MSG No. 227.133 $F_Sd\bar{3}m$ [Type IV, cubic]

Table 1: Wyckoff site: `16a`, site symmetry: `-43m`

No.	position	mapping
1	$\left[\frac{5}{8}, \frac{5}{8}, \frac{5}{8}\right]$	[1,8,9,10,17,18,19,20,21,22,23,24,26,27,28,29,30,31,35,36,37,38,39,40]
2	$\left[\frac{7}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[2,7,15,33,43,48,51,52,59,82,92,93,108,110,112,121,137,138,149,150,157,176,190,191]
3	$\left[\frac{7}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[3,4,11,34,44,45,50,55,63,81,91,96,101,102,109,128,142,143,156,158,160,169,185,186]
4	$\left[\frac{3}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[5,6,13,32,46,47,60,62,64,73,89,90,99,100,107,130,140,141,146,151,159,177,187,192]
5	$\left[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}\right]$	[12,14,16,25,41,42,53,54,61,80,94,95,98,103,111,129,139,144,147,148,155,178,188,189]
6	$\left[\frac{5}{8}, \frac{1}{8}, \frac{1}{8}\right]$	[49,56,57,58,65,66,67,68,69,70,71,72,74,75,76,77,78,79,83,84,85,86,87,88]
7	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[97,104,105,106,113,114,115,116,117,118,119,120,122,123,124,125,126,127,131,132,133,134,135,136]
8	$\left[\frac{1}{8}, \frac{1}{8}, \frac{5}{8}\right]$	[145,152,153,154,161,162,163,164,165,166,167,168,170,171,172,173,174,175,179,180,181,182,183,184]
9	$\left[\frac{5}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[193,200,201,202,209,210,211,212,213,214,215,216,218,219,220,221,222,223,227,228,229,230,231,232]
10	$\left[\frac{7}{8}, \frac{3}{8}, \frac{3}{8}\right]$	[194,199,207,225,235,240,243,244,251,274,284,285,300,302,304,313,329,330,341,342,349,368,382,383]
11	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[195,196,203,226,236,237,242,247,255,273,283,288,293,294,301,320,334,335,348,350,352,361,377,378]
12	$\left[\frac{3}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[197,198,205,224,238,239,252,254,256,265,281,282,291,292,299,322,332,333,338,343,351,369,379,384]
13	$\left[\frac{3}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[204,206,208,217,233,234,245,246,253,272,286,287,290,295,303,321,331,336,339,340,347,370,380,381]
14	$\left[\frac{5}{8}, \frac{1}{8}, \frac{5}{8}\right]$	[241,248,249,250,257,258,259,260,261,262,263,264,266,267,268,269,270,271,275,276,277,278,279,280]
15	$\left[\frac{1}{8}, \frac{5}{8}, \frac{5}{8}\right]$	[289,296,297,298,305,306,307,308,309,310,311,312,314,315,316,317,318,319,323,324,325,326,327,328]
16	$\left[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}\right]$	[337,344,345,346,353,354,355,356,357,358,359,360,362,363,364,365,366,367,371,372,373,374,375,376]

Table 2: Wyckoff site: `32b`, site symmetry: `.-3m`

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[1,12,14,16,17,18,25,36,38,40,41,42]
2	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[2,7,9,15,19,24,26,31,33,39,43,48]
3	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[3,4,10,11,20,21,27,28,34,35,44,45]
4	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[5,6,8,13,22,23,29,30,32,37,46,47]
5	$\left[\frac{1}{2}, 0, 0\right]$	[49,60,62,64,65,66,73,84,86,88,89,90]
6	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	[50,55,57,63,67,72,74,79,81,87,91,96]
7	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[51,52,58,59,68,69,75,76,82,83,92,93]
8	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[53,54,56,61,70,71,77,78,80,85,94,95]
9	$\left[0, \frac{1}{2}, 0\right]$	[97,108,110,112,113,114,121,132,134,136,137,138]
10	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[98,103,105,111,115,120,122,127,129,135,139,144]
11	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[99,100,106,107,116,117,123,124,130,131,140,141]
12	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	[101,102,104,109,118,119,125,126,128,133,142,143]
13	$\left[0, 0, \frac{1}{2}\right]$	[145,156,158,160,161,162,169,180,182,184,185,186]
14	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	[146,151,153,159,163,168,170,175,177,183,187,192]
15	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[147,148,154,155,164,165,171,172,178,179,188,189]
16	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	[149,150,152,157,166,167,173,174,176,181,190,191]
17	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[193,204,206,208,209,210,217,228,230,232,233,234]
18	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[194,199,201,207,211,216,218,223,225,231,235,240]
19	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	[195,196,202,203,212,213,219,220,226,227,236,237]
20	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[197,198,200,205,214,215,221,222,224,229,238,239]
21	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[241,252,254,256,257,258,265,276,278,280,281,282]

continued ...

