MSG No. 227.131 $Fd\bar{3}m'$ [Type III, cubic]

Table 1: Wyckoff site: `8a`, site symmetry: `-4'3m'`

No.	position	mapping
1	$\left[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}\right]$	[1,2,3,4,5,6,7,8,9,10,11,12,37,38,39,40,41,42,43,44,45,46,47,48]
2	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[13,17,18,32,34,36,62,70,71,76,77,81,111,115,120,121,126,131,160,164,165,170,171,175]
3	$\left[\frac{7}{8}, \frac{3}{8}, \frac{3}{8}\right]$	[14,22,23,28,29,33,61,65,66,80,82,84,112,116,117,122,123,127,159,163,168,169,174,179]
4	$\left[\frac{3}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[15,19,24,25,30,35,64,68,69,74,75,79,109,113,114,128,130,132,158,166,167,172,173,177]
5	$\left[\frac{3}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[16,20,21,26,27,31,63,67,72,73,78,83,110,118,119,124,125,129,157,161,162,176,178,180]
6	$\left[\frac{1}{8}, \frac{5}{8}, \frac{5}{8}\right]$	[49,50,51,52,53,54,55,56,57,58,59,60,85,86,87,88,89,90,91,92,93,94,95,96]
7	$\left[\frac{5}{8}, \frac{1}{8}, \frac{5}{8}\right]$	[97,98,99,100,101,102,103,104,105,106,107,108,133,134,135,136,137,138,139,140,141,142,143,144]
8	$\left[\frac{5}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[145,146,147,148,149,150,151,152,153,154,155,156,181,182,183,184,185,186,187,188,189,190,191,192]

Table 2: Wyckoff site: `8b`, site symmetry: `-4'3m'`

No.	position	mapping
1	$\left[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}\right]$	[1,5,6,44,46,48,50,58,59,88,89,93,99,103,108,133,138,143,148,152,153,182,183,187]
2	$\left[\frac{3}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[2,10,11,40,41,45,49,53,54,92,94,96,100,104,105,134,135,139,147,151,156,181,186,191]
3	$\left[\frac{7}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[3,7,12,37,42,47,52,56,57,86,87,91,97,101,102,140,142,144,146,154,155,184,185,189]
4	$\left[\frac{7}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[4,8,9,38,39,43,51,55,60,85,90,95,98,106,107,136,137,141,145,149,150,188,190,192]
5	$\left[\frac{5}{8}, \frac{5}{8}, \frac{5}{8}\right]$	[13,14,15,16,17,18,19,20,21,22,23,24,25,26,27,28,29,30,31,32,33,34,35,36]
6	$\left[\frac{5}{8}, \frac{1}{8}, \frac{1}{8}\right]$	[61,62,63,64,65,66,67,68,69,70,71,72,73,74,75,76,77,78,79,80,81,82,83,84]
7	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[109,110,111,112,113,114,115,116,117,118,119,120,121,122,123,124,125,126,127,128,129,130,131,132]
8	$\left[\frac{1}{8}, \frac{1}{8}, \frac{5}{8}\right]$	[157,158,159,160,161,162,163,164,165,166,167,168,169,170,171,172,173,174,175,176,177,178,179,180]

Table 3: Wyckoff site: `16c`, site symmetry: `.-3m`

No.	position	mapping
1	$[0, 0, 0]$	[1,5,6,13,17,18,32,34,36,44,46,48]
2	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	[2,10,11,14,22,23,28,29,33,40,41,45]
3	$\left[\frac{1}{4}, 0, \frac{1}{4}\right]$	[3,7,12,15,19,24,25,30,35,37,42,47]
4	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	[4,8,9,16,20,21,26,27,31,38,39,43]
5	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[49,53,54,61,65,66,80,82,84,92,94,96]
6	$\left[0, \frac{3}{4}, \frac{3}{4}\right]$	[50,58,59,62,70,71,76,77,81,88,89,93]
7	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[51,55,60,63,67,72,73,78,83,85,90,95]
8	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[52,56,57,64,68,69,74,75,79,86,87,91]
9	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[97,101,102,109,113,114,128,130,132,140,142,144]
10	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[98,106,107,110,118,119,124,125,129,136,137,141]
11	$\left[\frac{3}{4}, 0, \frac{3}{4}\right]$	[99,103,108,111,115,120,121,126,131,133,138,143]
12	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[100,104,105,112,116,117,122,123,127,134,135,139]
13	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[145,149,150,157,161,162,176,178,180,188,190,192]
14	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[146,154,155,158,166,167,172,173,177,184,185,189]
15	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[147,151,156,159,163,168,169,174,179,181,186,191]

continued ...

Table 3

No.	position	mapping
16	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	[148,152,153,160,164,165,170,171,175,182,183,187]

Table 4: Wyckoff site: 16d, site symmetry: .-3m

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[1,5,6,13,17,18,32,34,36,44,46,48]
2	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[2,10,11,14,22,23,28,29,33,40,41,45]
3	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[3,7,12,15,19,24,25,30,35,37,42,47]
4	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[4,8,9,16,20,21,26,27,31,38,39,43]
5	$\left[\frac{1}{2}, 0, 0\right]$	[49,53,54,61,65,66,80,82,84,92,94,96]
6	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[50,58,59,62,70,71,76,77,81,88,89,93]
7	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	[51,55,60,63,67,72,73,78,83,85,90,95]
8	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[52,56,57,64,68,69,74,75,79,86,87,91]
9	$\left[0, \frac{1}{2}, 0\right]$	[97,101,102,109,113,114,128,130,132,140,142,144]
10	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	[98,106,107,110,118,119,124,125,129,136,137,141]
11	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[99,103,108,111,115,120,121,126,131,133,138,143]
12	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[100,104,105,112,116,117,122,123,127,134,135,139]
13	$\left[0, 0, \frac{1}{2}\right]$	[145,149,150,157,161,162,176,178,180,188,190,192]
14	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	[146,154,155,158,166,167,172,173,177,184,185,189]
15	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	[147,151,156,159,163,168,169,174,179,181,186,191]
16	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[148,152,153,160,164,165,170,171,175,182,183,187]

Table 5: Wyckoff site: 32e, site symmetry: .3m'

