Table 1: Wyckoff site: `2a`, site symmetry: `m-3m'`

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

Table 2: Wyckoff site: `6b`, site symmetry: `4'/mm.m'`

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

Table 3: Wyckoff site: `8c`, site symmetry: `.-3'm'`

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

Table 4: Wyckoff site: `12d`, site symmetry: `-4m.2`

No.	position	mapping
1	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[1,8,13,14,26,27,33,34]
2	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	[2,3,9,10,25,32,37,38]
3	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[4,16,18,21,29,39,43,47]
4	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[5,15,19,23,28,40,42,45]
5	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	[6,11,20,22,31,36,41,48]
6	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[7,12,17,24,30,35,44,46]
7	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	[49,56,61,62,74,75,81,82]

continued ...

Table 4

No.	position	mapping
8	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	[50,51,57,58,73,80,85,86]
9	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[52,64,66,69,77,87,91,95]
10	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[53,63,67,71,76,88,90,93]
11	$\left[0, \frac{1}{4}, \frac{1}{2}\right]$	[54,59,68,70,79,84,89,96]
12	$\left[0, \frac{3}{4}, \frac{1}{2}\right]$	[55,60,65,72,78,83,92,94]

Table 5: Wyckoff site: `12e`, site symmetry: `4'm.m'`

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

Table 6: Wyckoff site: `16f`, site symmetry: `.3m'`

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

Table 7: Wyckoff site: 24g, site symmetry: 2mm..

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

Table 8: Wyckoff site: 24h, site symmetry: m.2'm'

No.	position	mapping
1	$[0, y, y]$	[1,32,61,86]
2	$\left[\frac{1}{2}, \frac{1}{2} - y, y + \frac{1}{2}\right]$	[2,27,58,81]
3	$\left[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - y\right]$	[3,26,57,82]
4	$\left[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}\right]$	[4,40,66,93]
5	$\left[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{2}\right]$	[5,39,67,95]
6	$\left[\frac{1}{2} - y, \frac{1}{2}, y + \frac{1}{2}\right]$	[6,35,68,94]
7	$\left[y + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}\right]$	[7,36,65,96]
8	$[0, -y, -y]$	[8,25,62,85]
9	$[0, y, -y]$	[9,34,51,74]
10	$[0, -y, y]$	[10,33,50,75]
11	$\left[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - y\right]$	[11,30,70,92]
12	$\left[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - y\right]$	[12,31,72,89]
13	$\left[\frac{1}{2}, y + \frac{1}{2}, y + \frac{1}{2}\right]$	[13,38,49,80]
14	$\left[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - y\right]$	[14,37,56,73]
15	$\left[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}\right]$	[15,29,71,91]

continued ...

Table 8

No.	position	mapping
16	$\left[\frac{1}{2}-y, \frac{1}{2}-y, \frac{1}{2}\right]$	[16,28,69,90]
17	$[y, 0, y]$	[17,48,55,84]
18	$[y, y, 0]$	[18,45,52,88]
19	$[-y, y, 0]$	[19,47,53,87]
20	$[-y, 0, y]$	[20,46,54,83]
21	$[-y, -y, 0]$	[21,42,64,76]
22	$[y, 0, -y]$	[22,44,59,78]
23	$[y, -y, 0]$	[23,43,63,77]
24	$[-y, 0, -y]$	[24,41,60,79]