Table 2

No.	position	mapping
22	$\left[\frac{3}{4}, 0, \frac{3}{4}\right]$	[242,247,249,255,259,264,266,271,273,279,283,288]
23	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[243,244,250,251,260,261,267,268,274,275,284,285]
24	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[245,246,248,253,262,263,269,270,272,277,286,287]
25	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[289,300,302,304,305,306,313,324,326,328,329,330]
26	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[290,295,297,303,307,312,314,319,321,327,331,336]
27	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[291,292,298,299,308,309,315,316,322,323,332,333]
28	$\left[0, \frac{3}{4}, \frac{3}{4}\right]$	[293,294,296,301,310,311,317,318,320,325,334,335]
29	$[0, 0, 0]$	[337,348,350,352,353,354,361,372,374,376,377,378]
30	$\left[\frac{1}{4}, 0, \frac{1}{4}\right]$	[338,343,345,351,355,360,362,367,369,375,379,384]
31	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	[339,340,346,347,356,357,363,364,370,371,380,381]
32	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	[341,342,344,349,358,359,365,366,368,373,382,383]

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

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[1,17,18,36,38,40,348,350,352,361,377,378]
2	$\left[0, \frac{1}{4}, 0\right]$	[2,7,15,33,43,48,345,355,360,362,367,375]
3	$\left[0, 0, \frac{1}{4}\right]$	[3,4,11,34,44,45,346,356,357,363,364,371]
4	$\left[\frac{1}{4}, 0, 0\right]$	[5,6,13,32,46,47,344,358,359,365,366,373]
5	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}\right]$	[8,22,23,29,30,37,341,342,349,368,382,383]
6	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{2}\right]$	[9,19,24,26,31,39,338,343,351,369,379,384]
7	$\left[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	[10,20,21,27,28,35,339,340,347,370,380,381]
8	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[12,14,16,25,41,42,337,353,354,372,374,376]
9	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[49,65,66,84,86,88,300,302,304,313,329,330]
10	$\left[0, \frac{3}{4}, \frac{1}{2}\right]$	[50,55,63,81,91,96,297,307,312,314,319,327]
11	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[51,52,59,82,92,93,298,308,309,315,316,323]
12	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}\right]$	[53,54,61,80,94,95,296,310,311,317,318,325]
13	$\left[\frac{3}{4}, 0, 0\right]$	[56,70,71,77,78,85,293,294,301,320,334,335]
14	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[57,67,72,74,79,87,290,295,303,321,331,336]
15	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[58,68,69,75,76,83,291,292,299,322,332,333]
16	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[60,62,64,73,89,90,289,305,306,324,326,328]
17	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[97,113,114,132,134,136,252,254,256,265,281,282]
18	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{2}\right]$	[98,103,111,129,139,144,249,259,264,266,271,279]
19	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[99,100,107,130,140,141,250,260,261,267,268,275]
20	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	[101,102,109,128,142,143,248,262,263,269,270,277]
21	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	[104,118,119,125,126,133,245,246,253,272,286,287]
22	$\left[0, \frac{3}{4}, 0\right]$	[105,115,120,122,127,135,242,247,255,273,283,288]
23	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[106,116,117,123,124,131,243,244,251,274,284,285]
24	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[108,110,112,121,137,138,241,257,258,276,278,280]
25	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[145,161,162,180,182,184,204,206,208,217,233,234]
26	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	[146,151,159,177,187,192,201,211,216,218,223,231]
27	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[147,148,155,178,188,189,202,212,213,219,220,227]
28	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	[149,150,157,176,190,191,200,214,215,221,222,229]
29	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[152,166,167,173,174,181,197,198,205,224,238,239]

continued ...

Table 3

No.	position	mapping
30	$\left[0,\ \frac{1}{4},\ \frac{1}{2}\right]$	[153,163,168,170,175,183,194,199,207,225,235,240]
31	$\left[0,\ 0,\ \frac{3}{4}\right]$	[154,164,165,171,172,179,195,196,203,226,236,237]
32	$\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$	[156,158,160,169,185,186,193,209,210,228,230,232]