No.	position	mapping
1	$[x, x, x]$	[1,5,6,44,46,48]
2	$\left[x, \frac{1}{4}-x, \frac{1}{4}-x\right]$	[2,10,11,40,41,45]
3	$\left[\frac{1}{4}-x, x, \frac{1}{4}-x\right]$	[3,7,12,37,42,47]
4	$\left[\frac{1}{4}-x, \frac{1}{4}-x, x\right]$	[4,8,9,38,39,43]
5	$[-x, -x, -x]$	[13,17,18,32,34,36]
6	$\left[-x, x+\frac{1}{4}, x+\frac{1}{4}\right]$	[14,22,23,28,29,33]
7	$\left[x+\frac{1}{4}, -x, x+\frac{1}{4}\right]$	[15,19,24,25,30,35]
8	$\left[x+\frac{1}{4}, x+\frac{1}{4}, -x\right]$	[16,20,21,26,27,31]
9	$\left[x, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[49,53,54,92,94,96]
10	$\left[x, \frac{3}{4}-x, \frac{3}{4}-x\right]$	[50,58,59,88,89,93]
11	$\left[\frac{1}{4}-x, x+\frac{1}{2}, \frac{3}{4}-x\right]$	[51,55,60,85,90,95]
12	$\left[\frac{1}{4}-x, \frac{3}{4}-x, x+\frac{1}{2}\right]$	[52,56,57,86,87,91]
13	$\left[-x, \frac{1}{2}-x, \frac{1}{2}-x\right]$	[61,65,66,80,82,84]
14	$\left[-x, x+\frac{3}{4}, x+\frac{3}{4}\right]$	[62,70,71,76,77,81]
15	$\left[x+\frac{1}{4}, \frac{1}{2}-x, x+\frac{3}{4}\right]$	[63,67,72,73,78,83]
16	$\left[x+\frac{1}{4}, x+\frac{3}{4}, \frac{1}{2}-x\right]$	[64,68,69,74,75,79]
17	$\left[x+\frac{1}{2}, x, x+\frac{1}{2}\right]$	[97,101,102,140,142,144]

continued ...

Table 5

No.	position	mapping
18	$\left[x+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{3}{4}-x\right]$	[98,106,107,136,137,141]
19	$\left[\frac{3}{4}-x,\ x,\ \frac{3}{4}-x\right]$	[99,103,108,133,138,143]
20	$\left[\frac{3}{4}-x,\ \frac{1}{4}-x,\ x+\frac{1}{2}\right]$	[100,104,105,134,135,139]
21	$\left[\frac{1}{2}-x,\ -x,\ \frac{1}{2}-x\right]$	[109,113,114,128,130,132]
22	$\left[\frac{1}{2}-x,\ x+\frac{1}{4},\ x+\frac{3}{4}\right]$	[110,118,119,124,125,129]
23	$\left[x+\frac{3}{4},\ -x,\ x+\frac{3}{4}\right]$	[111,115,120,121,126,131]
24	$\left[x+\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{2}-x\right]$	[112,116,117,122,123,127]
25	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ x\right]$	[145,149,150,188,190,192]
26	$\left[x+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{1}{4}-x\right]$	[146,154,155,184,185,189]
27	$\left[\frac{3}{4}-x,\ x+\frac{1}{2},\ \frac{1}{4}-x\right]$	[147,151,156,181,186,191]
28	$\left[\frac{3}{4}-x,\ \frac{3}{4}-x,\ x\right]$	[148,152,153,182,183,187]
29	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ -x\right]$	[157,161,162,176,178,180]
30	$\left[\frac{1}{2}-x,\ x+\frac{3}{4},\ x+\frac{1}{4}\right]$	[158,166,167,172,173,177]
31	$\left[x+\frac{3}{4},\ \frac{1}{2}-x,\ x+\frac{1}{4}\right]$	[159,163,168,169,174,179]
32	$\left[x+\frac{3}{4},\ x+\frac{3}{4},\ -x\right]$	[160,164,165,170,171,175]

Table 6: Wyckoff site: 48f, site symmetry: 2.m'm'

No.	position	mapping
1	$\left[x,\ \frac{1}{8},\ \frac{1}{8}\right]$	[1,2,45,46]
2	$\left[\frac{1}{4}-x,\ \frac{1}{8},\ \frac{1}{8}\right]$	[3,4,37,38]
3	$\left[\frac{1}{8},\ x,\ \frac{1}{8}\right]$	[5,12,42,44]
4	$\left[\frac{1}{8},\ \frac{1}{8},\ x\right]$	[6,9,39,48]
5	$\left[\frac{1}{8},\ \frac{1}{8},\ \frac{1}{4}-x\right]$	[7,11,40,47]
6	$\left[\frac{1}{8},\ \frac{1}{4}-x,\ \frac{1}{8}\right]$	[8,10,41,43]
7	$\left[-x,\ \frac{7}{8},\ \frac{7}{8}\right]$	[13,34,62,81]
8	$\left[-x,\ \frac{3}{8},\ \frac{3}{8}\right]$	[14,33,61,82]
9	$\left[x+\frac{1}{4},\ \frac{7}{8},\ \frac{3}{8}\right]$	[15,25,64,74]
10	$\left[x+\frac{1}{4},\ \frac{3}{8},\ \frac{7}{8}\right]$	[16,26,63,73]
11	$\left[\frac{7}{8},\ -x,\ \frac{7}{8}\right]$	[17,32,120,126]
12	$\left[\frac{7}{8},\ \frac{7}{8},\ -x\right]$	[18,36,165,171]
13	$\left[\frac{3}{8},\ \frac{7}{8},\ x+\frac{1}{4}\right]$	[19,35,167,172]
14	$\left[\frac{3}{8},\ x+\frac{1}{4},\ \frac{7}{8}\right]$	[20,31,118,125]
15	$\left[\frac{3}{8},\ \frac{3}{8},\ -x\right]$	[21,27,162,180]
16	$\left[\frac{7}{8},\ x+\frac{1}{4},\ \frac{3}{8}\right]$	[22,29,116,127]
17	$\left[\frac{7}{8},\ \frac{3}{8},\ x+\frac{1}{4}\right]$	[23,28,163,179]
18	$\left[\frac{3}{8},\ -x,\ \frac{3}{8}\right]$	[24,30,113,128]
19	$\left[x,\ \frac{5}{8},\ \frac{5}{8}\right]$	[49,50,93,94]
20	$\left[\frac{1}{4}-x,\ \frac{5}{8},\ \frac{5}{8}\right]$	[51,52,85,86]
21	$\left[\frac{1}{8},\ x+\frac{1}{2},\ \frac{5}{8}\right]$	[53,60,90,92]
22	$\left[\frac{1}{8},\ \frac{5}{8},\ x+\frac{1}{2}\right]$	[54,57,87,96]
23	$\left[\frac{1}{8},\ \frac{5}{8},\ \frac{3}{4}-x\right]$	[55,59,88,95]
24	$\left[\frac{1}{8},\ \frac{3}{4}-x,\ \frac{5}{8}\right]$	[56,58,89,91]
25	$\left[\frac{7}{8},\ \frac{1}{2}-x,\ \frac{3}{8}\right]$	[65,80,168,174]

continued ...

