MSG No. 210.55 F_S4_132 [Type IV, cubic]

Table 1: Wyckoff site: 16a, site symmetry: 23.

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

Table 2: Wyckoff site: 32b, site symmetry: .32

No.	position	mapping
1	$\left[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}\right]$	[1,12,14,16,17,18]
2	$\left[\frac{3}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[2,7,15,57,67,72]
3	$\left[\frac{3}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[3,4,11,82,92,93]
4	$\left[\frac{1}{8}, \frac{3}{8}, \frac{3}{8}\right]$	[5,6,13,32,46,47]
5	$\left[\frac{1}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[8,22,23,29,30,37]
6	$\left[\frac{7}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[9,19,24,50,55,63]
7	$\left[\frac{7}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[10,20,21,75,76,83]
8	$\left[\frac{1}{8}, \frac{5}{8}, \frac{5}{8}\right]$	[25,36,38,40,41,42]
9	$\left[\frac{3}{8}, \frac{5}{8}, \frac{7}{8}\right]$	[26,31,39,81,91,96]
10	$\left[\frac{3}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[27,28,35,58,68,69]
11	$\left[\frac{7}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[33,43,48,74,79,87]
12	$\left[\frac{7}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[34,44,45,51,52,59]
13	$\left[\frac{5}{8}, \frac{1}{8}, \frac{5}{8}\right]$	[49,60,62,64,65,66]
14	$\left[\frac{5}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[53,54,61,80,94,95]
15	$\left[\frac{5}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[56,70,71,77,78,85]
16	$\left[\frac{5}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[73,84,86,88,89,90]
17	$\left[\frac{1}{8}, \frac{1}{8}, \frac{5}{8}\right]$	[97,108,110,112,113,114]
18	$\left[\frac{3}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[98,103,111,153,163,168]
19	$\left[\frac{3}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[99,100,107,178,188,189]
20	$\left[\frac{1}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[101,102,109,128,142,143]
21	$\left[\frac{1}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[104,118,119,125,126,133]

continued ...

Table 2

No.	position	mapping
22	$\left[\frac{7}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[105,115,120,146,151,159]
23	$\left[\frac{7}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[106,116,117,171,172,179]
24	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[121,132,134,136,137,138]
25	$\left[\frac{3}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[122,127,135,177,187,192]
26	$\left[\frac{3}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[123,124,131,154,164,165]
27	$\left[\frac{7}{8}, \frac{5}{8}, \frac{7}{8}\right]$	[129,139,144,170,175,183]
28	$\left[\frac{7}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[130,140,141,147,148,155]
29	$\left[\frac{5}{8}, \frac{1}{8}, \frac{1}{8}\right]$	[145,156,158,160,161,162]
30	$\left[\frac{5}{8}, \frac{3}{8}, \frac{3}{8}\right]$	[149,150,157,176,190,191]
31	$\left[\frac{5}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[152,166,167,173,174,181]
32	$\left[\frac{5}{8}, \frac{5}{8}, \frac{5}{8}\right]$	[169,180,182,184,185,186]

Table 3: Wyckoff site: 32c, site symmetry: .32'

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

continued ...

Table 3

No.	position	mapping
30	$\left[\frac{1}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[81,91,96,146,151,159]
31	$\left[\frac{1}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[82,92,93,171,172,179]
32	$\left[\frac{3}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[84,86,88,97,113,114]

Table 4: Wyckoff site: 48d, site symmetry: 22'2'..

No.	position	mapping
1	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	[1,32,105,130]
2	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[2,27,110,133]
3	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	[3,26,109,134]
4	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[4,88,135,149]
5	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[5,87,136,148]
6	$\left[0, \frac{1}{4}, \frac{1}{2}\right]$	[6,59,108,151]
7	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{2}\right]$	[7,60,107,150]
8	$\left[0, \frac{3}{4}, \frac{3}{4}\right]$	[8,25,106,129]
9	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	[9,34,97,128]
10	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	[10,33,104,121]
11	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[11,54,103,156]
12	$\left[0, \frac{1}{4}, 0\right]$	[12,55,102,155]
13	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}\right]$	[13,38,99,122]
14	$\left[\frac{1}{4}, 0, 0\right]$	[14,37,98,123]
15	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[15,77,124,160]
16	$\left[0, 0, \frac{1}{4}\right]$	[16,76,125,159]
17	$\left[\frac{1}{4}, 0, \frac{1}{4}\right]$	[17,72,118,164]
18	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	[18,93,143,163]
19	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[19,95,141,162]
20	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	[20,70,120,161]
21	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	[21,90,139,167]
22	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	[22,68,113,168]
23	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[23,91,138,165]
24	$\left[\frac{3}{4}, 0, \frac{3}{4}\right]$	[24,65,116,166]
25	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[28,64,111,173]
26	$\left[0, 0, \frac{3}{4}\right]$	[29,63,112,172]
27	$\left[0, \frac{3}{4}, 0\right]$	[30,83,132,175]
28	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	[31,84,131,174]
29	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{2}\right]$	[35,78,127,180]
30	$\left[0, \frac{3}{4}, \frac{1}{2}\right]$	[36,79,126,179]
31	$\left[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	[39,53,100,184]
32	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[40,52,101,183]
33	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[41,96,142,188]
34	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[42,69,119,187]
35	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[43,71,117,186]
36	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[44,94,144,185]
37	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[45,66,115,191]

continued ...

Table 4

No.	position	mapping
38	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[46,92,137,192]
39	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[47,67,114,189]
40	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[48,89,140,190]
41	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[49,80,153,178]
42	$\left[\frac{3}{4}, 0, 0\right]$	[50,75,158,181]
43	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}\right]$	[51,74,157,182]
44	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[56,73,154,177]
45	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[57,82,145,176]
46	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[58,81,152,169]
47	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	[61,86,147,170]
48	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	[62,85,146,171]

Table 5: Wyckoff site: 48e, site symmetry: 2'.2'2

No.	position	mapping
1	$\left[\frac{1}{8}, 0, \frac{1}{4}\right]$	[1,14,104,133]
2	$\left[\frac{3}{8}, 0, \frac{1}{4}\right]$	[2,57,123,154]
3	$\left[\frac{3}{8}, \frac{1}{2}, \frac{1}{4}\right]$	[3,82,122,177]
4	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{8}\right]$	[4,93,160,162]
5	$\left[0, \frac{1}{4}, \frac{3}{8}\right]$	[5,47,115,159]
6	$\left[\frac{1}{4}, \frac{3}{8}, \frac{1}{2}\right]$	[6,46,107,188]
7	$\left[\frac{1}{4}, \frac{1}{8}, \frac{1}{2}\right]$	[7,72,108,113]
8	$\left[\frac{1}{8}, 0, \frac{3}{4}\right]$	[8,37,97,110]
9	$\left[\frac{7}{8}, 0, \frac{3}{4}\right]$	[9,50,106,171]
10	$\left[\frac{7}{8}, 0, \frac{1}{4}\right]$	[10,75,105,146]
11	$\left[\frac{1}{4}, \frac{3}{8}, 0\right]$	[11,92,102,142]
12	$\left[\frac{1}{4}, \frac{1}{8}, 0\right]$	[12,17,103,168]
13	$\left[\frac{1}{8}, \frac{1}{2}, \frac{1}{4}\right]$	[13,32,121,134]
14	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{8}\right]$	[15,67,149,191]
15	$\left[0, \frac{1}{4}, \frac{1}{8}\right]$	[16,18,141,148]
16	$\left[0, \frac{1}{4}, \frac{7}{8}\right]$	[19,63,101,143]
17	$\left[\frac{3}{4}, \frac{7}{8}, 0\right]$	[20,83,166,174]
18	$\left[0, \frac{3}{4}, \frac{1}{8}\right]$	[21,76,136,138]
19	$\left[\frac{1}{4}, \frac{7}{8}, 0\right]$	[22,30,131,164]
20	$\left[0, \frac{3}{4}, \frac{7}{8}\right]$	[23,29,139,183]
21	$\left[\frac{3}{4}, \frac{1}{8}, 0\right]$	[24,55,156,161]
22	$\left[\frac{1}{8}, \frac{1}{2}, \frac{3}{4}\right]$	[25,38,109,128]
23	$\left[\frac{3}{8}, \frac{1}{2}, \frac{3}{4}\right]$	[26,81,99,178]
24	$\left[\frac{3}{8}, 0, \frac{3}{4}\right]$	[27,58,98,153]
25	$\left[\frac{1}{2}, \frac{3}{4}, \frac{5}{8}\right]$	[28,69,184,186]
26	$\left[\frac{1}{4}, \frac{5}{8}, 0\right]$	[31,96,132,137]
27	$\left[\frac{7}{8}, \frac{1}{2}, \frac{1}{4}\right]$	[33,74,130,147]
28	$\left[\frac{7}{8}, \frac{1}{2}, \frac{3}{4}\right]$	[34,51,129,170]
29	$\left[\frac{1}{4}, \frac{7}{8}, \frac{1}{2}\right]$	[35,68,118,126]

continued ...

Table 5

No.	position	mapping
30	$\left[\frac{1}{4}, \frac{5}{8}, \frac{1}{2}\right]$	[36,41,127,192]
31	$\left[\frac{1}{2}, \frac{3}{4}, \frac{7}{8}\right]$	[39,91,167,173]
32	$\left[0, \frac{3}{4}, \frac{5}{8}\right]$	[40,42,117,172]
33	$\left[0, \frac{3}{4}, \frac{3}{8}\right]$	[43,87,119,125]
34	$\left[\frac{3}{4}, \frac{3}{8}, \frac{1}{2}\right]$	[44,59,150,190]
35	$\left[0, \frac{1}{4}, \frac{5}{8}\right]$	[45,52,112,114]
36	$\left[\frac{3}{4}, \frac{5}{8}, \frac{1}{2}\right]$	[48,79,180,185]
37	$\left[\frac{5}{8}, 0, \frac{3}{4}\right]$	[49,62,152,181]
38	$\left[\frac{1}{2}, \frac{1}{4}, \frac{7}{8}\right]$	[53,95,111,163]
39	$\left[\frac{3}{4}, \frac{3}{8}, 0\right]$	[54,94,140,155]
40	$\left[\frac{5}{8}, 0, \frac{1}{4}\right]$	[56,85,145,158]
41	$\left[\frac{3}{4}, \frac{1}{8}, \frac{1}{2}\right]$	[60,65,120,151]
42	$\left[\frac{5}{8}, \frac{1}{2}, \frac{3}{4}\right]$	[61,80,169,182]
43	$\left[\frac{1}{2}, \frac{1}{4}, \frac{5}{8}\right]$	[64,66,100,189]
44	$\left[\frac{3}{4}, \frac{7}{8}, \frac{1}{2}\right]$	[70,78,116,179]
45	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{8}\right]$	[71,77,135,187]
46	$\left[\frac{5}{8}, \frac{1}{2}, \frac{1}{4}\right]$	[73,86,157,176]
47	$\left[\frac{3}{4}, \frac{5}{8}, 0\right]$	[84,89,144,175]
48	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{8}\right]$	[88,90,124,165]