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

No.	position	mapping
1	$\left[\frac{5}{8},\ \frac{7}{8},\ \frac{7}{8}\right]$	[1,38,56,85,201,218,250,267]
2	$\left[\frac{7}{8},\ \frac{1}{8},\ \frac{1}{8}\right]$	[2,3,33,34,301,302,313,320]
3	$\left[\frac{1}{8},\ \frac{1}{8},\ \frac{3}{8}\right]$	[4,16,42,45,197,207,235,239]
4	$\left[\frac{1}{8},\ \frac{1}{8},\ \frac{7}{8}\right]$	[5,15,43,47,196,208,234,237]
5	$\left[\frac{1}{8},\ \frac{7}{8},\ \frac{1}{8}\right]$	[6,11,44,46,247,252,281,288]
6	$\left[\frac{1}{8},\ \frac{3}{8},\ \frac{1}{8}\right]$	[7,12,41,48,246,251,284,286]
7	$\left[\frac{5}{8},\ \frac{3}{8},\ \frac{3}{8}\right]$	[8,37,49,86,202,219,249,266]
8	$\left[\frac{5}{8},\ \frac{7}{8},\ \frac{3}{8}\right]$	[9,26,58,75,193,230,248,277]
9	$\left[\frac{5}{8},\ \frac{3}{8},\ \frac{7}{8}\right]$	[10,27,57,74,200,229,241,278]
10	$\left[\frac{3}{8},\ \frac{1}{8},\ \frac{1}{8}\right]$	[13,14,25,32,290,291,321,322]
11	$\left[\frac{7}{8},\ \frac{5}{8},\ \frac{7}{8}\right]$	[17,36,120,127,214,222,308,323]
12	$\left[\frac{7}{8},\ \frac{7}{8},\ \frac{5}{8}\right]$	[18,40,165,172,263,269,307,327]
13	$\left[\frac{3}{8},\ \frac{7}{8},\ \frac{5}{8}\right]$	[19,39,167,173,261,268,306,328]
14	$\left[\frac{3}{8},\ \frac{5}{8},\ \frac{7}{8}\right]$	[20,35,118,126,216,223,305,324]
15	$\left[\frac{3}{8},\ \frac{3}{8},\ \frac{5}{8}\right]$	[21,28,162,184,259,279,311,317]
16	$\left[\frac{7}{8},\ \frac{5}{8},\ \frac{3}{8}\right]$	[22,30,116,131,209,228,312,319]
17	$\left[\frac{7}{8},\ \frac{3}{8},\ \frac{5}{8}\right]$	[23,29,163,183,258,280,309,316]
18	$\left[\frac{3}{8},\ \frac{5}{8},\ \frac{3}{8}\right]$	[24,31,113,132,212,227,310,318]
19	$\left[\frac{7}{8},\ \frac{5}{8},\ \frac{5}{8}\right]$	[50,51,81,82,349,350,361,368]
20	$\left[\frac{1}{8},\ \frac{5}{8},\ \frac{7}{8}\right]$	[52,64,90,93,245,255,283,287]
21	$\left[\frac{1}{8},\ \frac{5}{8},\ \frac{3}{8}\right]$	[53,63,91,95,244,256,282,285]
22	$\left[\frac{1}{8},\ \frac{3}{8},\ \frac{5}{8}\right]$	[54,59,92,94,199,204,233,240]
23	$\left[\frac{1}{8},\ \frac{7}{8},\ \frac{5}{8}\right]$	[55,60,89,96,198,203,236,238]
24	$\left[\frac{3}{8},\ \frac{5}{8},\ \frac{5}{8}\right]$	[61,62,73,80,338,339,369,370]
25	$\left[\frac{7}{8},\ \frac{1}{8},\ \frac{3}{8}\right]$	[65,84,168,175,262,270,356,371]
26	$\left[\frac{7}{8},\ \frac{3}{8},\ \frac{1}{8}\right]$	[66,88,117,124,215,221,355,375]
27	$\left[\frac{3}{8},\ \frac{3}{8},\ \frac{1}{8}\right]$	[67,87,119,125,213,220,354,376]
28	$\left[\frac{3}{8},\ \frac{1}{8},\ \frac{3}{8}\right]$	[68,83,166,174,264,271,353,372]
29	$\left[\frac{3}{8},\ \frac{7}{8},\ \frac{1}{8}\right]$	[69,76,114,136,211,231,359,365]
30	$\left[\frac{7}{8},\ \frac{1}{8},\ \frac{7}{8}\right]$	[70,78,164,179,257,276,360,367]
31	$\left[\frac{7}{8},\ \frac{7}{8},\ \frac{1}{8}\right]$	[71,77,115,135,210,232,357,364]
32	$\left[\frac{3}{8},\ \frac{1}{8},\ \frac{7}{8}\right]$	[72,79,161,180,260,275,358,366]
33	$\left[\frac{1}{8},\ \frac{7}{8},\ \frac{3}{8}\right]$	[97,134,152,181,297,314,346,363]
34	$\left[\frac{3}{8},\ \frac{1}{8},\ \frac{5}{8}\right]$	[98,99,129,130,205,206,217,224]
35	$\left[\frac{5}{8},\ \frac{1}{8},\ \frac{7}{8}\right]$	[100,112,138,141,293,303,331,335]
36	$\left[\frac{5}{8},\ \frac{1}{8},\ \frac{3}{8}\right]$	[101,111,139,143,292,304,330,333]
37	$\left[\frac{5}{8},\ \frac{7}{8},\ \frac{5}{8}\right]$	[102,107,140,142,343,348,377,384]

continued ...

Table 4

No.	position	mapping
38	$\left[\frac{5}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[103,108,137,144,342,347,380,382]
39	$\left[\frac{1}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[104,133,145,182,298,315,345,362]
40	$\left[\frac{1}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[105,122,154,171,289,326,344,373]
41	$\left[\frac{1}{8}, \frac{3}{8}, \frac{3}{8}\right]$	[106,123,153,170,296,325,337,374]
42	$\left[\frac{7}{8}, \frac{1}{8}, \frac{5}{8}\right]$	[109,110,121,128,194,195,225,226]
43	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[146,147,177,178,253,254,265,272]
44	$\left[\frac{5}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[148,160,186,189,341,351,379,383]
45	$\left[\frac{5}{8}, \frac{5}{8}, \frac{7}{8}\right]$	[149,159,187,191,340,352,378,381]
46	$\left[\frac{5}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[150,155,188,190,295,300,329,336]
47	$\left[\frac{5}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[151,156,185,192,294,299,332,334]
48	$\left[\frac{7}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[157,158,169,176,242,243,273,274]

Table 5: Wyckoff site: 64e, site symmetry: .3m

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

continued ...