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

No.	position	mapping
1	$\left[\frac{1}{4}, y, \frac{1}{2}-y\right]$	[1,14]
2	$\left[\frac{3}{4}, y, y+\frac{1}{2}\right]$	[2,9]
3	$\left[\frac{3}{4}, -y, \frac{1}{2}-y\right]$	[3,10]
4	$\left[-y, y+\frac{1}{2}, \frac{1}{4}\right]$	[4,21]
5	$\left[y, y+\frac{1}{2}, \frac{3}{4}\right]$	[5,23]
6	$\left[\frac{1}{2}-y, \frac{3}{4}, -y\right]$	[6,22]
7	$\left[y+\frac{1}{2}, \frac{1}{4}, -y\right]$	[7,24]
8	$\left[\frac{1}{4}, -y, y+\frac{1}{2}\right]$	[8,13]
9	$\left[y+\frac{1}{2}, \frac{3}{4}, y\right]$	[11,20]
10	$\left[\frac{1}{2}-y, \frac{1}{4}, y\right]$	[12,17]
11	$\left[-y, \frac{1}{2}-y, \frac{3}{4}\right]$	[15,19]
12	$\left[y, \frac{1}{2}-y, \frac{1}{4}\right]$	[16,18]
13	$\left[\frac{3}{4}, -y, y+\frac{1}{2}\right]$	[25,38]
14	$\left[\frac{1}{4}, -y, \frac{1}{2}-y\right]$	[26,33]
15	$\left[\frac{1}{4}, y, y+\frac{1}{2}\right]$	[27,34]
16	$\left[y, \frac{1}{2}-y, \frac{3}{4}\right]$	[28,45]
17	$\left[-y, \frac{1}{2}-y, \frac{1}{4}\right]$	[29,47]
18	$\left[y+\frac{1}{2}, \frac{1}{4}, y\right]$	[30,46]
19	$\left[\frac{1}{2}-y, \frac{3}{4}, y\right]$	[31,48]
20	$\left[\frac{3}{4}, y, \frac{1}{2}-y\right]$	[32,37]
21	$\left[\frac{1}{2}-y, \frac{1}{4}, -y\right]$	[35,44]
22	$\left[y+\frac{1}{2}, \frac{3}{4}, -y\right]$	[36,41]
23	$\left[y, y+\frac{1}{2}, \frac{1}{4}\right]$	[39,43]
24	$\left[-y, y+\frac{1}{2}, \frac{3}{4}\right]$	[40,42]
25	$\left[\frac{3}{4}, y+\frac{1}{2}, -y\right]$	[49,62]
26	$\left[\frac{1}{4}, y+\frac{1}{2}, y\right]$	[50,57]
27	$\left[\frac{1}{4}, \frac{1}{2}-y, -y\right]$	[51,58]
28	$\left[\frac{1}{2}-y, y, \frac{3}{4}\right]$	[52,69]
29	$\left[y+\frac{1}{2}, y, \frac{1}{4}\right]$	[53,71]
30	$\left[-y, \frac{1}{4}, \frac{1}{2}-y\right]$	[54,70]
31	$\left[y, \frac{3}{4}, \frac{1}{2}-y\right]$	[55,72]

continued ...

4

Table 9

No.	position	mapping
32	$\left[\frac{3}{4}, \frac{1}{2} - y, y\right]$	[56,61]
33	$\left[y, \frac{1}{4}, y + \frac{1}{2}\right]$	[59,68]
34	$\left[-y, \frac{3}{4}, y + \frac{1}{2}\right]$	[60,65]
35	$\left[\frac{1}{2} - y, -y, \frac{1}{4}\right]$	[63,67]
36	$\left[y + \frac{1}{2}, -y, \frac{3}{4}\right]$	[64,66]
37	$\left[\frac{1}{4}, \frac{1}{2} - y, y\right]$	[73,86]
38	$\left[\frac{3}{4}, \frac{1}{2} - y, -y\right]$	[74,81]
39	$\left[\frac{3}{4}, y + \frac{1}{2}, y\right]$	[75,82]
40	$\left[y + \frac{1}{2}, -y, \frac{1}{4}\right]$	[76,93]
41	$\left[\frac{1}{2} - y, -y, \frac{3}{4}\right]$	[77,95]
42	$\left[y, \frac{3}{4}, y + \frac{1}{2}\right]$	[78,94]
43	$\left[-y, \frac{1}{4}, y + \frac{1}{2}\right]$	[79,96]
44	$\left[\frac{1}{4}, y + \frac{1}{2}, -y\right]$	[80,85]
45	$\left[-y, \frac{3}{4}, \frac{1}{2} - y\right]$	[83,92]
46	$\left[y, \frac{1}{4}, \frac{1}{2} - y\right]$	[84,89]
47	$\left[y + \frac{1}{2}, y, \frac{3}{4}\right]$	[87,91]
48	$\left[\frac{1}{2} - y, y, \frac{1}{4}\right]$	[88,90]

Table 10: Wyckoff site: 48j, site symmetry: m. .