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

No.	position	mapping
1	$\left[\frac{1}{8}, \frac{1}{4}, 0\right]$	[1,14,109,128]
2	$\left[\frac{3}{8}, \frac{1}{4}, \frac{1}{2}\right]$	[2,57,99,178]
3	$\left[\frac{3}{8}, \frac{1}{4}, 0\right]$	[3,82,98,153]
4	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{8}\right]$	[4,93,136,138]
5	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{8}\right]$	[5,47,135,187]
6	$\left[0, \frac{3}{8}, \frac{1}{4}\right]$	[6,46,140,155]
7	$\left[\frac{1}{2}, \frac{1}{8}, \frac{1}{4}\right]$	[7,72,156,161]
8	$\left[\frac{1}{8}, \frac{3}{4}, 0\right]$	[8,37,121,134]
9	$\left[\frac{7}{8}, \frac{1}{4}, 0\right]$	[9,50,130,147]
10	$\left[\frac{7}{8}, \frac{3}{4}, 0\right]$	[10,75,129,170]
11	$\left[\frac{1}{2}, \frac{3}{8}, \frac{1}{4}\right]$	[11,92,150,190]
12	$\left[0, \frac{1}{8}, \frac{1}{4}\right]$	[12,17,120,151]
13	$\left[\frac{1}{8}, \frac{1}{4}, \frac{1}{2}\right]$	[13,32,97,110]
14	$\left[\frac{1}{4}, 0, \frac{3}{8}\right]$	[15,67,119,125]
15	$\left[\frac{1}{4}, 0, \frac{1}{8}\right]$	[16,18,124,165]
16	$\left[\frac{3}{4}, 0, \frac{7}{8}\right]$	[19,63,167,173]
17	$\left[0, \frac{7}{8}, \frac{1}{4}\right]$	[20,83,118,126]
18	$\left[\frac{3}{4}, 0, \frac{1}{8}\right]$	[21,76,160,162]
19	$\left[0, \frac{7}{8}, \frac{3}{4}\right]$	[22,30,116,179]
20	$\left[\frac{1}{4}, 0, \frac{7}{8}\right]$	[23,29,111,163]
21	$\left[0, \frac{1}{8}, \frac{3}{4}\right]$	[24,55,108,113]

continued ...

Table 6

No.	position	mapping
22	$\left[\frac{1}{8}, \frac{3}{4}, \frac{1}{2}\right]$	[25,38,104,133]
23	$\left[\frac{3}{8}, \frac{3}{4}, 0\right]$	[26,81,123,154]
24	$\left[\frac{3}{8}, \frac{3}{4}, \frac{1}{2}\right]$	[27,58,122,177]
25	$\left[\frac{1}{4}, 0, \frac{5}{8}\right]$	[28,69,112,114]
26	$\left[\frac{1}{2}, \frac{5}{8}, \frac{3}{4}\right]$	[31,96,180,185]
27	$\left[\frac{7}{8}, \frac{3}{4}, \frac{1}{2}\right]$	[33,74,106,171]
28	$\left[\frac{7}{8}, \frac{1}{4}, \frac{1}{2}\right]$	[34,51,105,146]
29	$\left[\frac{1}{2}, \frac{7}{8}, \frac{3}{4}\right]$	[35,68,166,174]
30	$\left[0, \frac{5}{8}, \frac{3}{4}\right]$	[36,41,144,175]
31	$\left[\frac{1}{4}, \frac{1}{2}, \frac{7}{8}\right]$	[39,91,101,143]
32	$\left[\frac{1}{4}, \frac{1}{2}, \frac{5}{8}\right]$	[40,42,100,189]
33	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{8}\right]$	[43,87,149,191]
34	$\left[0, \frac{3}{8}, \frac{3}{4}\right]$	[44,59,102,142]
35	$\left[\frac{3}{4}, \frac{1}{2}, \frac{5}{8}\right]$	[45,52,184,186]
36	$\left[0, \frac{5}{8}, \frac{1}{4}\right]$	[48,79,132,137]
37	$\left[\frac{5}{8}, \frac{1}{4}, \frac{1}{2}\right]$	[49,62,157,176]
38	$\left[\frac{3}{4}, \frac{1}{2}, \frac{7}{8}\right]$	[53,95,139,183]
39	$\left[\frac{1}{2}, \frac{3}{8}, \frac{3}{4}\right]$	[54,94,107,188]
40	$\left[\frac{5}{8}, \frac{3}{4}, \frac{1}{2}\right]$	[56,85,169,182]
41	$\left[\frac{1}{2}, \frac{1}{8}, \frac{3}{4}\right]$	[60,65,103,168]
42	$\left[\frac{5}{8}, \frac{1}{4}, 0\right]$	[61,80,145,158]
43	$\left[\frac{3}{4}, 0, \frac{5}{8}\right]$	[64,66,117,172]
44	$\left[\frac{1}{2}, \frac{7}{8}, \frac{1}{4}\right]$	[70,78,131,164]
45	$\left[\frac{3}{4}, 0, \frac{3}{8}\right]$	[71,77,115,159]
46	$\left[\frac{5}{8}, \frac{3}{4}, 0\right]$	[73,86,152,181]
47	$\left[\frac{1}{2}, \frac{5}{8}, \frac{1}{4}\right]$	[84,89,127,192]
48	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{8}\right]$	[88,90,141,148]

Table 7: Wyckoff site: 64g, site symmetry: .3.

No.	position	mapping
1	$[x, x, x]$	[1,17,18]
2	$\left[x + \frac{1}{4}, \frac{1}{4} - x, x + \frac{1}{4}\right]$	[2,7,15]
3	$\left[x + \frac{1}{4}, x + \frac{1}{4}, \frac{1}{4} - x\right]$	[3,4,11]
4	$\left[\frac{1}{4} - x, x + \frac{1}{4}, x + \frac{1}{4}\right]$	[5,6,13]
5	$[x, -x, -x]$	[8,22,23]
6	$[-x, x, -x]$	[9,19,24]
7	$[-x, -x, x]$	[10,20,21]
8	$\left[\frac{1}{4} - x, \frac{1}{4} - x, \frac{1}{4} - x\right]$	[12,14,16]
9	$\left[x, x + \frac{1}{2}, x + \frac{1}{2}\right]$	[25,41,42]
10	$\left[x + \frac{1}{4}, \frac{3}{4} - x, x + \frac{3}{4}\right]$	[26,31,39]
11	$\left[x + \frac{1}{4}, x + \frac{3}{4}, \frac{3}{4} - x\right]$	[27,28,35]
12	$\left[\frac{1}{4} - x, x + \frac{3}{4}, x + \frac{3}{4}\right]$	[29,30,37]
13	$\left[x, \frac{1}{2} - x, \frac{1}{2} - x\right]$	[32,46,47]

continued ...

Table 7

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

continued ...

Table 7

No.	position	mapping
61	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	`[176,190,191]`
62	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ \frac{1}{2}-x\right]$	`[177,187,192]`
63	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ x+\frac{1}{2}\right]$	`[178,188,189]`
64	$\left[\frac{3}{4}-x,\ \frac{3}{4}-x,\ \frac{3}{4}-x\right]$	`[180,182,184]`

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

No.	position	mapping
1	$[x,\ 0,\ 0]$	`[1,8]`
2	$\left[x+\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	`[2,3]`
3	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}-x\right]$	`[4,16]`
4	$\left[\frac{1}{4},\ \frac{1}{4},\ x+\frac{1}{4}\right]$	`[5,15]`
5	$\left[\frac{1}{4},\ x+\frac{1}{4},\ \frac{1}{4}\right]$	`[6,11]`
6	$\left[\frac{1}{4},\ \frac{1}{4}-x,\ \frac{1}{4}\right]$	`[7,12]`
7	$[-x,\ 0,\ 0]$	`[9,10]`
8	$\left[\frac{1}{4}-x,\ \frac{1}{4},\ \frac{1}{4}\right]$	`[13,14]`
9	$[0,\ x,\ 0]$	`[17,24]`
10	$[0,\ 0,\ x]$	`[18,21]`
11	$[0,\ 0,\ -x]$	`[19,23]`
12	$[0,\ -x,\ 0]$	`[20,22]`
13	$\left[x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[25,32]`
14	$\left[x+\frac{1}{4},\ \frac{3}{4},\ \frac{3}{4}\right]$	`[26,27]`
15	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{3}{4}-x\right]$	`[28,40]`
16	$\left[\frac{1}{4},\ \frac{3}{4},\ x+\frac{3}{4}\right]$	`[29,39]`
17	$\left[\frac{1}{4},\ x+\frac{3}{4},\ \frac{3}{4}\right]$	`[30,35]`
18	$\left[\frac{1}{4},\ \frac{3}{4}-x,\ \frac{3}{4}\right]$	`[31,36]`
19	$\left[-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[33,34]`
20	$\left[\frac{1}{4}-x,\ \frac{3}{4},\ \frac{3}{4}\right]$	`[37,38]`
21	$\left[0,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[41,48]`
22	$\left[0,\ \frac{1}{2},\ x+\frac{1}{2}\right]$	`[42,45]`
23	$\left[0,\ \frac{1}{2},\ \frac{1}{2}-x\right]$	`[43,47]`
24	$\left[0,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[44,46]`
25	$\left[x+\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[49,56]`
26	$\left[x+\frac{3}{4},\ \frac{1}{4},\ \frac{3}{4}\right]$	`[50,51]`
27	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{3}{4}-x\right]$	`[52,64]`
28	$\left[\frac{3}{4},\ \frac{1}{4},\ x+\frac{3}{4}\right]$	`[53,63]`
29	$\left[\frac{3}{4},\ x+\frac{1}{4},\ \frac{3}{4}\right]$	`[54,59]`
30	$\left[\frac{3}{4},\ \frac{1}{4}-x,\ \frac{3}{4}\right]$	`[55,60]`
31	$\left[\frac{1}{2}-x,\ 0,\ \frac{1}{2}\right]$	`[57,58]`
32	$\left[\frac{3}{4}-x,\ \frac{1}{4},\ \frac{3}{4}\right]$	`[61,62]`
33	$\left[\frac{1}{2},\ x,\ \frac{1}{2}\right]$	`[65,72]`
34	$\left[\frac{1}{2},\ 0,\ x+\frac{1}{2}\right]$	`[66,69]`
35	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}-x\right]$	`[67,71]`
36	$\left[\frac{1}{2},\ -x,\ \frac{1}{2}\right]$	`[68,70]`

continued ...