Table 5

No.	position	mapping
30	$\left[\frac{3}{4}-x,\ x+\frac{1}{2},\ \frac{1}{4}-x\right]$	[153,163,168,170,175,183]
31	$\left[\frac{3}{4}-x,\ \frac{3}{4}-x,\ x\right]$	[154,164,165,171,172,179]
32	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ -x\right]$	[156,158,160,169,185,186]
33	$\left[x,\ x,\ x+\frac{1}{2}\right]$	[193,209,210,228,230,232]
34	$\left[x+\frac{1}{4},\ -x,\ x+\frac{3}{4}\right]$	[194,199,207,225,235,240]
35	$\left[x+\frac{1}{4},\ x+\frac{1}{4},\ \frac{1}{2}-x\right]$	[195,196,203,226,236,237]
36	$\left[-x,\ x+\frac{1}{4},\ x+\frac{3}{4}\right]$	[197,198,205,224,238,239]
37	$\left[x,\ \frac{1}{4}-x,\ \frac{3}{4}-x\right]$	[200,214,215,221,222,229]
38	$\left[\frac{1}{4}-x,\ x,\ \frac{3}{4}-x\right]$	[201,211,216,218,223,231]
39	$\left[\frac{1}{4}-x,\ \frac{1}{4}-x,\ x+\frac{1}{2}\right]$	[202,212,213,219,220,227]
40	$\left[-x,\ -x,\ \frac{1}{2}-x\right]$	[204,206,208,217,233,234]
41	$\left[x,\ x+\frac{1}{2},\ x\right]$	[241,257,258,276,278,280]
42	$\left[x+\frac{1}{4},\ \frac{1}{2}-x,\ x+\frac{1}{4}\right]$	[242,247,255,273,283,288]
43	$\left[x+\frac{1}{4},\ x+\frac{3}{4},\ -x\right]$	[243,244,251,274,284,285]
44	$\left[-x,\ x+\frac{3}{4},\ x+\frac{1}{4}\right]$	[245,246,253,272,286,287]
45	$\left[x,\ \frac{3}{4}-x,\ \frac{1}{4}-x\right]$	[248,262,263,269,270,277]
46	$\left[\frac{1}{4}-x,\ x+\frac{1}{2},\ \frac{1}{4}-x\right]$	[249,259,264,266,271,279]
47	$\left[\frac{1}{4}-x,\ \frac{3}{4}-x,\ x\right]$	[250,260,261,267,268,275]
48	$\left[-x,\ \frac{1}{2}-x,\ -x\right]$	[252,254,256,265,281,282]
49	$\left[x+\frac{1}{2},\ x,\ x\right]$	[289,305,306,324,326,328]
50	$\left[x+\frac{3}{4},\ -x,\ x+\frac{1}{4}\right]$	[290,295,303,321,331,336]
51	$\left[x+\frac{3}{4},\ x+\frac{1}{4},\ -x\right]$	[291,292,299,322,332,333]
52	$\left[\frac{1}{2}-x,\ x+\frac{1}{4},\ x+\frac{1}{4}\right]$	[293,294,301,320,334,335]
53	$\left[x+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{1}{4}-x\right]$	[296,310,311,317,318,325]
54	$\left[\frac{3}{4}-x,\ x,\ \frac{1}{4}-x\right]$	[297,307,312,314,319,327]
55	$\left[\frac{3}{4}-x,\ \frac{1}{4}-x,\ x\right]$	[298,308,309,315,316,323]
56	$\left[\frac{1}{2}-x,\ -x,\ -x\right]$	[300,302,304,313,329,330]
57	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ x+\frac{1}{2}\right]$	[337,353,354,372,374,376]
58	$\left[x+\frac{3}{4},\ \frac{1}{2}-x,\ x+\frac{3}{4}\right]$	[338,343,351,369,379,384]
59	$\left[x+\frac{3}{4},\ x+\frac{3}{4},\ \frac{1}{2}-x\right]$	[339,340,347,370,380,381]
60	$\left[\frac{1}{2}-x,\ x+\frac{3}{4},\ x+\frac{3}{4}\right]$	[341,342,349,368,382,383]
61	$\left[x+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{3}{4}-x\right]$	[344,358,359,365,366,373]
62	$\left[\frac{3}{4}-x,\ x+\frac{1}{2},\ \frac{3}{4}-x\right]$	[345,355,360,362,367,375]
63	$\left[\frac{3}{4}-x,\ \frac{3}{4}-x,\ x+\frac{1}{2}\right]$	[346,356,357,363,364,371]
64	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	[348,350,352,361,377,378]

Table 6: Wyckoff site: `96f`, site symmetry: `2'.22'`

No.	position	mapping
1	$\left[\frac{3}{4},\ \frac{5}{8},\ \frac{7}{8}\right]$	[1,157,200,350]
2	$\left[0,\ \frac{1}{8},\ \frac{7}{8}\right]$	[2,154,195,345]
3	$\left[0,\ \frac{1}{8},\ \frac{3}{8}\right]$	[3,153,194,346]
4	$\left[\frac{1}{8},\ \frac{7}{8},\ \frac{1}{4}\right]$	[4,114,256,357]
5	$\left[\frac{1}{8},\ \frac{7}{8},\ 0\right]$	[5,115,255,359]

continued ...