Table 6

No.	position	mapping
26	$\left[\frac{7}{8}, \frac{3}{8}, \frac{1}{2}-x\right]$	[66,84,117,123]
27	$\left[\frac{3}{8}, \frac{3}{8}, x+\frac{3}{4}\right]$	[67,83,119,124]
28	$\left[\frac{3}{8}, x+\frac{3}{4}, \frac{3}{8}\right]$	[68,79,166,173]
29	$\left[\frac{3}{8}, \frac{7}{8}, \frac{1}{2}-x\right]$	[69,75,114,132]
30	$\left[\frac{7}{8}, x+\frac{3}{4}, \frac{7}{8}\right]$	[70,77,164,175]
31	$\left[\frac{7}{8}, \frac{7}{8}, x+\frac{3}{4}\right]$	[71,76,115,131]
32	$\left[\frac{3}{8}, \frac{1}{2}-x, \frac{7}{8}\right]$	[72,78,161,176]
33	$\left[x+\frac{1}{2}, \frac{1}{8}, \frac{5}{8}\right]$	[97,98,141,142]
34	$\left[\frac{3}{4}-x, \frac{1}{8}, \frac{5}{8}\right]$	[99,100,133,134]
35	$\left[\frac{5}{8}, x, \frac{5}{8}\right]$	[101,108,138,140]
36	$\left[\frac{5}{8}, \frac{1}{8}, x+\frac{1}{2}\right]$	[102,105,135,144]
37	$\left[\frac{5}{8}, \frac{1}{8}, \frac{3}{4}-x\right]$	[103,107,136,143]
38	$\left[\frac{5}{8}, \frac{1}{4}-x, \frac{5}{8}\right]$	[104,106,137,139]
39	$\left[\frac{1}{2}-x, \frac{7}{8}, \frac{3}{8}\right]$	[109,130,158,177]
40	$\left[\frac{1}{2}-x, \frac{3}{8}, \frac{7}{8}\right]$	[110,129,157,178]
41	$\left[x+\frac{3}{4}, \frac{7}{8}, \frac{7}{8}\right]$	[111,121,160,170]
42	$\left[x+\frac{3}{4}, \frac{3}{8}, \frac{3}{8}\right]$	[112,122,159,169]
43	$\left[x+\frac{1}{2}, \frac{5}{8}, \frac{1}{8}\right]$	[145,146,189,190]
44	$\left[\frac{3}{4}-x, \frac{5}{8}, \frac{1}{8}\right]$	[147,148,181,182]
45	$\left[\frac{5}{8}, x+\frac{1}{2}, \frac{1}{8}\right]$	[149,156,186,188]
46	$\left[\frac{5}{8}, \frac{5}{8}, x\right]$	[150,153,183,192]
47	$\left[\frac{5}{8}, \frac{5}{8}, \frac{1}{4}-x\right]$	[151,155,184,191]
48	$\left[\frac{5}{8}, \frac{3}{4}-x, \frac{1}{8}\right]$	[152,154,185,187]

Table 7: Wyckoff site: 96g, site symmetry: ..m'

No.	position	mapping
1	$[x, x, z]$	[1,44]
2	$\left[x, \frac{1}{4}-x, \frac{1}{4}-z\right]$	[2,41]
3	$\left[\frac{1}{4}-x, x, \frac{1}{4}-z\right]$	[3,42]
4	$\left[\frac{1}{4}-x, \frac{1}{4}-x, z\right]$	[4,43]
5	$[z, x, x]$	[5,48]
6	$[x, z, x]$	[6,46]
7	$\left[\frac{1}{4}-x, z, \frac{1}{4}-x\right]$	[7,37]
8	$\left[\frac{1}{4}-z, \frac{1}{4}-x, x\right]$	[8,39]
9	$\left[\frac{1}{4}-x, \frac{1}{4}-z, x\right]$	[9,38]
10	$\left[z, \frac{1}{4}-x, \frac{1}{4}-x\right]$	[10,40]
11	$\left[x, \frac{1}{4}-z, \frac{1}{4}-x\right]$	[11,45]
12	$\left[\frac{1}{4}-z, x, \frac{1}{4}-x\right]$	[12,47]
13	$[-x, -x, -z]$	[13,32]
14	$\left[-x, x+\frac{1}{4}, z+\frac{1}{4}\right]$	[14,29]
15	$\left[x+\frac{1}{4}, -x, z+\frac{1}{4}\right]$	[15,30]
16	$\left[x+\frac{1}{4}, x+\frac{1}{4}, -z\right]$	[16,31]
17	$[-z, -x, -x]$	[17,36]

continued ...