Table 8

No.	position	mapping
37	$\left[x+\frac{1}{2},\ \frac{1}{2},\ 0\right]$	[73,80]
38	$\left[x+\frac{3}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$	[74,75]
39	$\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{4}-x\right]$	[76,88]
40	$\left[\frac{3}{4},\ \frac{3}{4},\ x+\frac{1}{4}\right]$	[77,87]
41	$\left[\frac{3}{4},\ x+\frac{3}{4},\ \frac{1}{4}\right]$	[78,83]
42	$\left[\frac{3}{4},\ \frac{3}{4}-x,\ \frac{1}{4}\right]$	[79,84]
43	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ 0\right]$	[81,82]
44	$\left[\frac{3}{4}-x,\ \frac{3}{4},\ \frac{1}{4}\right]$	[85,86]
45	$\left[\frac{1}{2},\ x+\frac{1}{2},\ 0\right]$	[89,96]
46	$\left[\frac{1}{2},\ \frac{1}{2},\ x\right]$	[90,93]
47	$\left[\frac{1}{2},\ \frac{1}{2},\ -x\right]$	[91,95]
48	$\left[\frac{1}{2},\ \frac{1}{2}-x,\ 0\right]$	[92,94]
49	$\left[x,\ 0,\ \frac{1}{2}\right]$	[97,104]
50	$\left[x+\frac{1}{4},\ \frac{1}{4},\ \frac{3}{4}\right]$	[98,99]
51	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{3}{4}-x\right]$	[100,112]
52	$\left[\frac{1}{4},\ \frac{1}{4},\ x+\frac{3}{4}\right]$	[101,111]
53	$\left[\frac{1}{4},\ x+\frac{1}{4},\ \frac{3}{4}\right]$	[102,107]
54	$\left[\frac{1}{4},\ \frac{1}{4}-x,\ \frac{3}{4}\right]$	[103,108]
55	$\left[-x,\ 0,\ \frac{1}{2}\right]$	[105,106]
56	$\left[\frac{1}{4}-x,\ \frac{1}{4},\ \frac{3}{4}\right]$	[109,110]
57	$\left[0,\ x,\ \frac{1}{2}\right]$	[113,120]
58	$\left[0,\ 0,\ x+\frac{1}{2}\right]$	[114,117]
59	$\left[0,\ 0,\ \frac{1}{2}-x\right]$	[115,119]
60	$\left[0,\ -x,\ \frac{1}{2}\right]$	[116,118]
61	$\left[x,\ \frac{1}{2},\ 0\right]$	[121,128]
62	$\left[x+\frac{1}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$	[122,123]
63	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{4}-x\right]$	[124,136]
64	$\left[\frac{1}{4},\ \frac{3}{4},\ x+\frac{1}{4}\right]$	[125,135]
65	$\left[\frac{1}{4},\ x+\frac{3}{4},\ \frac{1}{4}\right]$	[126,131]
66	$\left[\frac{1}{4},\ \frac{3}{4}-x,\ \frac{1}{4}\right]$	[127,132]
67	$\left[-x,\ \frac{1}{2},\ 0\right]$	[129,130]
68	$\left[\frac{1}{4}-x,\ \frac{3}{4},\ \frac{1}{4}\right]$	[133,134]
69	$\left[0,\ x+\frac{1}{2},\ 0\right]$	[137,144]
70	$\left[0,\ \frac{1}{2},\ x\right]$	[138,141]
71	$\left[0,\ \frac{1}{2},\ -x\right]$	[139,143]
72	$\left[0,\ \frac{1}{2}-x,\ 0\right]$	[140,142]
73	$\left[x+\frac{1}{2},\ 0,\ 0\right]$	[145,152]
74	$\left[x+\frac{3}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	[146,147]
75	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{4}-x\right]$	[148,160]
76	$\left[\frac{3}{4},\ \frac{1}{4},\ x+\frac{1}{4}\right]$	[149,159]
77	$\left[\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{4}\right]$	[150,155]
78	$\left[\frac{3}{4},\ \frac{1}{4}-x,\ \frac{1}{4}\right]$	[151,156]
79	$\left[\frac{1}{2}-x,\ 0,\ 0\right]$	[153,154]
80	$\left[\frac{3}{4}-x,\ \frac{1}{4},\ \frac{1}{4}\right]$	[157,158]
81	$\left[\frac{1}{2},\ x,\ 0\right]$	[161,168]
82	$\left[\frac{1}{2},\ 0,\ x\right]$	[162,165]
83	$\left[\frac{1}{2},\ 0,\ -x\right]$	[163,167]

continued ...

Table 8

No.	position	mapping
84	$\left[\frac{1}{2}, -x, 0\right]$	[164,166]
85	$\left[x+\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[169,176]
86	$\left[x+\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[170,171]
87	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}-x\right]$	[172,184]
88	$\left[\frac{3}{4}, \frac{3}{4}, x+\frac{3}{4}\right]$	[173,183]
89	$\left[\frac{3}{4}, x+\frac{3}{4}, \frac{3}{4}\right]$	[174,179]
90	$\left[\frac{3}{4}, \frac{3}{4}-x, \frac{3}{4}\right]$	[175,180]
91	$\left[\frac{1}{2}-x, \frac{1}{2}, \frac{1}{2}\right]$	[177,178]
92	$\left[\frac{3}{4}-x, \frac{3}{4}, \frac{3}{4}\right]$	[181,182]
93	$\left[\frac{1}{2}, x+\frac{1}{2}, \frac{1}{2}\right]$	[185,192]
94	$\left[\frac{1}{2}, \frac{1}{2}, x+\frac{1}{2}\right]$	[186,189]
95	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}-x\right]$	[187,191]
96	$\left[\frac{1}{2}, \frac{1}{2}-x, \frac{1}{2}\right]$	[188,190]

Table 9: Wyckoff site: 96i, site symmetry: 2'..

No.	position	mapping
1	$\left[x, 0, \frac{1}{4}\right]$	[1,104]
2	$\left[x+\frac{1}{4}, 0, \frac{1}{4}\right]$	[2,123]
3	$\left[x+\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[3,122]
4	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}-x\right]$	[4,160]
5	$\left[0, \frac{1}{4}, x+\frac{1}{4}\right]$	[5,159]
6	$\left[\frac{1}{4}, x+\frac{1}{4}, \frac{1}{2}\right]$	[6,107]
7	$\left[\frac{1}{4}, \frac{1}{4}-x, \frac{1}{2}\right]$	[7,108]
8	$\left[x, 0, \frac{3}{4}\right]$	[8,97]
9	$\left[-x, 0, \frac{3}{4}\right]$	[9,106]
10	$\left[-x, 0, \frac{1}{4}\right]$	[10,105]
11	$\left[\frac{1}{4}, x+\frac{1}{4}, 0\right]$	[11,102]
12	$\left[\frac{1}{4}, \frac{1}{4}-x, 0\right]$	[12,103]
13	$\left[\frac{1}{4}-x, \frac{1}{2}, \frac{1}{4}\right]$	[13,134]
14	$\left[\frac{1}{4}-x, 0, \frac{1}{4}\right]$	[14,133]
15	$\left[\frac{1}{2}, \frac{1}{4}, x+\frac{1}{4}\right]$	[15,149]
16	$\left[0, \frac{1}{4}, \frac{1}{4}-x\right]$	[16,148]
17	$\left[\frac{1}{4}, x, 0\right]$	[17,168]
18	$\left[0, \frac{1}{4}, x\right]$	[18,141]
19	$\left[0, \frac{1}{4}, -x\right]$	[19,143]
20	$\left[\frac{3}{4}, -x, 0\right]$	[20,166]
21	$\left[0, \frac{3}{4}, x\right]$	[21,138]
22	$\left[\frac{1}{4}, -x, 0\right]$	[22,164]
23	$\left[0, \frac{3}{4}, -x\right]$	[23,139]
24	$\left[\frac{3}{4}, x, 0\right]$	[24,161]
25	$\left[x, \frac{1}{2}, \frac{3}{4}\right]$	[25,128]
26	$\left[x+\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[26,99]
27	$\left[x+\frac{1}{4}, 0, \frac{3}{4}\right]$	[27,98]

continued ...

Table 9

No.	position	mapping
28	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{4} - x\right]$	[28,184]
29	$\left[0, \frac{3}{4}, x + \frac{3}{4}\right]$	[29,183]
30	$\left[\frac{1}{4}, x + \frac{3}{4}, 0\right]$	[30,131]
31	$\left[\frac{1}{4}, \frac{3}{4} - x, 0\right]$	[31,132]
32	$\left[x, \frac{1}{2}, \frac{1}{4}\right]$	[32,121]
33	$\left[-x, \frac{1}{2}, \frac{1}{4}\right]$	[33,130]
34	$\left[-x, \frac{1}{2}, \frac{3}{4}\right]$	[34,129]
35	$\left[\frac{1}{4}, x + \frac{3}{4}, \frac{1}{2}\right]$	[35,126]
36	$\left[\frac{1}{4}, \frac{3}{4} - x, \frac{1}{2}\right]$	[36,127]
37	$\left[\frac{1}{4} - x, 0, \frac{3}{4}\right]$	[37,110]
38	$\left[\frac{1}{4} - x, \frac{1}{2}, \frac{3}{4}\right]$	[38,109]
39	$\left[\frac{1}{2}, \frac{3}{4}, x + \frac{3}{4}\right]$	[39,173]
40	$\left[0, \frac{3}{4}, \frac{3}{4} - x\right]$	[40,172]
41	$\left[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{2}\right]$	[41,192]
42	$\left[0, \frac{3}{4}, x + \frac{1}{2}\right]$	[42,117]
43	$\left[0, \frac{3}{4}, \frac{1}{2} - x\right]$	[43,119]
44	$\left[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{2}\right]$	[44,190]
45	$\left[0, \frac{1}{4}, x + \frac{1}{2}\right]$	[45,114]
46	$\left[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{2}\right]$	[46,188]
47	$\left[0, \frac{1}{4}, \frac{1}{2} - x\right]$	[47,115]
48	$\left[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{2}\right]$	[48,185]
49	$\left[x + \frac{1}{2}, 0, \frac{3}{4}\right]$	[49,152]
50	$\left[x + \frac{3}{4}, 0, \frac{3}{4}\right]$	[50,171]
51	$\left[x + \frac{3}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[51,170]
52	$\left[0, \frac{1}{4}, \frac{3}{4} - x\right]$	[52,112]
53	$\left[\frac{1}{2}, \frac{1}{4}, x + \frac{3}{4}\right]$	[53,111]
54	$\left[\frac{3}{4}, x + \frac{1}{4}, 0\right]$	[54,155]
55	$\left[\frac{3}{4}, \frac{1}{4} - x, 0\right]$	[55,156]
56	$\left[x + \frac{1}{2}, 0, \frac{1}{4}\right]$	[56,145]
57	$\left[\frac{1}{2} - x, 0, \frac{1}{4}\right]$	[57,154]
58	$\left[\frac{1}{2} - x, 0, \frac{3}{4}\right]$	[58,153]
59	$\left[\frac{3}{4}, x + \frac{1}{4}, \frac{1}{2}\right]$	[59,150]
60	$\left[\frac{3}{4}, \frac{1}{4} - x, \frac{1}{2}\right]$	[60,151]
61	$\left[\frac{3}{4} - x, \frac{1}{2}, \frac{3}{4}\right]$	[61,182]
62	$\left[\frac{3}{4} - x, 0, \frac{3}{4}\right]$	[62,181]
63	$\left[0, \frac{1}{4}, x + \frac{3}{4}\right]$	[63,101]
64	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4} - x\right]$	[64,100]
65	$\left[\frac{3}{4}, x, \frac{1}{2}\right]$	[65,120]
66	$\left[\frac{1}{2}, \frac{1}{4}, x + \frac{1}{2}\right]$	[66,189]
67	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{2} - x\right]$	[67,191]
68	$\left[\frac{1}{4}, -x, \frac{1}{2}\right]$	[68,118]
69	$\left[\frac{1}{2}, \frac{3}{4}, x + \frac{1}{2}\right]$	[69,186]
70	$\left[\frac{3}{4}, -x, \frac{1}{2}\right]$	[70,116]
71	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{2} - x\right]$	[71,187]
72	$\left[\frac{1}{4}, x, \frac{1}{2}\right]$	[72,113]
73	$\left[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[73,176]
74	$\left[x + \frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[74,147]

continued ...