Table 6

No.	position	mapping
6	$\left[\frac{3}{8}, 0, \frac{1}{8}\right]$	[6,68,299,358]
7	$\left[\frac{7}{8}, \frac{1}{4}, \frac{1}{8}\right]$	[7,65,300,360]
8	$\left[\frac{3}{4}, \frac{5}{8}, \frac{3}{8}\right]$	[8,158,193,349]
9	$\left[\frac{1}{2}, \frac{5}{8}, \frac{3}{8}\right]$	[9,147,202,338]
10	$\left[\frac{1}{2}, \frac{5}{8}, \frac{7}{8}\right]$	[10,146,201,339]
11	$\left[\frac{7}{8}, 0, \frac{1}{8}\right]$	[11,70,294,356]
12	$\left[\frac{3}{8}, \frac{1}{4}, \frac{1}{8}\right]$	[12,72,295,353]
13	$\left[\frac{1}{4}, \frac{1}{8}, \frac{7}{8}\right]$	[13,145,206,344]
14	$\left[\frac{1}{4}, \frac{1}{8}, \frac{3}{8}\right]$	[14,152,205,337]
15	$\left[\frac{1}{8}, \frac{3}{8}, 0\right]$	[15,119,245,355]
16	$\left[\frac{1}{8}, \frac{3}{8}, \frac{1}{4}\right]$	[16,117,244,354]
17	$\left[\frac{7}{8}, \frac{3}{4}, \frac{5}{8}\right]$	[17,55,312,348]
18	$\left[\frac{5}{8}, \frac{7}{8}, \frac{3}{4}\right]$	[18,100,261,352]
19	$\left[\frac{5}{8}, \frac{7}{8}, \frac{1}{2}\right]$	[19,101,263,351]
20	$\left[\frac{3}{8}, \frac{1}{2}, \frac{5}{8}\right]$	[20,54,310,347]
21	$\left[\frac{5}{8}, \frac{3}{8}, \frac{3}{4}\right]$	[21,112,258,340]
22	$\left[\frac{7}{8}, \frac{1}{2}, \frac{5}{8}\right]$	[22,59,308,342]
23	$\left[\frac{5}{8}, \frac{3}{8}, \frac{1}{2}\right]$	[23,111,259,341]
24	$\left[\frac{3}{8}, \frac{3}{4}, \frac{5}{8}\right]$	[24,60,305,343]
25	$\left[\frac{1}{4}, \frac{3}{8}, \frac{1}{8}\right]$	[25,133,272,374]
26	$\left[\frac{1}{2}, \frac{7}{8}, \frac{5}{8}\right]$	[26,130,267,369]
27	$\left[\frac{1}{2}, \frac{3}{8}, \frac{5}{8}\right]$	[27,129,266,370]
28	$\left[\frac{3}{8}, \frac{5}{8}, \frac{3}{4}\right]$	[28,90,328,381]
29	$\left[\frac{7}{8}, \frac{5}{8}, \frac{1}{2}\right]$	[29,91,327,383]
30	$\left[\frac{5}{8}, \frac{1}{2}, \frac{3}{8}\right]$	[30,188,227,382]
31	$\left[\frac{5}{8}, \frac{3}{4}, \frac{3}{8}\right]$	[31,185,228,384]
32	$\left[\frac{1}{4}, \frac{7}{8}, \frac{1}{8}\right]$	[32,134,265,373]
33	$\left[0, \frac{3}{8}, \frac{1}{8}\right]$	[33,123,274,362]
34	$\left[0, \frac{7}{8}, \frac{1}{8}\right]$	[34,122,273,363]
35	$\left[\frac{5}{8}, \frac{1}{2}, \frac{7}{8}\right]$	[35,190,222,380]
36	$\left[\frac{5}{8}, \frac{3}{4}, \frac{7}{8}\right]$	[36,192,223,377]
37	$\left[\frac{3}{4}, \frac{3}{8}, \frac{5}{8}\right]$	[37,121,278,368]
38	$\left[\frac{3}{4}, \frac{7}{8}, \frac{5}{8}\right]$	[38,128,277,361]
39	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{2}\right]$	[39,95,317,379]
40	$\left[\frac{7}{8}, \frac{5}{8}, \frac{3}{4}\right]$	[40,93,316,378]
41	$\left[\frac{1}{8}, \frac{1}{4}, \frac{3}{8}\right]$	[41,175,240,372]
42	$\left[\frac{3}{8}, \frac{1}{8}, \frac{1}{4}\right]$	[42,76,333,376]
43	$\left[\frac{7}{8}, \frac{1}{8}, 0\right]$	[43,77,335,375]
44	$\left[\frac{1}{8}, 0, \frac{3}{8}\right]$	[44,174,238,371]
45	$\left[\frac{7}{8}, \frac{1}{8}, \frac{1}{4}\right]$	[45,88,330,364]
46	$\left[\frac{1}{8}, 0, \frac{7}{8}\right]$	[46,179,236,366]
47	$\left[\frac{3}{8}, \frac{1}{8}, 0\right]$	[47,87,331,365]
48	$\left[\frac{1}{8}, \frac{1}{4}, \frac{7}{8}\right]$	[48,180,233,367]
49	$\left[\frac{3}{4}, \frac{1}{8}, \frac{3}{8}\right]$	[49,109,248,302]
50	$\left[0, \frac{5}{8}, \frac{3}{8}\right]$	[50,106,243,297]
51	$\left[0, \frac{5}{8}, \frac{7}{8}\right]$	[51,105,242,298]
52	$\left[\frac{1}{8}, \frac{3}{8}, \frac{3}{4}\right]$	[52,162,208,309]

continued ...