Table 7

No.	position	mapping
18	$[-x,\ -z,\ -x]$	[18,34]
19	$\left[x+\frac{1}{4},\ -z,\ x+\frac{1}{4}\right]$	[19,25]
20	$\left[z+\frac{1}{4},\ x+\frac{1}{4},\ -x\right]$	[20,27]
21	$\left[x+\frac{1}{4},\ z+\frac{1}{4},\ -x\right]$	[21,26]
22	$\left[-z,\ x+\frac{1}{4},\ x+\frac{1}{4}\right]$	[22,28]
23	$\left[-x,\ z+\frac{1}{4},\ x+\frac{1}{4}\right]$	[23,33]
24	$\left[z+\frac{1}{4},\ -x,\ x+\frac{1}{4}\right]$	[24,35]
25	$\left[x,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[49,92]
26	$\left[x,\ \frac{3}{4}-x,\ \frac{3}{4}-z\right]$	[50,89]
27	$\left[\frac{1}{4}-x,\ x+\frac{1}{2},\ \frac{3}{4}-z\right]$	[51,90]
28	$\left[\frac{1}{4}-x,\ \frac{3}{4}-x,\ z+\frac{1}{2}\right]$	[52,91]
29	$\left[z,\ x+\frac{1}{2},\ x+\frac{1}{2}\right]$	[53,96]
30	$\left[x,\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$	[54,94]
31	$\left[\frac{1}{4}-x,\ z+\frac{1}{2},\ \frac{3}{4}-x\right]$	[55,85]
32	$\left[\frac{1}{4}-z,\ \frac{3}{4}-x,\ x+\frac{1}{2}\right]$	[56,87]
33	$\left[\frac{1}{4}-x,\ \frac{3}{4}-z,\ x+\frac{1}{2}\right]$	[57,86]
34	$\left[z,\ \frac{3}{4}-x,\ \frac{3}{4}-x\right]$	[58,88]
35	$\left[x,\ \frac{3}{4}-z,\ \frac{3}{4}-x\right]$	[59,93]
36	$\left[\frac{1}{4}-z,\ x+\frac{1}{2},\ \frac{3}{4}-x\right]$	[60,95]
37	$\left[-x,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[61,80]
38	$\left[-x,\ x+\frac{3}{4},\ z+\frac{3}{4}\right]$	[62,77]
39	$\left[x+\frac{1}{4},\ \frac{1}{2}-x,\ z+\frac{3}{4}\right]$	[63,78]
40	$\left[x+\frac{1}{4},\ x+\frac{3}{4},\ \frac{1}{2}-z\right]$	[64,79]
41	$\left[-z,\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	[65,84]
42	$\left[-x,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[66,82]
43	$\left[x+\frac{1}{4},\ \frac{1}{2}-z,\ x+\frac{3}{4}\right]$	[67,73]
44	$\left[z+\frac{1}{4},\ x+\frac{3}{4},\ \frac{1}{2}-x\right]$	[68,75]
45	$\left[x+\frac{1}{4},\ z+\frac{3}{4},\ \frac{1}{2}-x\right]$	[69,74]
46	$\left[-z,\ x+\frac{3}{4},\ x+\frac{3}{4}\right]$	[70,76]
47	$\left[-x,\ z+\frac{3}{4},\ x+\frac{3}{4}\right]$	[71,81]
48	$\left[z+\frac{1}{4},\ \frac{1}{2}-x,\ x+\frac{3}{4}\right]$	[72,83]
49	$\left[x+\frac{1}{2},\ x,\ z+\frac{1}{2}\right]$	[97,140]
50	$\left[x+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{3}{4}-z\right]$	[98,137]
51	$\left[\frac{3}{4}-x,\ x,\ \frac{3}{4}-z\right]$	[99,138]
52	$\left[\frac{3}{4}-x,\ \frac{1}{4}-x,\ z+\frac{1}{2}\right]$	[100,139]
53	$\left[z+\frac{1}{2},\ x,\ x+\frac{1}{2}\right]$	[101,144]
54	$\left[x+\frac{1}{2},\ z,\ x+\frac{1}{2}\right]$	[102,142]
55	$\left[\frac{3}{4}-x,\ z,\ \frac{3}{4}-x\right]$	[103,133]
56	$\left[\frac{3}{4}-z,\ \frac{1}{4}-x,\ x+\frac{1}{2}\right]$	[104,135]
57	$\left[\frac{3}{4}-x,\ \frac{1}{4}-z,\ x+\frac{1}{2}\right]$	[105,134]
58	$\left[z+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{3}{4}-x\right]$	[106,136]
59	$\left[x+\frac{1}{2},\ \frac{1}{4}-z,\ \frac{3}{4}-x\right]$	[107,141]
60	$\left[\frac{3}{4}-z,\ x,\ \frac{3}{4}-x\right]$	[108,143]
61	$\left[\frac{1}{2}-x,\ -x,\ \frac{1}{2}-z\right]$	[109,128]
62	$\left[\frac{1}{2}-x,\ x+\frac{1}{4},\ z+\frac{3}{4}\right]$	[110,125]
63	$\left[x+\frac{3}{4},\ -x,\ z+\frac{3}{4}\right]$	[111,126]
64	$\left[x+\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{2}-z\right]$	[112,127]

continued ...

Table 7

No.	position	mapping
65	$\left[\frac{1}{2}-z,\ -x,\ \frac{1}{2}-x\right]$	[113,132]
66	$\left[\frac{1}{2}-x,\ -z,\ \frac{1}{2}-x\right]$	[114,130]
67	$\left[x+\frac{3}{4},\ -z,\ x+\frac{3}{4}\right]$	[115,121]
68	$\left[z+\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{2}-x\right]$	[116,123]
69	$\left[x+\frac{3}{4},\ z+\frac{1}{4},\ \frac{1}{2}-x\right]$	[117,122]
70	$\left[\frac{1}{2}-z,\ x+\frac{1}{4},\ x+\frac{3}{4}\right]$	[118,124]
71	$\left[\frac{1}{2}-x,\ z+\frac{1}{4},\ x+\frac{3}{4}\right]$	[119,129]
72	$\left[z+\frac{3}{4},\ -x,\ x+\frac{3}{4}\right]$	[120,131]
73	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ z\right]$	[145,188]
74	$\left[x+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{1}{4}-z\right]$	[146,185]
75	$\left[\frac{3}{4}-x,\ x+\frac{1}{2},\ \frac{1}{4}-z\right]$	[147,186]
76	$\left[\frac{3}{4}-x,\ \frac{3}{4}-x,\ z\right]$	[148,187]
77	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ x\right]$	[149,192]
78	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ x\right]$	[150,190]
79	$\left[\frac{3}{4}-x,\ z+\frac{1}{2},\ \frac{1}{4}-x\right]$	[151,181]
80	$\left[\frac{3}{4}-z,\ \frac{3}{4}-x,\ x\right]$	[152,183]
81	$\left[\frac{3}{4}-x,\ \frac{3}{4}-z,\ x\right]$	[153,182]
82	$\left[z+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{1}{4}-x\right]$	[154,184]
83	$\left[x+\frac{1}{2},\ \frac{3}{4}-z,\ \frac{1}{4}-x\right]$	[155,189]
84	$\left[\frac{3}{4}-z,\ x+\frac{1}{2},\ \frac{1}{4}-x\right]$	[156,191]
85	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ -z\right]$	[157,176]
86	$\left[\frac{1}{2}-x,\ x+\frac{3}{4},\ z+\frac{1}{4}\right]$	[158,173]
87	$\left[x+\frac{3}{4},\ \frac{1}{2}-x,\ z+\frac{1}{4}\right]$	[159,174]
88	$\left[x+\frac{3}{4},\ x+\frac{3}{4},\ -z\right]$	[160,175]
89	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ -x\right]$	[161,180]
90	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ -x\right]$	[162,178]
91	$\left[x+\frac{3}{4},\ \frac{1}{2}-z,\ x+\frac{1}{4}\right]$	[163,169]
92	$\left[z+\frac{3}{4},\ x+\frac{3}{4},\ -x\right]$	[164,171]
93	$\left[x+\frac{3}{4},\ z+\frac{3}{4},\ -x\right]$	[165,170]
94	$\left[\frac{1}{2}-z,\ x+\frac{3}{4},\ x+\frac{1}{4}\right]$	[166,172]
95	$\left[\frac{1}{2}-x,\ z+\frac{3}{4},\ x+\frac{1}{4}\right]$	[167,177]
96	$\left[z+\frac{3}{4},\ \frac{1}{2}-x,\ x+\frac{1}{4}\right]$	[168,179]

Table 8: Wyckoff site: 96h, site symmetry: ..2'

No.	position	mapping
1	$[0,\ y,\ -y]$	[1,34]
2	$\left[0,\ \frac{1}{4}-y,\ y+\frac{1}{4}\right]$	[2,33]
3	$\left[\frac{1}{4},\ y,\ y+\frac{1}{4}\right]$	[3,25]
4	$\left[\frac{1}{4},\ \frac{1}{4}-y,\ -y\right]$	[4,26]
5	$[-y,\ 0,\ y]$	[5,32]
6	$[y,\ -y,\ 0]$	[6,36]
7	$\left[\frac{1}{4}-y,\ -y,\ \frac{1}{4}\right]$	[7,35]
8	$\left[y+\frac{1}{4},\ \frac{1}{4},\ y\right]$	[8,31]

continued ...