Table 9

No.	position	mapping
75	$\left[x+\frac{3}{4}, 0, \frac{1}{4}\right]$	[75,146]
76	$\left[0, \frac{3}{4}, \frac{1}{4}-x\right]$	[76,136]
77	$\left[\frac{1}{2}, \frac{3}{4}, x+\frac{1}{4}\right]$	[77,135]
78	$\left[\frac{3}{4}, x+\frac{3}{4}, \frac{1}{2}\right]$	[78,179]
79	$\left[\frac{3}{4}, \frac{3}{4}-x, \frac{1}{2}\right]$	[79,180]
80	$\left[x+\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	[80,169]
81	$\left[\frac{1}{2}-x, \frac{1}{2}, \frac{3}{4}\right]$	[81,178]
82	$\left[\frac{1}{2}-x, \frac{1}{2}, \frac{1}{4}\right]$	[82,177]
83	$\left[\frac{3}{4}, x+\frac{3}{4}, 0\right]$	[83,174]
84	$\left[\frac{3}{4}, \frac{3}{4}-x, 0\right]$	[84,175]
85	$\left[\frac{3}{4}-x, 0, \frac{1}{4}\right]$	[85,158]
86	$\left[\frac{3}{4}-x, \frac{1}{2}, \frac{1}{4}\right]$	[86,157]
87	$\left[0, \frac{3}{4}, x+\frac{1}{4}\right]$	[87,125]
88	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}-x\right]$	[88,124]
89	$\left[\frac{3}{4}, x+\frac{1}{2}, 0\right]$	[89,144]
90	$\left[\frac{1}{2}, \frac{3}{4}, x\right]$	[90,165]
91	$\left[\frac{1}{2}, \frac{3}{4}, -x\right]$	[91,167]
92	$\left[\frac{1}{4}, \frac{1}{2}-x, 0\right]$	[92,142]
93	$\left[\frac{1}{2}, \frac{1}{4}, x\right]$	[93,162]
94	$\left[\frac{3}{4}, \frac{1}{2}-x, 0\right]$	[94,140]
95	$\left[\frac{1}{2}, \frac{1}{4}, -x\right]$	[95,163]
96	$\left[\frac{1}{4}, x+\frac{1}{2}, 0\right]$	[96,137]

Table 10: Wyckoff site: 96j, site symmetry: 2'..

No.	position	mapping
1	$\left[x, \frac{1}{4}, 0\right]$	[1,128]
2	$\left[x+\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[2,99]
3	$\left[x+\frac{1}{4}, \frac{1}{4}, 0\right]$	[3,98]
4	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}-x\right]$	[4,136]
5	$\left[\frac{1}{4}, \frac{1}{2}, x+\frac{1}{4}\right]$	[5,135]
6	$\left[0, x+\frac{1}{4}, \frac{1}{4}\right]$	[6,155]
7	$\left[\frac{1}{2}, \frac{1}{4}-x, \frac{1}{4}\right]$	[7,156]
8	$\left[x, \frac{3}{4}, 0\right]$	[8,121]
9	$\left[-x, \frac{1}{4}, 0\right]$	[9,130]
10	$\left[-x, \frac{3}{4}, 0\right]$	[10,129]
11	$\left[\frac{1}{2}, x+\frac{1}{4}, \frac{1}{4}\right]$	[11,150]
12	$\left[0, \frac{1}{4}-x, \frac{1}{4}\right]$	[12,151]
13	$\left[\frac{1}{4}-x, \frac{1}{4}, \frac{1}{2}\right]$	[13,110]
14	$\left[\frac{1}{4}-x, \frac{1}{4}, 0\right]$	[14,109]
15	$\left[\frac{1}{4}, 0, x+\frac{1}{4}\right]$	[15,125]
16	$\left[\frac{1}{4}, 0, \frac{1}{4}-x\right]$	[16,124]
17	$\left[0, x, \frac{1}{4}\right]$	[17,120]
18	$\left[\frac{1}{4}, 0, x\right]$	[18,165]

continued ...

Table 10

No.	position	mapping
19	$\left[\frac{3}{4}, 0, -x\right]$	[19,167]
20	$\left[0, -x, \frac{1}{4}\right]$	[20,118]
21	$\left[\frac{3}{4}, 0, x\right]$	[21,162]
22	$\left[0, -x, \frac{3}{4}\right]$	[22,116]
23	$\left[\frac{1}{4}, 0, -x\right]$	[23,163]
24	$\left[0, x, \frac{3}{4}\right]$	[24,113]
25	$\left[x, \frac{3}{4}, \frac{1}{2}\right]$	[25,104]
26	$\left[x+\frac{1}{4}, \frac{3}{4}, 0\right]$	[26,123]
27	$\left[x+\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[27,122]
28	$\left[\frac{1}{4}, 0, \frac{3}{4}-x\right]$	[28,112]
29	$\left[\frac{1}{4}, 0, x+\frac{3}{4}\right]$	[29,111]
30	$\left[0, x+\frac{3}{4}, \frac{3}{4}\right]$	[30,179]
31	$\left[\frac{1}{2}, \frac{3}{4}-x, \frac{3}{4}\right]$	[31,180]
32	$\left[x, \frac{1}{4}, \frac{1}{2}\right]$	[32,97]
33	$\left[-x, \frac{3}{4}, \frac{1}{2}\right]$	[33,106]
34	$\left[-x, \frac{1}{4}, \frac{1}{2}\right]$	[34,105]
35	$\left[\frac{1}{2}, x+\frac{3}{4}, \frac{3}{4}\right]$	[35,174]
36	$\left[0, \frac{3}{4}-x, \frac{3}{4}\right]$	[36,175]
37	$\left[\frac{1}{4}-x, \frac{3}{4}, 0\right]$	[37,134]
38	$\left[\frac{1}{4}-x, \frac{3}{4}, \frac{1}{2}\right]$	[38,133]
39	$\left[\frac{1}{4}, \frac{1}{2}, x+\frac{3}{4}\right]$	[39,101]
40	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}-x\right]$	[40,100]
41	$\left[0, x+\frac{1}{2}, \frac{3}{4}\right]$	[41,144]
42	$\left[\frac{1}{4}, \frac{1}{2}, x+\frac{1}{2}\right]$	[42,189]
43	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}-x\right]$	[43,191]
44	$\left[0, \frac{1}{2}-x, \frac{3}{4}\right]$	[44,142]
45	$\left[\frac{3}{4}, \frac{1}{2}, x+\frac{1}{2}\right]$	[45,186]
46	$\left[0, \frac{1}{2}-x, \frac{1}{4}\right]$	[46,140]
47	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}-x\right]$	[47,187]
48	$\left[0, x+\frac{1}{2}, \frac{1}{4}\right]$	[48,137]
49	$\left[x+\frac{1}{2}, \frac{1}{4}, \frac{1}{2}\right]$	[49,176]
50	$\left[x+\frac{3}{4}, \frac{1}{4}, 0\right]$	[50,147]
51	$\left[x+\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[51,146]
52	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}-x\right]$	[52,184]
53	$\left[\frac{3}{4}, \frac{1}{2}, x+\frac{3}{4}\right]$	[53,183]
54	$\left[\frac{1}{2}, x+\frac{1}{4}, \frac{3}{4}\right]$	[54,107]
55	$\left[0, \frac{1}{4}-x, \frac{3}{4}\right]$	[55,108]
56	$\left[x+\frac{1}{2}, \frac{3}{4}, \frac{1}{2}\right]$	[56,169]
57	$\left[\frac{1}{2}-x, \frac{1}{4}, \frac{1}{2}\right]$	[57,178]
58	$\left[\frac{1}{2}-x, \frac{3}{4}, \frac{1}{2}\right]$	[58,177]
59	$\left[0, x+\frac{1}{4}, \frac{3}{4}\right]$	[59,102]
60	$\left[\frac{1}{2}, \frac{1}{4}-x, \frac{3}{4}\right]$	[60,103]
61	$\left[\frac{3}{4}-x, \frac{1}{4}, 0\right]$	[61,158]
62	$\left[\frac{3}{4}-x, \frac{1}{4}, \frac{1}{2}\right]$	[62,157]
63	$\left[\frac{3}{4}, 0, x+\frac{3}{4}\right]$	[63,173]
64	$\left[\frac{3}{4}, 0, \frac{3}{4}-x\right]$	[64,172]
65	$\left[\frac{1}{2}, x, \frac{3}{4}\right]$	[65,168]

continued ...