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

Table 10

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

Table 11: Wyckoff site: `48k`, site symmetry: `..m'`

No.	position	mapping
1	$[x, x, z]$	[1,84]
2	$\left[x+\frac{1}{2}, \frac{1}{2}-z, x+\frac{1}{2}\right]$	[2,91]
3	$\left[x+\frac{1}{2}, z+\frac{1}{2}, \frac{1}{2}-x\right]$	[3,93]
4	$\left[z+\frac{1}{2}, x+\frac{1}{2}, \frac{1}{2}-x\right]$	[4,92]
5	$\left[\frac{1}{2}-z, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[5,94]
6	$\left[\frac{1}{2}-x, x+\frac{1}{2}, z+\frac{1}{2}\right]$	[6,80]
7	$\left[x+\frac{1}{2}, \frac{1}{2}-x, z+\frac{1}{2}\right]$	[7,81]
8	$[x, -x, -z]$	[8,78]
9	$[-x, x, -z]$	[9,79]
10	$[-x, -x, z]$	[10,83]
11	$\left[x+\frac{1}{2}, x+\frac{1}{2}, \frac{1}{2}-z\right]$	[11,82]
12	$\left[\frac{1}{2}-x, \frac{1}{2}-x, \frac{1}{2}-z\right]$	[12,73]
13	$\left[\frac{1}{2}-x, z+\frac{1}{2}, x+\frac{1}{2}\right]$	[13,95]
14	$\left[\frac{1}{2}-x, \frac{1}{2}-z, \frac{1}{2}-x\right]$	[14,90]
15	$\left[z+\frac{1}{2}, \frac{1}{2}-x, x+\frac{1}{2}\right]$	[15,96]

continued ...

Table 11

No.	position	mapping
16	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	[16,89]
17	$[z,\ x,\ x]$	[17,88]
18	$[x,\ z,\ x]$	[18,86]
19	$[-x,\ z,\ -x]$	[19,74]
20	$[-z,\ -x,\ x]$	[20,76]
21	$[-x,\ -z,\ x]$	[21,75]
22	$[z,\ -x,\ -x]$	[22,77]
23	$[x,\ -z,\ -x]$	[23,85]
24	$[-z,\ x,\ -x]$	[24,87]
25	$[-x,\ -x,\ -z]$	[25,60]
26	$\left[\frac{1}{2}-x,\ z+\frac{1}{2},\ \frac{1}{2}-x\right]$	[26,67]
27	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ x+\frac{1}{2}\right]$	[27,69]
28	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ x+\frac{1}{2}\right]$	[28,68]
29	$\left[z+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	[29,70]
30	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[30,56]
31	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[31,57]
32	$[-x,\ x,\ z]$	[32,54]
33	$[x,\ -x,\ z]$	[33,55]
34	$[x,\ x,\ -z]$	[34,59]
35	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	[35,58]
36	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[36,49]
37	$\left[x+\frac{1}{2},\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[37,71]
38	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$	[38,66]
39	$\left[\frac{1}{2}-z,\ x+\frac{1}{2},\ \frac{1}{2}-x\right]$	[39,72]
40	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ x+\frac{1}{2}\right]$	[40,65]
41	$[-z,\ -x,\ -x]$	[41,64]
42	$[-x,\ -z,\ -x]$	[42,62]
43	$[x,\ -z,\ x]$	[43,50]
44	$[z,\ x,\ -x]$	[44,52]
45	$[x,\ z,\ -x]$	[45,51]
46	$[-z,\ x,\ x]$	[46,53]
47	$[-x,\ z,\ x]$	[47,61]
48	$[z,\ -x,\ x]$	[48,63]

Table 12: Wyckoff site: 96l, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$\left[x+\frac{1}{2},\ \frac{1}{2}-z,\ y+\frac{1}{2}\right]$	[2]
3	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ \frac{1}{2}-y\right]$	[3]
4	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-x\right]$	[4]
5	$\left[\frac{1}{2}-z,\ y+\frac{1}{2},\ x+\frac{1}{2}\right]$	[5]
6	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[6]
7	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	[7]

continued ...