Table 8

No.	position	mapping
9	$\left[\frac{1}{4}-y,\, y+\frac{1}{4},\, 0\right]$	[9,27]
10	$\left[-y,\, \frac{1}{4},\, \frac{1}{4}-y\right]$	[10,29]
11	$\left[y,\, y+\frac{1}{4},\, \frac{1}{4}\right]$	[11,28]
12	$\left[y+\frac{1}{4},\, 0,\, \frac{1}{4}-y\right]$	[12,30]
13	$[0,\, -y,\, y]$	[13,46]
14	$\left[0,\, y+\frac{1}{4},\, \frac{1}{4}-y\right]$	[14,45]
15	$\left[\frac{1}{4},\, -y,\, \frac{1}{4}-y\right]$	[15,37]
16	$\left[\frac{1}{4},\, y+\frac{1}{4},\, y\right]$	[16,38]
17	$[y,\, 0,\, -y]$	[17,44]
18	$[-y,\, y,\, 0]$	[18,48]
19	$\left[y+\frac{1}{4},\, y,\, \frac{1}{4}\right]$	[19,47]
20	$\left[\frac{1}{4}-y,\, \frac{1}{4},\, -y\right]$	[20,43]
21	$\left[y+\frac{1}{4},\, \frac{1}{4}-y,\, 0\right]$	[21,39]
22	$\left[y,\, \frac{1}{4},\, y+\frac{1}{4}\right]$	[22,41]
23	$\left[-y,\, \frac{1}{4}-y,\, \frac{1}{4}\right]$	[23,40]
24	$\left[\frac{1}{4}-y,\, 0,\, y+\frac{1}{4}\right]$	[24,42]
25	$\left[0,\, y+\frac{1}{2},\, \frac{1}{2}-y\right]$	[49,82]
26	$\left[0,\, \frac{3}{4}-y,\, y+\frac{3}{4}\right]$	[50,81]
27	$\left[\frac{1}{4},\, y+\frac{1}{2},\, y+\frac{3}{4}\right]$	[51,73]
28	$\left[\frac{1}{4},\, \frac{3}{4}-y,\, \frac{1}{2}-y\right]$	[52,74]
29	$\left[-y,\, \frac{1}{2},\, y+\frac{1}{2}\right]$	[53,80]
30	$\left[y,\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[54,84]
31	$\left[\frac{1}{4}-y,\, \frac{1}{2}-y,\, \frac{3}{4}\right]$	[55,83]
32	$\left[y+\frac{1}{4},\, \frac{3}{4},\, y+\frac{1}{2}\right]$	[56,79]
33	$\left[\frac{1}{4}-y,\, y+\frac{3}{4},\, \frac{1}{2}\right]$	[57,75]
34	$\left[-y,\, \frac{3}{4},\, \frac{3}{4}-y\right]$	[58,77]
35	$\left[y,\, y+\frac{3}{4},\, \frac{3}{4}\right]$	[59,76]
36	$\left[y+\frac{1}{4},\, \frac{1}{2},\, \frac{3}{4}-y\right]$	[60,78]
37	$\left[0,\, \frac{1}{2}-y,\, y+\frac{1}{2}\right]$	[61,94]
38	$\left[0,\, y+\frac{3}{4},\, \frac{3}{4}-y\right]$	[62,93]
39	$\left[\frac{1}{4},\, \frac{1}{2}-y,\, \frac{3}{4}-y\right]$	[63,85]
40	$\left[\frac{1}{4},\, y+\frac{3}{4},\, y+\frac{1}{2}\right]$	[64,86]
41	$\left[y,\, \frac{1}{2},\, \frac{1}{2}-y\right]$	[65,92]
42	$\left[-y,\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[66,96]
43	$\left[y+\frac{1}{4},\, y+\frac{1}{2},\, \frac{3}{4}\right]$	[67,95]
44	$\left[\frac{1}{4}-y,\, \frac{3}{4},\, \frac{1}{2}-y\right]$	[68,91]
45	$\left[y+\frac{1}{4},\, \frac{3}{4}-y,\, \frac{1}{2}\right]$	[69,87]
46	$\left[y,\, \frac{3}{4},\, y+\frac{3}{4}\right]$	[70,89]
47	$\left[-y,\, \frac{3}{4}-y,\, \frac{3}{4}\right]$	[71,88]
48	$\left[\frac{1}{4}-y,\, \frac{1}{2},\, y+\frac{3}{4}\right]$	[72,90]
49	$\left[\frac{1}{2},\, y,\, \frac{1}{2}-y\right]$	[97,130]
50	$\left[\frac{1}{2},\, \frac{1}{4}-y,\, y+\frac{3}{4}\right]$	[98,129]
51	$\left[\frac{3}{4},\, y,\, y+\frac{3}{4}\right]$	[99,121]
52	$\left[\frac{3}{4},\, \frac{1}{4}-y,\, \frac{1}{2}-y\right]$	[100,122]
53	$\left[\frac{1}{2}-y,\, 0,\, y+\frac{1}{2}\right]$	[101,128]
54	$\left[y+\frac{1}{2},\, -y,\, \frac{1}{2}\right]$	[102,132]
55	$\left[\frac{3}{4}-y,\, -y,\, \frac{3}{4}\right]$	[103,131]

continued ...