Table 10

No.	position	mapping
66	$\left[\frac{3}{4}, 0, x+\frac{1}{2}\right]$	[66,117]
67	$\left[\frac{1}{4}, 0, \frac{1}{2}-x\right]$	[67,119]
68	$\left[\frac{1}{2}, -x, \frac{3}{4}\right]$	[68,166]
69	$\left[\frac{1}{4}, 0, x+\frac{1}{2}\right]$	[69,114]
70	$\left[\frac{1}{2}, -x, \frac{1}{4}\right]$	[70,164]
71	$\left[\frac{3}{4}, 0, \frac{1}{2}-x\right]$	[71,115]
72	$\left[\frac{1}{2}, x, \frac{1}{4}\right]$	[72,161]
73	$\left[x+\frac{1}{2}, \frac{3}{4}, 0\right]$	[73,152]
74	$\left[x+\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[74,171]
75	$\left[x+\frac{3}{4}, \frac{3}{4}, 0\right]$	[75,170]
76	$\left[\frac{3}{4}, 0, \frac{1}{4}-x\right]$	[76,160]
77	$\left[\frac{3}{4}, 0, x+\frac{1}{4}\right]$	[77,159]
78	$\left[\frac{1}{2}, x+\frac{3}{4}, \frac{1}{4}\right]$	[78,131]
79	$\left[0, \frac{3}{4}-x, \frac{1}{4}\right]$	[79,132]
80	$\left[x+\frac{1}{2}, \frac{1}{4}, 0\right]$	[80,145]
81	$\left[\frac{1}{2}-x, \frac{3}{4}, 0\right]$	[81,154]
82	$\left[\frac{1}{2}-x, \frac{1}{4}, 0\right]$	[82,153]
83	$\left[0, x+\frac{3}{4}, \frac{1}{4}\right]$	[83,126]
84	$\left[\frac{1}{2}, \frac{3}{4}-x, \frac{1}{4}\right]$	[84,127]
85	$\left[\frac{3}{4}-x, \frac{3}{4}, \frac{1}{2}\right]$	[85,182]
86	$\left[\frac{3}{4}-x, \frac{3}{4}, 0\right]$	[86,181]
87	$\left[\frac{3}{4}, \frac{1}{2}, x+\frac{1}{4}\right]$	[87,149]
88	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}-x\right]$	[88,148]
89	$\left[\frac{1}{2}, x+\frac{1}{2}, \frac{1}{4}\right]$	[89,192]
90	$\left[\frac{3}{4}, \frac{1}{2}, x\right]$	[90,141]
91	$\left[\frac{1}{4}, \frac{1}{2}, -x\right]$	[91,143]
92	$\left[\frac{1}{2}, \frac{1}{2}-x, \frac{1}{4}\right]$	[92,190]
93	$\left[\frac{1}{4}, \frac{1}{2}, x\right]$	[93,138]
94	$\left[\frac{1}{2}, \frac{1}{2}-x, \frac{3}{4}\right]$	[94,188]
95	$\left[\frac{3}{4}, \frac{1}{2}, -x\right]$	[95,139]
96	$\left[\frac{1}{2}, x+\frac{1}{2}, \frac{3}{4}\right]$	[96,185]

Table 11: Wyckoff site: 96k, site symmetry: ..2

No.	position	mapping
1	$\left[\frac{1}{8}, y, \frac{1}{4}-y\right]$	[1,14]
2	$\left[\frac{3}{8}, y, y+\frac{1}{4}\right]$	[2,57]
3	$\left[\frac{3}{8}, \frac{1}{2}-y, \frac{1}{4}-y\right]$	[3,82]
4	$\left[\frac{1}{2}-y, y+\frac{1}{4}, \frac{1}{8}\right]$	[4,93]
5	$\left[y, y+\frac{1}{4}, \frac{3}{8}\right]$	[5,47]
6	$\left[\frac{1}{4}-y, \frac{3}{8}, \frac{1}{2}-y\right]$	[6,46]
7	$\left[y+\frac{1}{4}, \frac{1}{8}, \frac{1}{2}-y\right]$	[7,72]
8	$\left[\frac{1}{8}, -y, y+\frac{3}{4}\right]$	[8,37]
9	$\left[\frac{7}{8}, y, y+\frac{3}{4}\right]$	[9,50]

continued ...

Table 11

No.	position	mapping
10	$\left[\frac{7}{8},\ -y,\ \frac{1}{4}-y\right]$	[10,75]
11	$\left[y+\frac{1}{4},\ \frac{3}{8},\ y\right]$	[11,92]
12	$\left[\frac{1}{4}-y,\ \frac{1}{8},\ y\right]$	[12,17]
13	$\left[\frac{1}{8},\ \frac{1}{2}-y,\ y+\frac{1}{4}\right]$	[13,32]
14	$\left[\frac{1}{2}-y,\ \frac{1}{4}-y,\ \frac{3}{8}\right]$	[15,67]
15	$\left[y,\ \frac{1}{4}-y,\ \frac{1}{8}\right]$	[16,18]
16	$\left[-y,\ \frac{1}{4}-y,\ \frac{7}{8}\right]$	[19,63]
17	$\left[y+\frac{3}{4},\ \frac{7}{8},\ y\right]$	[20,83]
18	$\left[-y,\ y+\frac{3}{4},\ \frac{1}{8}\right]$	[21,76]
19	$\left[\frac{1}{4}-y,\ \frac{7}{8},\ -y\right]$	[22,30]
20	$\left[y,\ y+\frac{3}{4},\ \frac{7}{8}\right]$	[23,29]
21	$\left[y+\frac{3}{4},\ \frac{1}{8},\ -y\right]$	[24,55]
22	$\left[\frac{1}{8},\ y+\frac{1}{2},\ \frac{3}{4}-y\right]$	[25,38]
23	$\left[\frac{3}{8},\ y+\frac{1}{2},\ y+\frac{3}{4}\right]$	[26,81]
24	$\left[\frac{3}{8},\ -y,\ \frac{3}{4}-y\right]$	[27,58]
25	$\left[\frac{1}{2}-y,\ y+\frac{3}{4},\ \frac{5}{8}\right]$	[28,69]
26	$\left[y+\frac{1}{4},\ \frac{5}{8},\ -y\right]$	[31,96]
27	$\left[\frac{7}{8},\ y+\frac{1}{2},\ y+\frac{1}{4}\right]$	[33,74]
28	$\left[\frac{7}{8},\ \frac{1}{2}-y,\ \frac{3}{4}-y\right]$	[34,51]
29	$\left[y+\frac{1}{4},\ \frac{7}{8},\ y+\frac{1}{2}\right]$	[35,68]
30	$\left[\frac{1}{4}-y,\ \frac{5}{8},\ y+\frac{1}{2}\right]$	[36,41]
31	$\left[\frac{1}{2}-y,\ \frac{3}{4}-y,\ \frac{7}{8}\right]$	[39,91]
32	$\left[y,\ \frac{3}{4}-y,\ \frac{5}{8}\right]$	[40,42]
33	$\left[-y,\ \frac{3}{4}-y,\ \frac{3}{8}\right]$	[43,87]
34	$\left[y+\frac{3}{4},\ \frac{3}{8},\ y+\frac{1}{2}\right]$	[44,59]
35	$\left[-y,\ y+\frac{1}{4},\ \frac{5}{8}\right]$	[45,52]
36	$\left[y+\frac{3}{4},\ \frac{5}{8},\ \frac{1}{2}-y\right]$	[48,79]
37	$\left[\frac{5}{8},\ y,\ \frac{3}{4}-y\right]$	[49,62]
38	$\left[y+\frac{1}{2},\ y+\frac{1}{4},\ \frac{7}{8}\right]$	[53,95]
39	$\left[\frac{3}{4}-y,\ \frac{3}{8},\ -y\right]$	[54,94]
40	$\left[\frac{5}{8},\ -y,\ y+\frac{1}{4}\right]$	[56,85]
41	$\left[\frac{3}{4}-y,\ \frac{1}{8},\ y+\frac{1}{2}\right]$	[60,65]
42	$\left[\frac{5}{8},\ \frac{1}{2}-y,\ y+\frac{3}{4}\right]$	[61,80]
43	$\left[y+\frac{1}{2},\ \frac{1}{4}-y,\ \frac{5}{8}\right]$	[64,66]
44	$\left[\frac{3}{4}-y,\ \frac{7}{8},\ \frac{1}{2}-y\right]$	[70,78]
45	$\left[y+\frac{1}{2},\ y+\frac{3}{4},\ \frac{3}{8}\right]$	[71,77]
46	$\left[\frac{5}{8},\ y+\frac{1}{2},\ \frac{1}{4}-y\right]$	[73,86]
47	$\left[\frac{3}{4}-y,\ \frac{5}{8},\ y\right]$	[84,89]
48	$\left[y+\frac{1}{2},\ \frac{3}{4}-y,\ \frac{1}{8}\right]$	[88,90]
49	$\left[\frac{1}{8},\ y,\ \frac{3}{4}-y\right]$	[97,110]
50	$\left[\frac{3}{8},\ y,\ y+\frac{3}{4}\right]$	[98,153]
51	$\left[\frac{3}{8},\ \frac{1}{2}-y,\ \frac{3}{4}-y\right]$	[99,178]
52	$\left[\frac{1}{2}-y,\ y+\frac{1}{4},\ \frac{5}{8}\right]$	[100,189]
53	$\left[y,\ y+\frac{1}{4},\ \frac{7}{8}\right]$	[101,143]
54	$\left[\frac{1}{4}-y,\ \frac{3}{8},\ -y\right]$	[102,142]
55	$\left[y+\frac{1}{4},\ \frac{1}{8},\ -y\right]$	[103,168]
56	$\left[\frac{1}{8},\ -y,\ y+\frac{1}{4}\right]$	[104,133]

continued ...