Table 6

No.	position	mapping
53	$\left[\frac{1}{8}, \frac{3}{8}, \frac{1}{2}\right]$	[53,163,207,311]
54	$\left[\frac{3}{4}, \frac{1}{8}, \frac{7}{8}\right]$	[56,110,241,301]
55	$\left[\frac{1}{2}, \frac{1}{8}, \frac{7}{8}\right]$	[57,99,250,290]
56	$\left[\frac{1}{2}, \frac{1}{8}, \frac{3}{8}\right]$	[58,98,249,291]
57	$\left[\frac{1}{4}, \frac{5}{8}, \frac{3}{8}\right]$	[61,97,254,296]
58	$\left[\frac{1}{4}, \frac{5}{8}, \frac{7}{8}\right]$	[62,104,253,289]
59	$\left[\frac{1}{8}, \frac{7}{8}, \frac{1}{2}\right]$	[63,167,197,307]
60	$\left[\frac{1}{8}, \frac{7}{8}, \frac{3}{4}\right]$	[64,165,196,306]
61	$\left[\frac{5}{8}, \frac{3}{8}, \frac{1}{4}\right]$	[66,148,213,304]
62	$\left[\frac{5}{8}, \frac{3}{8}, 0\right]$	[67,149,215,303]
63	$\left[\frac{5}{8}, \frac{7}{8}, \frac{1}{4}\right]$	[69,160,210,292]
64	$\left[\frac{5}{8}, \frac{7}{8}, 0\right]$	[71,159,211,293]
65	$\left[\frac{1}{4}, \frac{7}{8}, \frac{5}{8}\right]$	[73,181,224,326]
66	$\left[\frac{1}{2}, \frac{3}{8}, \frac{1}{8}\right]$	[74,178,219,321]
67	$\left[\frac{1}{2}, \frac{7}{8}, \frac{1}{8}\right]$	[75,177,218,322]
68	$\left[\frac{5}{8}, 0, \frac{7}{8}\right]$	[78,140,275,334]
69	$\left[\frac{5}{8}, \frac{1}{4}, \frac{7}{8}\right]$	[79,137,276,336]
70	$\left[\frac{1}{4}, \frac{3}{8}, \frac{5}{8}\right]$	[80,182,217,325]
71	$\left[0, \frac{7}{8}, \frac{5}{8}\right]$	[81,171,226,314]
72	$\left[0, \frac{3}{8}, \frac{5}{8}\right]$	[82,170,225,315]
73	$\left[\frac{5}{8}, 0, \frac{3}{8}\right]$	[83,142,270,332]
74	$\left[\frac{5}{8}, \frac{1}{4}, \frac{3}{8}\right]$	[84,144,271,329]
75	$\left[\frac{3}{4}, \frac{7}{8}, \frac{1}{8}\right]$	[85,169,230,320]
76	$\left[\frac{3}{4}, \frac{3}{8}, \frac{1}{8}\right]$	[86,176,229,313]
77	$\left[\frac{1}{8}, \frac{3}{4}, \frac{7}{8}\right]$	[89,127,288,324]
78	$\left[\frac{1}{8}, \frac{1}{2}, \frac{7}{8}\right]$	[92,126,286,323]
79	$\left[\frac{1}{8}, \frac{1}{2}, \frac{3}{8}\right]$	[94,131,284,318]
80	$\left[\frac{1}{8}, \frac{3}{4}, \frac{3}{8}\right]$	[96,132,281,319]
81	$\left[\frac{7}{8}, 0, \frac{5}{8}\right]$	[102,164,203,262]
82	$\left[\frac{3}{8}, \frac{1}{4}, \frac{5}{8}\right]$	[103,161,204,264]
83	$\left[\frac{3}{8}, 0, \frac{5}{8}\right]$	[107,166,198,260]
84	$\left[\frac{7}{8}, \frac{1}{4}, \frac{5}{8}\right]$	[108,168,199,257]
85	$\left[\frac{3}{8}, \frac{3}{4}, \frac{1}{8}\right]$	[113,151,216,252]
86	$\left[\frac{7}{8}, \frac{1}{2}, \frac{1}{8}\right]$	[116,150,214,251]
87	$\left[\frac{3}{8}, \frac{1}{2}, \frac{1}{8}\right]$	[118,155,212,246]
88	$\left[\frac{7}{8}, \frac{3}{4}, \frac{1}{8}\right]$	[120,156,209,247]
89	$\left[\frac{7}{8}, \frac{5}{8}, \frac{1}{4}\right]$	[124,186,232,285]
90	$\left[\frac{3}{8}, \frac{5}{8}, 0\right]$	[125,187,231,287]
91	$\left[\frac{7}{8}, \frac{5}{8}, 0\right]$	[135,191,221,283]
92	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{4}\right]$	[136,189,220,282]
93	$\left[\frac{7}{8}, \frac{1}{8}, \frac{3}{4}\right]$	[138,172,237,280]
94	$\left[\frac{3}{8}, \frac{1}{8}, \frac{1}{2}\right]$	[139,173,239,279]
95	$\left[\frac{3}{8}, \frac{1}{8}, \frac{3}{4}\right]$	[141,184,234,268]
96	$\left[\frac{7}{8}, \frac{1}{8}, \frac{1}{2}\right]$	[143,183,235,269]

Table 7: Wyckoff site: 96g, site symmetry: 2.mm

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

continued ...