Table 8

No.	position	mapping
56	$\left[y+\frac{3}{4},\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[104,127]
57	$\left[\frac{3}{4}-y,\ y+\frac{1}{4},\ \frac{1}{2}\right]$	[105,123]
58	$\left[\frac{1}{2}-y,\ \frac{1}{4},\ \frac{3}{4}-y\right]$	[106,125]
59	$\left[y+\frac{1}{2},\ y+\frac{1}{4},\ \frac{3}{4}\right]$	[107,124]
60	$\left[y+\frac{3}{4},\ 0,\ \frac{3}{4}-y\right]$	[108,126]
61	$\left[\frac{1}{2},\ -y,\ y+\frac{1}{2}\right]$	[109,142]
62	$\left[\frac{1}{2},\ y+\frac{1}{4},\ \frac{3}{4}-y\right]$	[110,141]
63	$\left[\frac{3}{4},\ -y,\ \frac{3}{4}-y\right]$	[111,133]
64	$\left[\frac{3}{4},\ y+\frac{1}{4},\ y+\frac{1}{2}\right]$	[112,134]
65	$\left[y+\frac{1}{2},\ 0,\ \frac{1}{2}-y\right]$	[113,140]
66	$\left[\frac{1}{2}-y,\ y,\ \frac{1}{2}\right]$	[114,144]
67	$\left[y+\frac{3}{4},\ y,\ \frac{3}{4}\right]$	[115,143]
68	$\left[\frac{3}{4}-y,\ \frac{1}{4},\ \frac{1}{2}-y\right]$	[116,139]
69	$\left[y+\frac{3}{4},\ \frac{1}{4}-y,\ \frac{1}{2}\right]$	[117,135]
70	$\left[y+\frac{1}{2},\ \frac{1}{4},\ y+\frac{3}{4}\right]$	[118,137]
71	$\left[\frac{1}{2}-y,\ \frac{1}{4}-y,\ \frac{3}{4}\right]$	[119,136]
72	$\left[\frac{3}{4}-y,\ 0,\ y+\frac{3}{4}\right]$	[120,138]
73	$\left[\frac{1}{2},\ y+\frac{1}{2},\ -y\right]$	[145,178]
74	$\left[\frac{1}{2},\ \frac{3}{4}-y,\ y+\frac{1}{4}\right]$	[146,177]
75	$\left[\frac{3}{4},\ y+\frac{1}{2},\ y+\frac{1}{4}\right]$	[147,169]
76	$\left[\frac{3}{4},\ \frac{3}{4}-y,\ -y\right]$	[148,170]
77	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ y\right]$	[149,176]
78	$\left[y+\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	[150,180]
79	$\left[\frac{3}{4}-y,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[151,179]
80	$\left[y+\frac{3}{4},\ \frac{3}{4},\ y\right]$	[152,175]
81	$\left[\frac{3}{4}-y,\ y+\frac{3}{4},\ 0\right]$	[153,171]
82	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ \frac{1}{4}-y\right]$	[154,173]
83	$\left[y+\frac{1}{2},\ y+\frac{3}{4},\ \frac{1}{4}\right]$	[155,172]
84	$\left[y+\frac{3}{4},\ \frac{1}{2},\ \frac{1}{4}-y\right]$	[156,174]
85	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ y\right]$	[157,190]
86	$\left[\frac{1}{2},\ y+\frac{3}{4},\ \frac{1}{4}-y\right]$	[158,189]
87	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ \frac{1}{4}-y\right]$	[159,181]
88	$\left[\frac{3}{4},\ y+\frac{3}{4},\ y\right]$	[160,182]
89	$\left[y+\frac{1}{2},\ \frac{1}{2},\ -y\right]$	[161,188]
90	$\left[\frac{1}{2}-y,\ y+\frac{1}{2},\ 0\right]$	[162,192]
91	$\left[y+\frac{3}{4},\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[163,191]
92	$\left[\frac{3}{4}-y,\ \frac{3}{4},\ -y\right]$	[164,187]
93	$\left[y+\frac{3}{4},\ \frac{3}{4}-y,\ 0\right]$	[165,183]
94	$\left[y+\frac{1}{2},\ \frac{3}{4},\ y+\frac{1}{4}\right]$	[166,185]
95	$\left[\frac{1}{2}-y,\ \frac{3}{4}-y,\ \frac{1}{4}\right]$	[167,184]
96	$\left[\frac{3}{4}-y,\ \frac{1}{2},\ y+\frac{1}{4}\right]$	[168,186]

Table 9: Wyckoff site: `192i`, site symmetry: `1`

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

continued ...

Table 9

No.	position	mapping
47	$\left[\frac{1}{4}-z,\, y,\, \frac{1}{4}-x\right]$	[47]
48	$[z,\, y,\, x]$	[48]
49	$\left[x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[49]
50	$\left[x,\, \frac{3}{4}-y,\, \frac{3}{4}-z\right]$	[50]
51	$\left[\frac{1}{4}-x,\, y+\frac{1}{2},\, \frac{3}{4}-z\right]$	[51]
52	$\left[\frac{1}{4}-x,\, \frac{3}{4}-y,\, z+\frac{1}{2}\right]$	[52]
53	$\left[z,\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[53]
54	$\left[y,\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[54]
55	$\left[\frac{1}{4}-y,\, z+\frac{1}{2},\, \frac{3}{4}-x\right]$	[55]
56	$\left[\frac{1}{4}-z,\, \frac{3}{4}-x,\, y+\frac{1}{2}\right]$	[56]
57	$\left[\frac{1}{4}-y,\, \frac{3}{4}-z,\, x+\frac{1}{2}\right]$	[57]
58	$\left[z,\, \frac{3}{4}-x,\, \frac{3}{4}-y\right]$	[58]
59	$\left[y,\, \frac{3}{4}-z,\, \frac{3}{4}-x\right]$	[59]
60	$\left[\frac{1}{4}-z,\, x+\frac{1}{2},\, \frac{3}{4}-y\right]$	[60]
61	$\left[-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[61]
62	$\left[-x,\, y+\frac{3}{4},\, z+\frac{3}{4}\right]$	[62]
63	$\left[x+\frac{1}{4},\, \frac{1}{2}-y,\, z+\frac{3}{4}\right]$	[63]
64	$\left[x+\frac{1}{4},\, y+\frac{3}{4},\, \frac{1}{2}-z\right]$	[64]
65	$\left[-z,\, \frac{1}{2}-x,\, \frac{1}{2}-y\right]$	[65]
66	$\left[-y,\, \frac{1}{2}-z,\, \frac{1}{2}-x\right]$	[66]
67	$\left[y+\frac{1}{4},\, \frac{1}{2}-z,\, x+\frac{3}{4}\right]$	[67]
68	$\left[z+\frac{1}{4},\, x+\frac{3}{4},\, \frac{1}{2}-y\right]$	[68]
69	$\left[y+\frac{1}{4},\, z+\frac{3}{4},\, \frac{1}{2}-x\right]$	[69]
70	$\left[-z,\, x+\frac{3}{4},\, y+\frac{3}{4}\right]$	[70]
71	$\left[-y,\, z+\frac{3}{4},\, x+\frac{3}{4}\right]$	[71]
72	$\left[z+\frac{1}{4},\, \frac{1}{2}-x,\, y+\frac{3}{4}\right]$	[72]
73	$\left[x+\frac{1}{4},\, \frac{1}{2}-z,\, y+\frac{3}{4}\right]$	[73]
74	$\left[x+\frac{1}{4},\, z+\frac{3}{4},\, \frac{1}{2}-y\right]$	[74]
75	$\left[z+\frac{1}{4},\, y+\frac{3}{4},\, \frac{1}{2}-x\right]$	[75]
76	$\left[-z,\, y+\frac{3}{4},\, x+\frac{3}{4}\right]$	[76]
77	$\left[-y,\, x+\frac{3}{4},\, z+\frac{3}{4}\right]$	[77]
78	$\left[y+\frac{1}{4},\, \frac{1}{2}-x,\, z+\frac{3}{4}\right]$	[78]
79	$\left[y+\frac{1}{4},\, x+\frac{3}{4},\, \frac{1}{2}-z\right]$	[79]
80	$\left[-y,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[80]
81	$\left[-x,\, z+\frac{3}{4},\, y+\frac{3}{4}\right]$	[81]
82	$\left[-x,\, \frac{1}{2}-z,\, \frac{1}{2}-y\right]$	[82]
83	$\left[z+\frac{1}{4},\, \frac{1}{2}-y,\, x+\frac{3}{4}\right]$	[83]
84	$\left[-z,\, \frac{1}{2}-y,\, \frac{1}{2}-x\right]$	[84]
85	$\left[\frac{1}{4}-x,\, z+\frac{1}{2},\, \frac{3}{4}-y\right]$	[85]
86	$\left[\frac{1}{4}-x,\, \frac{3}{4}-z,\, y+\frac{1}{2}\right]$	[86]
87	$\left[\frac{1}{4}-z,\, \frac{3}{4}-y,\, x+\frac{1}{2}\right]$	[87]
88	$\left[z,\, \frac{3}{4}-y,\, \frac{3}{4}-x\right]$	[88]
89	$\left[y,\, \frac{3}{4}-x,\, \frac{3}{4}-z\right]$	[89]
90	$\left[\frac{1}{4}-y,\, x+\frac{1}{2},\, \frac{3}{4}-z\right]$	[90]
91	$\left[\frac{1}{4}-y,\, \frac{3}{4}-x,\, z+\frac{1}{2}\right]$	[91]
92	$\left[y,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[92]
93	$\left[x,\, \frac{3}{4}-z,\, \frac{3}{4}-y\right]$	[93]