Table 11

No.	position	mapping
57	$\left[\frac{7}{8},\ y,\ y+\frac{1}{4}\right]$	[105,146]
58	$\left[\frac{7}{8},\ -y,\ \frac{3}{4}-y\right]$	[106,171]
59	$\left[y+\frac{1}{4},\ \frac{3}{8},\ y+\frac{1}{2}\right]$	[107,188]
60	$\left[\frac{1}{4}-y,\ \frac{1}{8},\ y+\frac{1}{2}\right]$	[108,113]
61	$\left[\frac{1}{8},\ \frac{1}{2}-y,\ y+\frac{3}{4}\right]$	[109,128]
62	$\left[\frac{1}{2}-y,\ \frac{1}{4}-y,\ \frac{7}{8}\right]$	[111,163]
63	$\left[y,\ \frac{1}{4}-y,\ \frac{5}{8}\right]$	[112,114]
64	$\left[-y,\ \frac{1}{4}-y,\ \frac{3}{8}\right]$	[115,159]
65	$\left[y+\frac{3}{4},\ \frac{7}{8},\ y+\frac{1}{2}\right]$	[116,179]
66	$\left[-y,\ y+\frac{3}{4},\ \frac{5}{8}\right]$	[117,172]
67	$\left[\frac{1}{4}-y,\ \frac{7}{8},\ \frac{1}{2}-y\right]$	[118,126]
68	$\left[y,\ y+\frac{3}{4},\ \frac{3}{8}\right]$	[119,125]
69	$\left[y+\frac{3}{4},\ \frac{1}{8},\ \frac{1}{2}-y\right]$	[120,151]
70	$\left[\frac{1}{8},\ y+\frac{1}{2},\ \frac{1}{4}-y\right]$	[121,134]
71	$\left[\frac{3}{8},\ y+\frac{1}{2},\ y+\frac{1}{4}\right]$	[122,177]
72	$\left[\frac{3}{8},\ -y,\ \frac{1}{4}-y\right]$	[123,154]
73	$\left[\frac{1}{2}-y,\ y+\frac{3}{4},\ \frac{1}{8}\right]$	[124,165]
74	$\left[y+\frac{1}{4},\ \frac{5}{8},\ \frac{1}{2}-y\right]$	[127,192]
75	$\left[\frac{7}{8},\ y+\frac{1}{2},\ y+\frac{3}{4}\right]$	[129,170]
76	$\left[\frac{7}{8},\ \frac{1}{2}-y,\ \frac{1}{4}-y\right]$	[130,147]
77	$\left[y+\frac{1}{4},\ \frac{7}{8},\ y\right]$	[131,164]
78	$\left[\frac{1}{4}-y,\ \frac{5}{8},\ y\right]$	[132,137]
79	$\left[\frac{1}{2}-y,\ \frac{3}{4}-y,\ \frac{3}{8}\right]$	[135,187]
80	$\left[y,\ \frac{3}{4}-y,\ \frac{1}{8}\right]$	[136,138]
81	$\left[-y,\ \frac{3}{4}-y,\ \frac{7}{8}\right]$	[139,183]
82	$\left[y+\frac{3}{4},\ \frac{3}{8},\ y\right]$	[140,155]
83	$\left[-y,\ y+\frac{1}{4},\ \frac{1}{8}\right]$	[141,148]
84	$\left[y+\frac{3}{4},\ \frac{5}{8},\ -y\right]$	[144,175]
85	$\left[\frac{5}{8},\ y,\ \frac{1}{4}-y\right]$	[145,158]
86	$\left[y+\frac{1}{2},\ y+\frac{1}{4},\ \frac{3}{8}\right]$	[149,191]
87	$\left[\frac{3}{4}-y,\ \frac{3}{8},\ \frac{1}{2}-y\right]$	[150,190]
88	$\left[\frac{5}{8},\ -y,\ y+\frac{3}{4}\right]$	[152,181]
89	$\left[\frac{3}{4}-y,\ \frac{1}{8},\ y\right]$	[156,161]
90	$\left[\frac{5}{8},\ \frac{1}{2}-y,\ y+\frac{1}{4}\right]$	[157,176]
91	$\left[y+\frac{1}{2},\ \frac{1}{4}-y,\ \frac{1}{8}\right]$	[160,162]
92	$\left[\frac{3}{4}-y,\ \frac{7}{8},\ -y\right]$	[166,174]
93	$\left[y+\frac{1}{2},\ y+\frac{3}{4},\ \frac{7}{8}\right]$	[167,173]
94	$\left[\frac{5}{8},\ y+\frac{1}{2},\ \frac{3}{4}-y\right]$	[169,182]
95	$\left[\frac{3}{4}-y,\ \frac{5}{8},\ y+\frac{1}{2}\right]$	[180,185]
96	$\left[y+\frac{1}{2},\ \frac{3}{4}-y,\ \frac{5}{8}\right]$	[184,186]

Table 12: Wyckoff site: `96l`, site symmetry: `..2'`

No.	position	mapping
1	$\left[\frac{1}{8}, y, y+\frac{1}{4}\right]$	[1,133]
2	$\left[\frac{3}{8}, -y, y+\frac{1}{4}\right]$	[2,154]
3	$\left[\frac{3}{8}, y+\frac{1}{2}, \frac{1}{4}-y\right]$	[3,177]
4	$\left[y+\frac{1}{2}, y+\frac{1}{4}, \frac{1}{8}\right]$	[4,162]
5	$\left[-y, y+\frac{1}{4}, \frac{3}{8}\right]$	[5,115]
6	$\left[\frac{1}{4}-y, \frac{3}{8}, y+\frac{1}{2}\right]$	[6,188]
7	$\left[y+\frac{1}{4}, \frac{1}{8}, y+\frac{1}{2}\right]$	[7,113]
8	$\left[\frac{1}{8}, -y, \frac{3}{4}-y\right]$	[8,110]
9	$\left[\frac{7}{8}, y, \frac{3}{4}-y\right]$	[9,171]
10	$\left[\frac{7}{8}, -y, y+\frac{1}{4}\right]$	[10,146]
11	$\left[y+\frac{1}{4}, \frac{3}{8}, -y\right]$	[11,142]
12	$\left[\frac{1}{4}-y, \frac{1}{8}, -y\right]$	[12,168]
13	$\left[\frac{1}{8}, y+\frac{1}{2}, y+\frac{1}{4}\right]$	[13,121]
14	$\left[\frac{1}{8}, -y, \frac{1}{4}-y\right]$	[14,104]
15	$\left[y+\frac{1}{2}, \frac{1}{4}-y, \frac{3}{8}\right]$	[15,191]
16	$\left[-y, \frac{1}{4}-y, \frac{1}{8}\right]$	[16,141]
17	$\left[y+\frac{1}{4}, \frac{1}{8}, y\right]$	[17,103]
18	$\left[y, y+\frac{1}{4}, \frac{1}{8}\right]$	[18,148]
19	$\left[-y, y+\frac{1}{4}, \frac{7}{8}\right]$	[19,101]
20	$\left[\frac{3}{4}-y, \frac{7}{8}, y\right]$	[20,174]
21	$\left[-y, \frac{3}{4}-y, \frac{1}{8}\right]$	[21,136]
22	$\left[y+\frac{1}{4}, \frac{7}{8}, -y\right]$	[22,131]
23	$\left[y, \frac{3}{4}-y, \frac{7}{8}\right]$	[23,183]
24	$\left[\frac{3}{4}-y, \frac{1}{8}, -y\right]$	[24,156]
25	$\left[\frac{1}{8}, y+\frac{1}{2}, y+\frac{3}{4}\right]$	[25,109]
26	$\left[\frac{3}{8}, \frac{1}{2}-y, y+\frac{3}{4}\right]$	[26,178]
27	$\left[\frac{3}{8}, y, \frac{3}{4}-y\right]$	[27,153]
28	$\left[y+\frac{1}{2}, y+\frac{3}{4}, \frac{5}{8}\right]$	[28,186]
29	$\left[-y, y+\frac{3}{4}, \frac{7}{8}\right]$	[29,139]
30	$\left[\frac{1}{4}-y, \frac{7}{8}, y\right]$	[30,164]
31	$\left[y+\frac{1}{4}, \frac{5}{8}, y\right]$	[31,137]
32	$\left[\frac{1}{8}, \frac{1}{2}-y, \frac{1}{4}-y\right]$	[32,134]
33	$\left[\frac{7}{8}, y+\frac{1}{2}, \frac{1}{4}-y\right]$	[33,147]
34	$\left[\frac{7}{8}, \frac{1}{2}-y, y+\frac{3}{4}\right]$	[34,170]
35	$\left[y+\frac{1}{4}, \frac{7}{8}, \frac{1}{2}-y\right]$	[35,118]
36	$\left[\frac{1}{4}-y, \frac{5}{8}, \frac{1}{2}-y\right]$	[36,192]
37	$\left[\frac{1}{8}, y, y+\frac{3}{4}\right]$	[37,97]
38	$\left[\frac{1}{8}, \frac{1}{2}-y, \frac{3}{4}-y\right]$	[38,128]
39	$\left[y+\frac{1}{2}, \frac{3}{4}-y, \frac{7}{8}\right]$	[39,167]
40	$\left[-y, \frac{3}{4}-y, \frac{5}{8}\right]$	[40,117]
41	$\left[y+\frac{1}{4}, \frac{5}{8}, y+\frac{1}{2}\right]$	[41,127]
42	$\left[y, y+\frac{3}{4}, \frac{5}{8}\right]$	[42,172]
43	$\left[-y, y+\frac{3}{4}, \frac{3}{8}\right]$	[43,125]
44	$\left[\frac{3}{4}-y, \frac{3}{8}, y+\frac{1}{2}\right]$	[44,150]
45	$\left[-y, \frac{1}{4}-y, \frac{5}{8}\right]$	[45,112]
46	$\left[y+\frac{1}{4}, \frac{3}{8}, \frac{1}{2}-y\right]$	[46,107]

continued ...

Table 12

No.	position	mapping
47	$\left[y,\ \frac{1}{4}-y,\ \frac{3}{8}\right]$	[47,159]
48	$\left[\frac{3}{4}-y,\ \frac{5}{8},\ \frac{1}{2}-y\right]$	[48,180]
49	$\left[\frac{5}{8},\ y,\ y+\frac{3}{4}\right]$	[49,181]
50	$\left[\frac{7}{8},\ -y,\ y+\frac{3}{4}\right]$	[50,106]
51	$\left[\frac{7}{8},\ y+\frac{1}{2},\ \frac{3}{4}-y\right]$	[51,129]
52	$\left[y,\ y+\frac{1}{4},\ \frac{5}{8}\right]$	[52,114]
53	$\left[\frac{1}{2}-y,\ y+\frac{1}{4},\ \frac{7}{8}\right]$	[53,163]
54	$\left[\frac{3}{4}-y,\ \frac{3}{8},\ y\right]$	[54,140]
55	$\left[y+\frac{3}{4},\ \frac{1}{8},\ y\right]$	[55,161]
56	$\left[\frac{5}{8},\ -y,\ \frac{1}{4}-y\right]$	[56,158]
57	$\left[\frac{3}{8},\ y,\ \frac{1}{4}-y\right]$	[57,123]
58	$\left[\frac{3}{8},\ -y,\ y+\frac{3}{4}\right]$	[58,98]
59	$\left[y+\frac{3}{4},\ \frac{3}{8},\ \frac{1}{2}-y\right]$	[59,190]
60	$\left[\frac{3}{4}-y,\ \frac{1}{8},\ \frac{1}{2}-y\right]$	[60,120]
61	$\left[\frac{5}{8},\ y+\frac{1}{2},\ y+\frac{3}{4}\right]$	[61,169]
62	$\left[\frac{5}{8},\ -y,\ \frac{3}{4}-y\right]$	[62,152]
63	$\left[y,\ \frac{1}{4}-y,\ \frac{7}{8}\right]$	[63,143]
64	$\left[\frac{1}{2}-y,\ \frac{1}{4}-y,\ \frac{5}{8}\right]$	[64,189]
65	$\left[y+\frac{3}{4},\ \frac{1}{8},\ y+\frac{1}{2}\right]$	[65,151]
66	$\left[y+\frac{1}{2},\ y+\frac{1}{4},\ \frac{5}{8}\right]$	[66,100]
67	$\left[\frac{1}{2}-y,\ y+\frac{1}{4},\ \frac{3}{8}\right]$	[67,149]
68	$\left[\frac{1}{4}-y,\ \frac{7}{8},\ y+\frac{1}{2}\right]$	[68,126]
69	$\left[\frac{1}{2}-y,\ \frac{3}{4}-y,\ \frac{5}{8}\right]$	[69,184]
70	$\left[y+\frac{3}{4},\ \frac{7}{8},\ \frac{1}{2}-y\right]$	[70,179]
71	$\left[y+\frac{1}{2},\ \frac{3}{4}-y,\ \frac{3}{8}\right]$	[71,135]
72	$\left[\frac{1}{4}-y,\ \frac{1}{8},\ \frac{1}{2}-y\right]$	[72,108]
73	$\left[\frac{5}{8},\ y+\frac{1}{2},\ y+\frac{1}{4}\right]$	[73,157]
74	$\left[\frac{7}{8},\ \frac{1}{2}-y,\ y+\frac{1}{4}\right]$	[74,130]
75	$\left[\frac{7}{8},\ y,\ \frac{1}{4}-y\right]$	[75,105]
76	$\left[y,\ y+\frac{3}{4},\ \frac{1}{8}\right]$	[76,138]
77	$\left[\frac{1}{2}-y,\ y+\frac{3}{4},\ \frac{3}{8}\right]$	[77,187]
78	$\left[\frac{3}{4}-y,\ \frac{7}{8},\ y+\frac{1}{2}\right]$	[78,116]
79	$\left[y+\frac{3}{4},\ \frac{5}{8},\ y+\frac{1}{2}\right]$	[79,185]
80	$\left[\frac{5}{8},\ \frac{1}{2}-y,\ \frac{3}{4}-y\right]$	[80,182]
81	$\left[\frac{3}{8},\ y+\frac{1}{2},\ \frac{3}{4}-y\right]$	[81,99]
82	$\left[\frac{3}{8},\ \frac{1}{2}-y,\ y+\frac{1}{4}\right]$	[82,122]
83	$\left[y+\frac{3}{4},\ \frac{7}{8},\ -y\right]$	[83,166]
84	$\left[\frac{3}{4}-y,\ \frac{5}{8},\ -y\right]$	[84,144]
85	$\left[\frac{5}{8},\ y,\ y+\frac{1}{4}\right]$	[85,145]
86	$\left[\frac{5}{8},\ \frac{1}{2}-y,\ \frac{1}{4}-y\right]$	[86,176]
87	$\left[y,\ \frac{3}{4}-y,\ \frac{3}{8}\right]$	[87,119]
88	$\left[\frac{1}{2}-y,\ \frac{3}{4}-y,\ \frac{1}{8}\right]$	[88,165]
89	$\left[y+\frac{3}{4},\ \frac{5}{8},\ y\right]$	[89,175]
90	$\left[y+\frac{1}{2},\ y+\frac{3}{4},\ \frac{1}{8}\right]$	[90,124]
91	$\left[\frac{1}{2}-y,\ y+\frac{3}{4},\ \frac{7}{8}\right]$	[91,173]
92	$\left[\frac{1}{4}-y,\ \frac{3}{8},\ y\right]$	[92,102]
93	$\left[\frac{1}{2}-y,\ \frac{1}{4}-y,\ \frac{1}{8}\right]$	[93,160]