Table 7

No.	position	mapping
47	$\left[\frac{1}{8}, \frac{1}{8}, \frac{1}{4} - x\right]$	[163,167,173,183]
48	$\left[\frac{1}{8}, \frac{3}{4} - x, \frac{5}{8}\right]$	[164,166,174,179]
49	$\left[x, \frac{5}{8}, \frac{1}{8}\right]$	[193,200,229,230]
50	$\left[x + \frac{1}{4}, \frac{3}{8}, \frac{3}{8}\right]$	[194,225,243,274]
51	$\left[x + \frac{1}{4}, \frac{7}{8}, \frac{7}{8}\right]$	[195,226,242,273]
52	$\left[\frac{7}{8}, \frac{7}{8}, \frac{1}{2} - x\right]$	[196,237,352,378]
53	$\left[\frac{3}{8}, \frac{7}{8}, x + \frac{3}{4}\right]$	[197,239,351,379]
54	$\left[\frac{3}{8}, x + \frac{1}{4}, \frac{3}{8}\right]$	[198,238,299,332]
55	$\left[\frac{7}{8}, -x, \frac{3}{8}\right]$	[199,240,300,329]
56	$\left[\frac{1}{4} - x, \frac{5}{8}, \frac{1}{8}\right]$	[201,202,218,219]
57	$\left[\frac{7}{8}, x + \frac{1}{4}, \frac{7}{8}\right]$	[203,236,294,334]
58	$\left[\frac{3}{8}, -x, \frac{7}{8}\right]$	[204,233,295,336]
59	$\left[-x, \frac{7}{8}, \frac{3}{8}\right]$	[205,224,254,265]
60	$\left[-x, \frac{3}{8}, \frac{7}{8}\right]$	[206,217,253,272]
61	$\left[\frac{7}{8}, \frac{3}{8}, x + \frac{3}{4}\right]$	[207,235,341,383]
62	$\left[\frac{3}{8}, \frac{3}{8}, \frac{1}{2} - x\right]$	[208,234,340,381]
63	$\left[\frac{5}{8}, x, \frac{1}{8}\right]$	[209,216,223,228]
64	$\left[\frac{5}{8}, \frac{5}{8}, x + \frac{1}{2}\right]$	[210,213,220,232]
65	$\left[\frac{5}{8}, \frac{5}{8}, \frac{3}{4} - x\right]$	[211,215,221,231]
66	$\left[\frac{5}{8}, \frac{1}{4} - x, \frac{1}{8}\right]$	[212,214,222,227]
67	$\left[x, \frac{1}{8}, \frac{5}{8}\right]$	[241,248,277,278]
68	$\left[\frac{7}{8}, \frac{3}{8}, -x\right]$	[244,285,304,330]
69	$\left[\frac{3}{8}, \frac{3}{8}, x + \frac{1}{4}\right]$	[245,287,303,331]
70	$\left[\frac{3}{8}, x + \frac{3}{4}, \frac{7}{8}\right]$	[246,286,347,380]
71	$\left[\frac{7}{8}, \frac{1}{2} - x, \frac{7}{8}\right]$	[247,288,348,377]
72	$\left[\frac{1}{4} - x, \frac{1}{8}, \frac{5}{8}\right]$	[249,250,266,267]
73	$\left[\frac{7}{8}, x + \frac{3}{4}, \frac{3}{8}\right]$	[251,284,342,382]
74	$\left[\frac{3}{8}, \frac{1}{2} - x, \frac{3}{8}\right]$	[252,281,343,384]
75	$\left[\frac{7}{8}, \frac{7}{8}, x + \frac{1}{4}\right]$	[255,283,293,335]
76	$\left[\frac{3}{8}, \frac{7}{8}, -x\right]$	[256,282,292,333]
77	$\left[\frac{5}{8}, x + \frac{1}{2}, \frac{5}{8}\right]$	[257,264,271,276]
78	$\left[\frac{5}{8}, \frac{1}{8}, x\right]$	[258,261,268,280]
79	$\left[\frac{5}{8}, \frac{1}{8}, \frac{1}{4} - x\right]$	[259,263,269,279]
80	$\left[\frac{5}{8}, \frac{3}{4} - x, \frac{5}{8}\right]$	[260,262,270,275]
81	$\left[x + \frac{1}{2}, \frac{5}{8}, \frac{5}{8}\right]$	[289,296,325,326]
82	$\left[x + \frac{3}{4}, \frac{3}{8}, \frac{7}{8}\right]$	[290,321,339,370]
83	$\left[x + \frac{3}{4}, \frac{7}{8}, \frac{3}{8}\right]$	[291,322,338,369]
84	$\left[\frac{3}{4} - x, \frac{5}{8}, \frac{5}{8}\right]$	[297,298,314,315]
85	$\left[\frac{1}{2} - x, \frac{7}{8}, \frac{7}{8}\right]$	[301,320,350,361]
86	$\left[\frac{1}{2} - x, \frac{3}{8}, \frac{3}{8}\right]$	[302,313,349,368]
87	$\left[\frac{1}{8}, x, \frac{5}{8}\right]$	[305,312,319,324]
88	$\left[\frac{1}{8}, \frac{5}{8}, x\right]$	[306,309,316,328]
89	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{4} - x\right]$	[307,311,317,327]
90	$\left[\frac{1}{8}, \frac{1}{4} - x, \frac{5}{8}\right]$	[308,310,318,323]
91	$\left[x + \frac{1}{2}, \frac{1}{8}, \frac{1}{8}\right]$	[337,344,373,374]
92	$\left[\frac{3}{4} - x, \frac{1}{8}, \frac{1}{8}\right]$	[345,346,362,363]
93	$\left[\frac{1}{8}, x + \frac{1}{2}, \frac{1}{8}\right]$	[353,360,367,372]