continued ...

Table 9

No.	position	mapping
94	$\left[x,\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[94]
95	$\left[\frac{1}{4}-z,\, y+\frac{1}{2},\, \frac{3}{4}-x\right]$	[95]
96	$\left[z,\, y+\frac{1}{2},\, x+\frac{1}{2}\right]$	[96]
97	$\left[x+\frac{1}{2},\, y,\, z+\frac{1}{2}\right]$	[97]
98	$\left[x+\frac{1}{2},\, \frac{1}{4}-y,\, \frac{3}{4}-z\right]$	[98]
99	$\left[\frac{3}{4}-x,\, y,\, \frac{3}{4}-z\right]$	[99]
100	$\left[\frac{3}{4}-x,\, \frac{1}{4}-y,\, z+\frac{1}{2}\right]$	[100]
101	$\left[z+\frac{1}{2},\, x,\, y+\frac{1}{2}\right]$	[101]
102	$\left[y+\frac{1}{2},\, z,\, x+\frac{1}{2}\right]$	[102]
103	$\left[\frac{3}{4}-y,\, z,\, \frac{3}{4}-x\right]$	[103]
104	$\left[\frac{3}{4}-z,\, \frac{1}{4}-x,\, y+\frac{1}{2}\right]$	[104]
105	$\left[\frac{3}{4}-y,\, \frac{1}{4}-z,\, x+\frac{1}{2}\right]$	[105]
106	$\left[z+\frac{1}{2},\, \frac{1}{4}-x,\, \frac{3}{4}-y\right]$	[106]
107	$\left[y+\frac{1}{2},\, \frac{1}{4}-z,\, \frac{3}{4}-x\right]$	[107]
108	$\left[\frac{3}{4}-z,\, x,\, \frac{3}{4}-y\right]$	[108]
109	$\left[\frac{1}{2}-x,\, -y,\, \frac{1}{2}-z\right]$	[109]
110	$\left[\frac{1}{2}-x,\, y+\frac{1}{4},\, z+\frac{3}{4}\right]$	[110]
111	$\left[x+\frac{3}{4},\, -y,\, z+\frac{3}{4}\right]$	[111]
112	$\left[x+\frac{3}{4},\, y+\frac{1}{4},\, \frac{1}{2}-z\right]$	[112]
113	$\left[\frac{1}{2}-z,\, -x,\, \frac{1}{2}-y\right]$	[113]
114	$\left[\frac{1}{2}-y,\, -z,\, \frac{1}{2}-x\right]$	[114]
115	$\left[y+\frac{3}{4},\, -z,\, x+\frac{3}{4}\right]$	[115]
116	$\left[z+\frac{3}{4},\, x+\frac{1}{4},\, \frac{1}{2}-y\right]$	[116]
117	$\left[y+\frac{3}{4},\, z+\frac{1}{4},\, \frac{1}{2}-x\right]$	[117]
118	$\left[\frac{1}{2}-z,\, x+\frac{1}{4},\, y+\frac{3}{4}\right]$	[118]
119	$\left[\frac{1}{2}-y,\, z+\frac{1}{4},\, x+\frac{3}{4}\right]$	[119]
120	$\left[z+\frac{3}{4},\, -x,\, y+\frac{3}{4}\right]$	[120]
121	$\left[x+\frac{3}{4},\, -z,\, y+\frac{3}{4}\right]$	[121]
122	$\left[x+\frac{3}{4},\, z+\frac{1}{4},\, \frac{1}{2}-y\right]$	[122]
123	$\left[z+\frac{3}{4},\, y+\frac{1}{4},\, \frac{1}{2}-x\right]$	[123]
124	$\left[\frac{1}{2}-z,\, y+\frac{1}{4},\, x+\frac{3}{4}\right]$	[124]
125	$\left[\frac{1}{2}-y,\, x+\frac{1}{4},\, z+\frac{3}{4}\right]$	[125]
126	$\left[y+\frac{3}{4},\, -x,\, z+\frac{3}{4}\right]$	[126]
127	$\left[y+\frac{3}{4},\, x+\frac{1}{4},\, \frac{1}{2}-z\right]$	[127]
128	$\left[\frac{1}{2}-y,\, -x,\, \frac{1}{2}-z\right]$	[128]
129	$\left[\frac{1}{2}-x,\, z+\frac{1}{4},\, y+\frac{3}{4}\right]$	[129]
130	$\left[\frac{1}{2}-x,\, -z,\, \frac{1}{2}-y\right]$	[130]
131	$\left[z+\frac{3}{4},\, -y,\, x+\frac{3}{4}\right]$	[131]
132	$\left[\frac{1}{2}-z,\, -y,\, \frac{1}{2}-x\right]$	[132]
133	$\left[\frac{3}{4}-x,\, z,\, \frac{3}{4}-y\right]$	[133]
134	$\left[\frac{3}{4}-x,\, \frac{1}{4}-z,\, y+\frac{1}{2}\right]$	[134]
135	$\left[\frac{3}{4}-z,\, \frac{1}{4}-y,\, x+\frac{1}{2}\right]$	[135]
136	$\left[z+\frac{1}{2},\, \frac{1}{4}-y,\, \frac{3}{4}-x\right]$	[136]
137	$\left[y+\frac{1}{2},\, \frac{1}{4}-x,\, \frac{3}{4}-z\right]$	[137]
138	$\left[\frac{3}{4}-y,\, x,\, \frac{3}{4}-z\right]$	[138]
139	$\left[\frac{3}{4}-y,\, \frac{1}{4}-x,\, z+\frac{1}{2}\right]$	[139]
140	$\left[y+\frac{1}{2},\, x,\, z+\frac{1}{2}\right]$	[140]