continued ...

Table 12

No.	position	mapping
94	$\left[y+\frac{3}{4},\ \frac{3}{8},\ -y\right]$	[94,155]
95	$\left[y+\frac{1}{2},\ \frac{1}{4}-y,\ \frac{7}{8}\right]$	[95,111]
96	$\left[\frac{1}{4}-y,\ \frac{5}{8},\ -y\right]$	[96,132]

Table 13: Wyckoff site: 192m, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$\left[x+\frac{1}{4},\ \frac{1}{4}-z,\ y+\frac{1}{4}\right]$	[2]
3	$\left[x+\frac{1}{4},\ z+\frac{1}{4},\ \frac{1}{4}-y\right]$	[3]
4	$\left[z+\frac{1}{4},\ y+\frac{1}{4},\ \frac{1}{4}-x\right]$	[4]
5	$\left[\frac{1}{4}-z,\ y+\frac{1}{4},\ x+\frac{1}{4}\right]$	[5]
6	$\left[\frac{1}{4}-y,\ x+\frac{1}{4},\ z+\frac{1}{4}\right]$	[6]
7	$\left[y+\frac{1}{4},\ \frac{1}{4}-x,\ z+\frac{1}{4}\right]$	[7]
8	$[x,\ -y,\ -z]$	[8]
9	$[-x,\ y,\ -z]$	[9]
10	$[-x,\ -y,\ z]$	[10]
11	$\left[y+\frac{1}{4},\ x+\frac{1}{4},\ \frac{1}{4}-z\right]$	[11]
12	$\left[\frac{1}{4}-y,\ \frac{1}{4}-x,\ \frac{1}{4}-z\right]$	[12]
13	$\left[\frac{1}{4}-x,\ z+\frac{1}{4},\ y+\frac{1}{4}\right]$	[13]
14	$\left[\frac{1}{4}-x,\ \frac{1}{4}-z,\ \frac{1}{4}-y\right]$	[14]
15	$\left[z+\frac{1}{4},\ \frac{1}{4}-y,\ x+\frac{1}{4}\right]$	[15]
16	$\left[\frac{1}{4}-z,\ \frac{1}{4}-y,\ \frac{1}{4}-x\right]$	[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	$\left[x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[25]
26	$\left[x+\frac{1}{4},\ \frac{3}{4}-z,\ y+\frac{3}{4}\right]$	[26]
27	$\left[x+\frac{1}{4},\ z+\frac{3}{4},\ \frac{3}{4}-y\right]$	[27]
28	$\left[z+\frac{1}{4},\ y+\frac{3}{4},\ \frac{3}{4}-x\right]$	[28]
29	$\left[\frac{1}{4}-z,\ y+\frac{3}{4},\ x+\frac{3}{4}\right]$	[29]
30	$\left[\frac{1}{4}-y,\ x+\frac{3}{4},\ z+\frac{3}{4}\right]$	[30]
31	$\left[y+\frac{1}{4},\ \frac{3}{4}-x,\ z+\frac{3}{4}\right]$	[31]
32	$\left[x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[32]
33	$\left[-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[33]
34	$\left[-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[34]
35	$\left[y+\frac{1}{4},\ x+\frac{3}{4},\ \frac{3}{4}-z\right]$	[35]
36	$\left[\frac{1}{4}-y,\ \frac{3}{4}-x,\ \frac{3}{4}-z\right]$	[36]
37	$\left[\frac{1}{4}-x,\ z+\frac{3}{4},\ y+\frac{3}{4}\right]$	[37]

continued ...

Table 13

No.	position	mapping
38	$\left[\frac{1}{4}-x,\ \frac{3}{4}-z,\ \frac{3}{4}-y\right]$	[38]
39	$\left[z+\frac{1}{4},\ \frac{3}{4}-y,\ x+\frac{3}{4}\right]$	[39]
40	$\left[\frac{1}{4}-z,\ \frac{3}{4}-y,\ \frac{3}{4}-x\right]$	[40]
41	$\left[z,\ x+\frac{1}{2},\ y+\frac{1}{2}\right]$	[41]
42	$\left[y,\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$	[42]
43	$\left[-y,\ z+\frac{1}{2},\ \frac{1}{2}-x\right]$	[43]
44	$\left[-z,\ \frac{1}{2}-x,\ y+\frac{1}{2}\right]$	[44]
45	$\left[-y,\ \frac{1}{2}-z,\ x+\frac{1}{2}\right]$	[45]
46	$\left[z,\ \frac{1}{2}-x,\ \frac{1}{2}-y\right]$	[46]
47	$\left[y,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[47]
48	$\left[-z,\ x+\frac{1}{2},\ \frac{1}{2}-y\right]$	[48]
49	$\left[x+\frac{1}{2},\ y,\ z+\frac{1}{2}\right]$	[49]
50	$\left[x+\frac{3}{4},\ \frac{1}{4}-z,\ y+\frac{3}{4}\right]$	[50]
51	$\left[x+\frac{3}{4},\ z+\frac{1}{4},\ \frac{3}{4}-y\right]$	[51]
52	$\left[z+\frac{3}{4},\ y+\frac{1}{4},\ \frac{3}{4}-x\right]$	[52]
53	$\left[\frac{3}{4}-z,\ y+\frac{1}{4},\ x+\frac{3}{4}\right]$	[53]
54	$\left[\frac{3}{4}-y,\ x+\frac{1}{4},\ z+\frac{3}{4}\right]$	[54]
55	$\left[y+\frac{3}{4},\ \frac{1}{4}-x,\ z+\frac{3}{4}\right]$	[55]
56	$\left[x+\frac{1}{2},\ -y,\ \frac{1}{2}-z\right]$	[56]
57	$\left[\frac{1}{2}-x,\ y,\ \frac{1}{2}-z\right]$	[57]
58	$\left[\frac{1}{2}-x,\ -y,\ z+\frac{1}{2}\right]$	[58]
59	$\left[y+\frac{3}{4},\ x+\frac{1}{4},\ \frac{3}{4}-z\right]$	[59]
60	$\left[\frac{3}{4}-y,\ \frac{1}{4}-x,\ \frac{3}{4}-z\right]$	[60]
61	$\left[\frac{3}{4}-x,\ z+\frac{1}{4},\ y+\frac{3}{4}\right]$	[61]
62	$\left[\frac{3}{4}-x,\ \frac{1}{4}-z,\ \frac{3}{4}-y\right]$	[62]
63	$\left[z+\frac{3}{4},\ \frac{1}{4}-y,\ x+\frac{3}{4}\right]$	[63]
64	$\left[\frac{3}{4}-z,\ \frac{1}{4}-y,\ \frac{3}{4}-x\right]$	[64]
65	$\left[z+\frac{1}{2},\ x,\ y+\frac{1}{2}\right]$	[65]
66	$\left[y+\frac{1}{2},\ z,\ x+\frac{1}{2}\right]$	[66]
67	$\left[\frac{1}{2}-y,\ z,\ \frac{1}{2}-x\right]$	[67]
68	$\left[\frac{1}{2}-z,\ -x,\ y+\frac{1}{2}\right]$	[68]
69	$\left[\frac{1}{2}-y,\ -z,\ x+\frac{1}{2}\right]$	[69]
70	$\left[z+\frac{1}{2},\ -x,\ \frac{1}{2}-y\right]$	[70]
71	$\left[y+\frac{1}{2},\ -z,\ \frac{1}{2}-x\right]$	[71]
72	$\left[\frac{1}{2}-z,\ x,\ \frac{1}{2}-y\right]$	[72]
73	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[73]
74	$\left[x+\frac{3}{4},\ \frac{3}{4}-z,\ y+\frac{1}{4}\right]$	[74]
75	$\left[x+\frac{3}{4},\ z+\frac{3}{4},\ \frac{1}{4}-y\right]$	[75]
76	$\left[z+\frac{3}{4},\ y+\frac{3}{4},\ \frac{1}{4}-x\right]$	[76]
77	$\left[\frac{3}{4}-z,\ y+\frac{3}{4},\ x+\frac{1}{4}\right]$	[77]
78	$\left[\frac{3}{4}-y,\ x+\frac{3}{4},\ z+\frac{1}{4}\right]$	[78]
79	$\left[y+\frac{3}{4},\ \frac{3}{4}-x,\ z+\frac{1}{4}\right]$	[79]
80	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[80]
81	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ -z\right]$	[81]
82	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	[82]
83	$\left[y+\frac{3}{4},\ x+\frac{3}{4},\ \frac{1}{4}-z\right]$	[83]
84	$\left[\frac{3}{4}-y,\ \frac{3}{4}-x,\ \frac{1}{4}-z\right]$	[84]

continued ...

