-x, \frac{3}{4}, \frac{3}{4}]$	[52,63]
29	$[\frac{1}{4}, x, \frac{3}{4}]$	[53,84]
30	$[\frac{1}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[54,93]

continued ...

Table 9

No.	position	mapping
31	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[55,95]
32	$[\frac{3}{4}, -x, \frac{3}{4}]$	[56,82]
33	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[57,90]
34	$[\frac{1}{4}, -x, \frac{1}{4}]$	[58,80]
35	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[59,91]
36	$[\frac{3}{4}, x, \frac{1}{4}]$	[60,77]
37	$[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[65,96]
38	$[\frac{1}{4}, \frac{3}{4}, x]$	[66,81]
39	$[\frac{3}{4}, \frac{3}{4}, -x]$	[67,83]
40	$[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[68,94]
41	$[\frac{3}{4}, \frac{1}{4}, x]$	[69,78]
42	$[\frac{1}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[70,92]
43	$[\frac{1}{4}, \frac{1}{4}, -x]$	[71,79]
44	$[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[72,89]
45	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[73,86]
46	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[74,85]
47	$[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$	[75,88]
48	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]$	[76,87]

Table 10: Wyckoff site: **96j**, 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	$[y, z, x]$	[6]
7	$[-y, z, -x]$	[7]
8	$[-z, -x, y]$	[8]
9	$[-y, -z, x]$	[9]
10	$[z, -x, -y]$	[10]
11	$[y, -z, -x]$	[11]
12	$[-z, x, -y]$	[12]
13	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[13]
14	$[x, \frac{1}{2} - y, \frac{1}{2} - z]$	[14]
15	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[15]
16	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[16]
17	$[z, x + \frac{1}{2}, y + \frac{1}{2}]$	[17]
18	$[y, z + \frac{1}{2}, x + \frac{1}{2}]$	[18]
19	$[-y, z + \frac{1}{2}, \frac{1}{2} - x]$	[19]
20	$[-z, \frac{1}{2} - x, y + \frac{1}{2}]$	[20]
21	$[-y, \frac{1}{2} - z, x + \frac{1}{2}]$	[21]
22	$[z, \frac{1}{2} - x, \frac{1}{2} - y]$	[22]

continued ...

Table 10

No.	position	mapping
23	$[y, \frac{1}{2} - z, \frac{1}{2} - x]$	[23]
24	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[24]
25	$[x + \frac{1}{2}, y, z + \frac{1}{2}]$	[25]
26	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[26]
27	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[27]
28	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[28]
29	$[z + \frac{1}{2}, x, y + \frac{1}{2}]$	[29]
30	$[y + \frac{1}{2}, z, x + \frac{1}{2}]$	[30]
31	$[\frac{1}{2} - y, z, \frac{1}{2} - x]$	[31]
32	$[\frac{1}{2} - z, -x, y + \frac{1}{2}]$	[32]
33	$[\frac{1}{2} - y, -z, x + \frac{1}{2}]$	[33]
34	$[z + \frac{1}{2}, -x, \frac{1}{2} - y]$	[34]
35	$[y + \frac{1}{2}, -z, \frac{1}{2} - x]$	[35]
36	$[\frac{1}{2} - z, x, \frac{1}{2} - y]$	[36]
37	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[37]
38	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[38]
39	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[39]
40	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[40]
41	$[z + \frac{1}{2}, x + \frac{1}{2}, y]$	[41]
42	$[y + \frac{1}{2}, z + \frac{1}{2}, x]$	[42]
43	$[\frac{1}{2} - y, z + \frac{1}{2}, -x]$	[43]
44	$[\frac{1}{2} - z, \frac{1}{2} - x, y]$	[44]
45	$[\frac{1}{2} - y, \frac{1}{2} - z, x]$	[45]
46	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[46]
47	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[47]
48	$[\frac{1}{2} - z, x + \frac{1}{2}, -y]$	[48]
49	$[x, y, z + \frac{1}{2}]$	[49]
50	$[x, -y, \frac{1}{2} - z]$	[50]
51	$[-x, y, \frac{1}{2} - z]$	[51]
52	$[-x, -y, z + \frac{1}{2}]$	[52]
53	$[z, x, y + \frac{1}{2}]$	[53]
54	$[y, z, x + \frac{1}{2}]$	[54]
55	$[-y, z, \frac{1}{2} - x]$	[55]
56	$[-z, -x, y + \frac{1}{2}]$	[56]
57	$[-y, -z, x + \frac{1}{2}]$	[57]
58	$[z, -x, \frac{1}{2} - y]$	[58]
59	$[y, -z, \frac{1}{2} - x]$	[59]
60	$[-z, x, \frac{1}{2} - y]$	[60]
61	$[x, y + \frac{1}{2}, z]$	[61]
62	$[x, \frac{1}{2} - y, -z]$	[62]
63	$[-x, y + \frac{1}{2}, -z]$	[63]
64	$[-x, \frac{1}{2} - y, z]$	[64]
65	$[z, x + \frac{1}{2}, y]$	[65]
66	$[y, z + \frac{1}{2}, x]$	[66]
67	$[-y, z + \frac{1}{2}, -x]$	[67]
68	$[-z, \frac{1}{2} - x, y]$	[68]
69	$[-y, \frac{1}{2} - z, x]$	[69]

continued ...

Table 10

No.	position	mapping
70	$[z, \frac{1}{2} - x, -y]$	[70]
71	$[y, \frac{1}{2} - z, -x]$	[71]
72	$[-z, x + \frac{1}{2}, -y]$	[72]
73	$[x + \frac{1}{2}, y, z]$	[73]
74	$[x + \frac{1}{2}, -y, -z]$	[74]
75	$[\frac{1}{2} - x, y, -z]$	[75]
76	$[\frac{1}{2} - x, -y, z]$	[76]
77	$[z + \frac{1}{2}, x, y]$	[77]
78	$[y + \frac{1}{2}, z, x]$	[78]
79	$[\frac{1}{2} - y, z, -x]$	[79]
80	$[\frac{1}{2} - z, -x, y]$	[80]
81	$[\frac{1}{2} - y, -z, x]$	[81]
82	$[z + \frac{1}{2}, -x, -y]$	[82]
83	$[y + \frac{1}{2}, -z, -x]$	[83]
84	$[\frac{1}{2} - z, x, -y]$	[84]
85	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[85]
86	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[86]
87	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[87]
88	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[88]
89	$[z + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}]$	[89]
90	$[y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}]$	[90]
91	$[\frac{1}{2} - y, z + \frac{1}{2}, \frac{1}{2} - x]$	[91]
92	$[\frac{1}{2} - z, \frac{1}{2} - x, y + \frac{1}{2}]$	[92]
93	$[\frac{1}{2} - y, \frac{1}{2} - z, x + \frac{1}{2}]$	[93]
94	$[z + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - y]$	[94]
95	$[y + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - x]$	[95]
96	$[\frac{1}{2} - z, x + \frac{1}{2}, \frac{1}{2} - y]$	[96]