continued ...

Table 9

No.	position	mapping
141	$\left[x+\frac{1}{2},\ \frac{1}{4}-z,\ \frac{3}{4}-y\right]$	[141]
142	$\left[x+\frac{1}{2},\ z,\ y+\frac{1}{2}\right]$	[142]
143	$\left[\frac{3}{4}-z,\ y,\ \frac{3}{4}-x\right]$	[143]
144	$\left[z+\frac{1}{2},\ y,\ x+\frac{1}{2}\right]$	[144]
145	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[145]
146	$\left[x+\frac{1}{2},\ \frac{3}{4}-y,\ \frac{1}{4}-z\right]$	[146]
147	$\left[\frac{3}{4}-x,\ y+\frac{1}{2},\ \frac{1}{4}-z\right]$	[147]
148	$\left[\frac{3}{4}-x,\ \frac{3}{4}-y,\ z\right]$	[148]
149	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ y\right]$	[149]
150	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ x\right]$	[150]
151	$\left[\frac{3}{4}-y,\ z+\frac{1}{2},\ \frac{1}{4}-x\right]$	[151]
152	$\left[\frac{3}{4}-z,\ \frac{3}{4}-x,\ y\right]$	[152]
153	$\left[\frac{3}{4}-y,\ \frac{3}{4}-z,\ x\right]$	[153]
154	$\left[z+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{1}{4}-y\right]$	[154]
155	$\left[y+\frac{1}{2},\ \frac{3}{4}-z,\ \frac{1}{4}-x\right]$	[155]
156	$\left[\frac{3}{4}-z,\ x+\frac{1}{2},\ \frac{1}{4}-y\right]$	[156]
157	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ -z\right]$	[157]
158	$\left[\frac{1}{2}-x,\ y+\frac{3}{4},\ z+\frac{1}{4}\right]$	[158]
159	$\left[x+\frac{3}{4},\ \frac{1}{2}-y,\ z+\frac{1}{4}\right]$	[159]
160	$\left[x+\frac{3}{4},\ y+\frac{3}{4},\ -z\right]$	[160]
161	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ -y\right]$	[161]
162	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ -x\right]$	[162]
163	$\left[y+\frac{3}{4},\ \frac{1}{2}-z,\ x+\frac{1}{4}\right]$	[163]
164	$\left[z+\frac{3}{4},\ x+\frac{3}{4},\ -y\right]$	[164]
165	$\left[y+\frac{3}{4},\ z+\frac{3}{4},\ -x\right]$	[165]
166	$\left[\frac{1}{2}-z,\ x+\frac{3}{4},\ y+\frac{1}{4}\right]$	[166]
167	$\left[\frac{1}{2}-y,\ z+\frac{3}{4},\ x+\frac{1}{4}\right]$	[167]
168	$\left[z+\frac{3}{4},\ \frac{1}{2}-x,\ y+\frac{1}{4}\right]$	[168]
169	$\left[x+\frac{3}{4},\ \frac{1}{2}-z,\ y+\frac{1}{4}\right]$	[169]
170	$\left[x+\frac{3}{4},\ z+\frac{3}{4},\ -y\right]$	[170]
171	$\left[z+\frac{3}{4},\ y+\frac{3}{4},\ -x\right]$	[171]
172	$\left[\frac{1}{2}-z,\ y+\frac{3}{4},\ x+\frac{1}{4}\right]$	[172]
173	$\left[\frac{1}{2}-y,\ x+\frac{3}{4},\ z+\frac{1}{4}\right]$	[173]
174	$\left[y+\frac{3}{4},\ \frac{1}{2}-x,\ z+\frac{1}{4}\right]$	[174]
175	$\left[y+\frac{3}{4},\ x+\frac{3}{4},\ -z\right]$	[175]
176	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ -z\right]$	[176]
177	$\left[\frac{1}{2}-x,\ z+\frac{3}{4},\ y+\frac{1}{4}\right]$	[177]
178	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ -y\right]$	[178]
179	$\left[z+\frac{3}{4},\ \frac{1}{2}-y,\ x+\frac{1}{4}\right]$	[179]
180	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ -x\right]$	[180]
181	$\left[\frac{3}{4}-x,\ z+\frac{1}{2},\ \frac{1}{4}-y\right]$	[181]
182	$\left[\frac{3}{4}-x,\ \frac{3}{4}-z,\ y\right]$	[182]
183	$\left[\frac{3}{4}-z,\ \frac{3}{4}-y,\ x\right]$	[183]
184	$\left[z+\frac{1}{2},\ \frac{3}{4}-y,\ \frac{1}{4}-x\right]$	[184]
185	$\left[y+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{1}{4}-z\right]$	[185]
186	$\left[\frac{3}{4}-y,\ x+\frac{1}{2},\ \frac{1}{4}-z\right]$	[186]
187	$\left[\frac{3}{4}-y,\ \frac{3}{4}-x,\ z\right]$	[187]

continued ...

Table 9

No.	position	mapping
188	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z\right]$	[188]
189	$\left[x+\frac{1}{2},\, \frac{3}{4}-z,\, \frac{1}{4}-y\right]$	[189]
190	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, y\right]$	[190]
191	$\left[\frac{3}{4}-z,\, y+\frac{1}{2},\, \frac{1}{4}-x\right]$	[191]
192	$\left[z+\frac{1}{2},\, y+\frac{1}{2},\, x\right]$	[192]