Table 13

No.	position	mapping
85	$\left[\frac{3}{4}-x,\, z+\frac{3}{4},\, y+\frac{1}{4}\right]$	[85]
86	$\left[\frac{3}{4}-x,\, \frac{3}{4}-z,\, \frac{1}{4}-y\right]$	[86]
87	$\left[z+\frac{3}{4},\, \frac{3}{4}-y,\, x+\frac{1}{4}\right]$	[87]
88	$\left[\frac{3}{4}-z,\, \frac{3}{4}-y,\, \frac{1}{4}-x\right]$	[88]
89	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, y\right]$	[89]
90	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, x\right]$	[90]
91	$\left[\frac{1}{2}-y,\, z+\frac{1}{2},\, -x\right]$	[91]
92	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, y\right]$	[92]
93	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, x\right]$	[93]
94	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, -y\right]$	[94]
95	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, -x\right]$	[95]
96	$\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, -y\right]$	[96]
97	$\left[x,\, y,\, z+\frac{1}{2}\right]$	[97]
98	$\left[x+\frac{1}{4},\, \frac{1}{4}-z,\, y+\frac{3}{4}\right]$	[98]
99	$\left[x+\frac{1}{4},\, z+\frac{1}{4},\, \frac{3}{4}-y\right]$	[99]
100	$\left[z+\frac{1}{4},\, y+\frac{1}{4},\, \frac{3}{4}-x\right]$	[100]
101	$\left[\frac{1}{4}-z,\, y+\frac{1}{4},\, x+\frac{3}{4}\right]$	[101]
102	$\left[\frac{1}{4}-y,\, x+\frac{1}{4},\, z+\frac{3}{4}\right]$	[102]
103	$\left[y+\frac{1}{4},\, \frac{1}{4}-x,\, z+\frac{3}{4}\right]$	[103]
104	$\left[x,\, -y,\, \frac{1}{2}-z\right]$	[104]
105	$\left[-x,\, y,\, \frac{1}{2}-z\right]$	[105]
106	$\left[-x,\, -y,\, z+\frac{1}{2}\right]$	[106]
107	$\left[y+\frac{1}{4},\, x+\frac{1}{4},\, \frac{3}{4}-z\right]$	[107]
108	$\left[\frac{1}{4}-y,\, \frac{1}{4}-x,\, \frac{3}{4}-z\right]$	[108]
109	$\left[\frac{1}{4}-x,\, z+\frac{1}{4},\, y+\frac{3}{4}\right]$	[109]
110	$\left[\frac{1}{4}-x,\, \frac{1}{4}-z,\, \frac{3}{4}-y\right]$	[110]
111	$\left[z+\frac{1}{4},\, \frac{1}{4}-y,\, x+\frac{3}{4}\right]$	[111]
112	$\left[\frac{1}{4}-z,\, \frac{1}{4}-y,\, \frac{3}{4}-x\right]$	[112]
113	$\left[z,\, x,\, y+\frac{1}{2}\right]$	[113]
114	$\left[y,\, z,\, x+\frac{1}{2}\right]$	[114]
115	$\left[-y,\, z,\, \frac{1}{2}-x\right]$	[115]
116	$\left[-z,\, -x,\, y+\frac{1}{2}\right]$	[116]
117	$\left[-y,\, -z,\, x+\frac{1}{2}\right]$	[117]
118	$\left[z,\, -x,\, \frac{1}{2}-y\right]$	[118]
119	$\left[y,\, -z,\, \frac{1}{2}-x\right]$	[119]
120	$\left[-z,\, x,\, \frac{1}{2}-y\right]$	[120]
121	$\left[x,\, y+\frac{1}{2},\, z\right]$	[121]
122	$\left[x+\frac{1}{4},\, \frac{3}{4}-z,\, y+\frac{1}{4}\right]$	[122]
123	$\left[x+\frac{1}{4},\, z+\frac{3}{4},\, \frac{1}{4}-y\right]$	[123]
124	$\left[z+\frac{1}{4},\, y+\frac{3}{4},\, \frac{1}{4}-x\right]$	[124]
125	$\left[\frac{1}{4}-z,\, y+\frac{3}{4},\, x+\frac{1}{4}\right]$	[125]
126	$\left[\frac{1}{4}-y,\, x+\frac{3}{4},\, z+\frac{1}{4}\right]$	[126]
127	$\left[y+\frac{1}{4},\, \frac{3}{4}-x,\, z+\frac{1}{4}\right]$	[127]
128	$\left[x,\, \frac{1}{2}-y,\, -z\right]$	[128]
129	$\left[-x,\, y+\frac{1}{2},\, -z\right]$	[129]
130	$\left[-x,\, \frac{1}{2}-y,\, z\right]$	[130]
131	$\left[y+\frac{1}{4},\, x+\frac{3}{4},\, \frac{1}{4}-z\right]$	[131]

continued ...

Table 13

No.	position	mapping
132	$\left[\frac{1}{4}-y,\ \frac{3}{4}-x,\ \frac{1}{4}-z\right]$	[132]
133	$\left[\frac{1}{4}-x,\ z+\frac{3}{4},\ y+\frac{1}{4}\right]$	[133]
134	$\left[\frac{1}{4}-x,\ \frac{3}{4}-z,\ \frac{1}{4}-y\right]$	[134]
135	$\left[z+\frac{1}{4},\ \frac{3}{4}-y,\ x+\frac{1}{4}\right]$	[135]
136	$\left[\frac{1}{4}-z,\ \frac{3}{4}-y,\ \frac{1}{4}-x\right]$	[136]
137	$\left[z,\ x+\frac{1}{2},\ y\right]$	[137]
138	$\left[y,\ z+\frac{1}{2},\ x\right]$	[138]
139	$\left[-y,\ z+\frac{1}{2},\ -x\right]$	[139]
140	$\left[-z,\ \frac{1}{2}-x,\ y\right]$	[140]
141	$\left[-y,\ \frac{1}{2}-z,\ x\right]$	[141]
142	$\left[z,\ \frac{1}{2}-x,\ -y\right]$	[142]
143	$\left[y,\ \frac{1}{2}-z,\ -x\right]$	[143]
144	$\left[-z,\ x+\frac{1}{2},\ -y\right]$	[144]
145	$\left[x+\frac{1}{2},\ y,\ z\right]$	[145]
146	$\left[x+\frac{3}{4},\ \frac{1}{4}-z,\ y+\frac{1}{4}\right]$	[146]
147	$\left[x+\frac{3}{4},\ z+\frac{1}{4},\ \frac{1}{4}-y\right]$	[147]
148	$\left[z+\frac{3}{4},\ y+\frac{1}{4},\ \frac{1}{4}-x\right]$	[148]
149	$\left[\frac{3}{4}-z,\ y+\frac{1}{4},\ x+\frac{1}{4}\right]$	[149]
150	$\left[\frac{3}{4}-y,\ x+\frac{1}{4},\ z+\frac{1}{4}\right]$	[150]
151	$\left[y+\frac{3}{4},\ \frac{1}{4}-x,\ z+\frac{1}{4}\right]$	[151]
152	$\left[x+\frac{1}{2},\ -y,\ -z\right]$	[152]
153	$\left[\frac{1}{2}-x,\ y,\ -z\right]$	[153]
154	$\left[\frac{1}{2}-x,\ -y,\ z\right]$	[154]
155	$\left[y+\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{4}-z\right]$	[155]
156	$\left[\frac{3}{4}-y,\ \frac{1}{4}-x,\ \frac{1}{4}-z\right]$	[156]
157	$\left[\frac{3}{4}-x,\ z+\frac{1}{4},\ y+\frac{1}{4}\right]$	[157]
158	$\left[\frac{3}{4}-x,\ \frac{1}{4}-z,\ \frac{1}{4}-y\right]$	[158]
159	$\left[z+\frac{3}{4},\ \frac{1}{4}-y,\ x+\frac{1}{4}\right]$	[159]
160	$\left[\frac{3}{4}-z,\ \frac{1}{4}-y,\ \frac{1}{4}-x\right]$	[160]
161	$\left[z+\frac{1}{2},\ x,\ y\right]$	[161]
162	$\left[y+\frac{1}{2},\ z,\ x\right]$	[162]
163	$\left[\frac{1}{2}-y,\ z,\ -x\right]$	[163]
164	$\left[\frac{1}{2}-z,\ -x,\ y\right]$	[164]
165	$\left[\frac{1}{2}-y,\ -z,\ x\right]$	[165]
166	$\left[z+\frac{1}{2},\ -x,\ -y\right]$	[166]
167	$\left[y+\frac{1}{2},\ -z,\ -x\right]$	[167]
168	$\left[\frac{1}{2}-z,\ x,\ -y\right]$	[168]
169	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[169]
170	$\left[x+\frac{3}{4},\ \frac{3}{4}-z,\ y+\frac{3}{4}\right]$	[170]
171	$\left[x+\frac{3}{4},\ z+\frac{3}{4},\ \frac{3}{4}-y\right]$	[171]
172	$\left[z+\frac{3}{4},\ y+\frac{3}{4},\ \frac{3}{4}-x\right]$	[172]
173	$\left[\frac{3}{4}-z,\ y+\frac{3}{4},\ x+\frac{3}{4}\right]$	[173]
174	$\left[\frac{3}{4}-y,\ x+\frac{3}{4},\ z+\frac{3}{4}\right]$	[174]
175	$\left[y+\frac{3}{4},\ \frac{3}{4}-x,\ z+\frac{3}{4}\right]$	[175]
176	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[176]
177	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[177]
178	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[178]

continued ...

Table 13

No.	position	mapping
179	$\left[y+\frac{3}{4},\, x+\frac{3}{4},\, \frac{3}{4}-z\right]$	[179]
180	$\left[\frac{3}{4}-y,\, \frac{3}{4}-x,\, \frac{3}{4}-z\right]$	[180]
181	$\left[\frac{3}{4}-x,\, z+\frac{3}{4},\, y+\frac{3}{4}\right]$	[181]
182	$\left[\frac{3}{4}-x,\, \frac{3}{4}-z,\, \frac{3}{4}-y\right]$	[182]
183	$\left[z+\frac{3}{4},\, \frac{3}{4}-y,\, x+\frac{3}{4}\right]$	[183]
184	$\left[\frac{3}{4}-z,\, \frac{3}{4}-y,\, \frac{3}{4}-x\right]$	[184]
185	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[185]
186	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[186]
187	$\left[\frac{1}{2}-y,\, z+\frac{1}{2},\, \frac{1}{2}-x\right]$	[187]
188	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, y+\frac{1}{2}\right]$	[188]
189	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, x+\frac{1}{2}\right]$	[189]
190	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, \frac{1}{2}-y\right]$	[190]
191	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, \frac{1}{2}-x\right]$	[191]
192	$\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, \frac{1}{2}-y\right]$	[192]