Table 12

No.	position	mapping
8	$[x, -y, -z]$	[8]
9	$[-x, y, -z]$	[9]
10	$[-x, -y, z]$	[10]
11	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[12]
13	$[\frac{1}{2} - x, z + \frac{1}{2}, y + \frac{1}{2}]$	[13]
14	$[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y]$	[14]
15	$[z + \frac{1}{2}, \frac{1}{2} - y, x + \frac{1}{2}]$	[15]
16	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2} - x]$	[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	$[-x, -y, -z]$	[25]
26	$[\frac{1}{2} - x, z + \frac{1}{2}, \frac{1}{2} - y]$	[26]
27	$[\frac{1}{2} - x, \frac{1}{2} - z, y + \frac{1}{2}]$	[27]
28	$[\frac{1}{2} - z, \frac{1}{2} - y, x + \frac{1}{2}]$	[28]
29	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - x]$	[29]
30	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[30]
31	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[31]
32	$[-x, y, z]$	[32]
33	$[x, -y, z]$	[33]
34	$[x, y, -z]$	[34]
35	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[35]
36	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[36]
37	$[x + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[37]
38	$[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[38]
39	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2} - x]$	[39]
40	$[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}]$	[40]
41	$[-z, -x, -y]$	[41]
42	$[-y, -z, -x]$	[42]
43	$[y, -z, x]$	[43]
44	$[z, x, -y]$	[44]
45	$[y, z, -x]$	[45]
46	$[-z, x, y]$	[46]
47	$[-y, z, x]$	[47]
48	$[z, -x, y]$	[48]
49	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[49]
50	$[x, -z, y]$	[50]
51	$[x, z, -y]$	[51]
52	$[z, y, -x]$	[52]
53	$[-z, y, x]$	[53]
54	$[-y, x, z]$	[54]

continued ...

Table 12

No.	position	mapping
55	$[y, -x, z]$	[55]
56	$\left[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z\right]$	[56]
57	$\left[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z\right]$	[57]
58	$\left[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}\right]$	[58]
59	$[y, x, -z]$	[59]
60	$[-y, -x, -z]$	[60]
61	$[-x, z, y]$	[61]
62	$[-x, -z, -y]$	[62]
63	$[z, -y, x]$	[63]
64	$[-z, -y, -x]$	[64]
65	$\left[z + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}\right]$	[65]
66	$\left[y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}\right]$	[66]
67	$\left[\frac{1}{2} - y, z + \frac{1}{2}, \frac{1}{2} - x\right]$	[67]
68	$\left[\frac{1}{2} - z, \frac{1}{2} - x, y + \frac{1}{2}\right]$	[68]
69	$\left[\frac{1}{2} - y, \frac{1}{2} - z, x + \frac{1}{2}\right]$	[69]
70	$\left[z + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - y\right]$	[70]
71	$\left[y + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - x\right]$	[71]
72	$\left[\frac{1}{2} - z, x + \frac{1}{2}, \frac{1}{2} - y\right]$	[72]
73	$\left[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z\right]$	[73]
74	$[-x, z, -y]$	[74]
75	$[-x, -z, y]$	[75]
76	$[-z, -y, x]$	[76]
77	$[z, -y, -x]$	[77]
78	$[y, -x, -z]$	[78]
79	$[-y, x, -z]$	[79]
80	$\left[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}\right]$	[80]
81	$\left[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}\right]$	[81]
82	$\left[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z\right]$	[82]
83	$[-y, -x, z]$	[83]
84	$[y, x, z]$	[84]
85	$[x, -z, -y]$	[85]
86	$[x, z, y]$	[86]
87	$[-z, y, -x]$	[87]
88	$[z, y, x]$	[88]
89	$\left[\frac{1}{2} - z, \frac{1}{2} - x, \frac{1}{2} - y\right]$	[89]
90	$\left[\frac{1}{2} - y, \frac{1}{2} - z, \frac{1}{2} - x\right]$	[90]
91	$\left[y + \frac{1}{2}, \frac{1}{2} - z, x + \frac{1}{2}\right]$	[91]
92	$\left[z + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - y\right]$	[92]
93	$\left[y + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - x\right]$	[93]
94	$\left[\frac{1}{2} - z, x + \frac{1}{2}, y + \frac{1}{2}\right]$	[94]
95	$\left[\frac{1}{2} - y, z + \frac{1}{2}, x + \frac{1}{2}\right]$	[95]
96	$\left[z + \frac{1}{2}, \frac{1}{2} - x, y + \frac{1}{2}\right]$	[96]