Table 1: Wyckoff site: 4a, site symmetry: 4'32'

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	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[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	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[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	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[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: 4'32'

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

Table 4: Wyckoff site: 24d, site symmetry: 2.2'2'

No.	position	mapping
1	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	[1,21,26,46]
2	$\left[0, \frac{3}{4}, \frac{3}{4}\right]$	[2,22,25,45]
3	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	[3,14,28,37]
4	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	[4,13,27,38]
5	$\left[\frac{1}{4}, 0, \frac{1}{4}\right]$	[5,18,60,68]
6	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	[6,15,81,96]
7	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[7,16,83,95]
8	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	[8,17,58,67]
9	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	[9,24,78,87]

continued ...

Table 4

No.	position	mapping
10	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	[10,19,56,65]
11	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[11,23,79,88]
12	$\left[\frac{3}{4}, 0, \frac{3}{4}\right]$	[12,20,53,66]
13	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[29,42,84,92]
14	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[30,39,57,72]
15	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[31,40,59,71]
16	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[32,41,82,91]
17	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[33,48,54,63]
18	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[34,43,80,89]
19	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[35,47,55,64]
20	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[36,44,77,90]
21	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[49,69,74,94]
22	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[50,70,73,93]
23	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[51,62,76,85]
24	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[52,61,75,86]

Table 5: Wyckoff site: 24e, site symmetry: 4'..

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

Table 6: Wyckoff site: `32f`, site symmetry: `.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	$[x, -x, x]$	[13,18,23]
6	$[x, x, -x]$	[14,15,19]
7	$[-x, x, x]$	[16,17,21]
8	$[-x, -x, -x]$	[20,22,24]
9	$[x, x+\frac{1}{2}, x+\frac{1}{2}]$	[25,29,30]
10	$[x, \frac{1}{2}-x, \frac{1}{2}-x]$	[26,34,35]
11	$[-x, x+\frac{1}{2}, \frac{1}{2}-x]$	[27,31,36]
12	$[-x, \frac{1}{2}-x, x+\frac{1}{2}]$	[28,32,33]
13	$[x, \frac{1}{2}-x, x+\frac{1}{2}]$	[37,42,47]
14	$[x, x+\frac{1}{2}, \frac{1}{2}-x]$	[38,39,43]
15	$[-x, x+\frac{1}{2}, x+\frac{1}{2}]$	[40,41,45]
16	$[-x, \frac{1}{2}-x, \frac{1}{2}-x]$	[44,46,48]
17	$[x+\frac{1}{2}, x, x+\frac{1}{2}]$	[49,53,54]
18	$[x+\frac{1}{2}, -x, \frac{1}{2}-x]$	[50,58,59]
19	$[\frac{1}{2}-x, x, \frac{1}{2}-x]$	[51,55,60]
20	$[\frac{1}{2}-x, -x, x+\frac{1}{2}]$	[52,56,57]
21	$[x+\frac{1}{2}, -x, x+\frac{1}{2}]$	[61,66,71]
22	$[x+\frac{1}{2}, x, \frac{1}{2}-x]$	[62,63,67]
23	$[\frac{1}{2}-x, x, x+\frac{1}{2}]$	[64,65,69]
24	$[\frac{1}{2}-x, -x, \frac{1}{2}-x]$	[68,70,72]
25	$[x+\frac{1}{2}, x+\frac{1}{2}, x]$	[73,77,78]
26	$[x+\frac{1}{2}, \frac{1}{2}-x, -x]$	[74,82,83]
27	$[\frac{1}{2}-x, x+\frac{1}{2}, -x]$	[75,79,84]
28	$[\frac{1}{2}-x, \frac{1}{2}-x, x]$	[76,80,81]
29	$[x+\frac{1}{2}, \frac{1}{2}-x, x]$	[85,90,95]
30	$[x+\frac{1}{2}, x+\frac{1}{2}, -x]$	[86,87,91]
31	$[\frac{1}{2}-x, x+\frac{1}{2}, x]$	[88,89,93]
32	$[\frac{1}{2}-x, \frac{1}{2}-x, -x]$	[92,94,96]

Table 7: Wyckoff site: `48g`, site symmetry: `..2'`

No.	position	mapping
1	$[0, y, y]$	[1,21]
2	$[0, -y, -y]$	[2,22]
3	$[0, y, -y]$	[3,14]
4	$[0, -y, y]$	[4,13]
5	$[y, 0, y]$	[5,18]
6	$[y, y, 0]$	[6,15]
7	$[-y, y, 0]$	[7,16]

continued …

Table 7

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

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

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

continued ...

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Table 8

No.	position	mapping
47	$\left[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}\right]$	[83,95]
48	$\left[\frac{1}{2} - y, 0, -y\right]$	[84,92]

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

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

continued ...

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Table 9

No.	position	mapping
39	$\left[\frac{1}{4}, \frac{1}{4}, x + \frac{1}{2}\right]$	[47,64]
40	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - x\right]$	[48,63]
41	$\left[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[49,74]
42	$\left[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[50,73]
43	$\left[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}\right]$	[51,76]
44	$\left[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}\right]$	[52,75]
45	$\left[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[61,86]
46	$\left[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[62,85]
47	$\left[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}\right]$	[69,94]
48	$\left[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}\right]$	[70,93]

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	$[x, -z, y]$	[13]
14	$[x, z, -y]$	[14]
15	$[z, y, -x]$	[15]
16	$[-z, y, x]$	[16]
17	$[-y, x, z]$	[17]
18	$[y, -x, z]$	[18]
19	$[y, x, -z]$	[19]
20	$[-y, -x, -z]$	[20]
21	$[-x, z, y]$	[21]
22	$[-x, -z, -y]$	[22]
23	$[z, -y, x]$	[23]
24	$[-z, -y, -x]$	[24]
25	$\left[x, y + \frac{1}{2}, z + \frac{1}{2}\right]$	[25]
26	$\left[x, \frac{1}{2} - y, \frac{1}{2} - z\right]$	[26]
27	$\left[-x, y + \frac{1}{2}, \frac{1}{2} - z\right]$	[27]
28	$\left[-x, \frac{1}{2} - y, z + \frac{1}{2}\right]$	[28]
29	$\left[z, x + \frac{1}{2}, y + \frac{1}{2}\right]$	[29]
30	$\left[y, z + \frac{1}{2}, x + \frac{1}{2}\right]$	[30]

continued ...

Table 10

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

continued ...

Table 10

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