continued ...

Table 7

No.	position	mapping
94	$\left[\frac{1}{8}, \frac{1}{8}, x+\frac{1}{2}\right]$	[354,357,364,376]
95	$\left[\frac{1}{8}, \frac{1}{8}, \frac{3}{4}-x\right]$	[355,359,365,375]
96	$\left[\frac{1}{8}, \frac{3}{4}-x, \frac{1}{8}\right]$	[356,358,366,371]

Table 8: Wyckoff site: 192h, site symmetry: 2'..

No.	position	mapping
1	$\left[x, \frac{5}{8}, \frac{7}{8}\right]$	[1,200]
2	$\left[x+\frac{1}{4}, \frac{1}{8}, \frac{7}{8}\right]$	[2,195]
3	$\left[x+\frac{1}{4}, \frac{1}{8}, \frac{3}{8}\right]$	[3,194]
4	$\left[\frac{1}{8}, \frac{7}{8}, -x\right]$	[4,256]
5	$\left[\frac{1}{8}, \frac{7}{8}, x+\frac{1}{4}\right]$	[5,255]
6	$\left[\frac{3}{8}, x+\frac{1}{4}, \frac{1}{8}\right]$	[6,299]
7	$\left[\frac{7}{8}, -x, \frac{1}{8}\right]$	[7,300]
8	$\left[x, \frac{5}{8}, \frac{3}{8}\right]$	[8,193]
9	$\left[\frac{1}{4}-x, \frac{5}{8}, \frac{3}{8}\right]$	[9,202]
10	$\left[\frac{1}{4}-x, \frac{5}{8}, \frac{7}{8}\right]$	[10,201]
11	$\left[\frac{7}{8}, x+\frac{1}{4}, \frac{1}{8}\right]$	[11,294]
12	$\left[\frac{3}{8}, -x, \frac{1}{8}\right]$	[12,295]
13	$\left[-x, \frac{1}{8}, \frac{7}{8}\right]$	[13,206]
14	$\left[-x, \frac{1}{8}, \frac{3}{8}\right]$	[14,205]
15	$\left[\frac{1}{8}, \frac{3}{8}, x+\frac{1}{4}\right]$	[15,245]
16	$\left[\frac{1}{8}, \frac{3}{8}, -x\right]$	[16,244]
17	$\left[\frac{7}{8}, x, \frac{5}{8}\right]$	[17,312]
18	$\left[\frac{5}{8}, \frac{7}{8}, x\right]$	[18,261]
19	$\left[\frac{5}{8}, \frac{7}{8}, \frac{1}{4}-x\right]$	[19,263]
20	$\left[\frac{3}{8}, \frac{1}{4}-x, \frac{5}{8}\right]$	[20,310]
21	$\left[\frac{5}{8}, \frac{3}{8}, x\right]$	[21,258]
22	$\left[\frac{7}{8}, \frac{1}{4}-x, \frac{5}{8}\right]$	[22,308]
23	$\left[\frac{5}{8}, \frac{3}{8}, \frac{1}{4}-x\right]$	[23,259]
24	$\left[\frac{3}{8}, x, \frac{5}{8}\right]$	[24,305]
25	$\left[-x, \frac{3}{8}, \frac{1}{8}\right]$	[25,272]
26	$\left[\frac{1}{4}-x, \frac{7}{8}, \frac{5}{8}\right]$	[26,267]
27	$\left[\frac{1}{4}-x, \frac{3}{8}, \frac{5}{8}\right]$	[27,266]
28	$\left[\frac{3}{8}, \frac{5}{8}, x\right]$	[28,328]
29	$\left[\frac{7}{8}, \frac{5}{8}, \frac{1}{4}-x\right]$	[29,327]
30	$\left[\frac{5}{8}, \frac{1}{4}-x, \frac{3}{8}\right]$	[30,227]
31	$\left[\frac{5}{8}, x, \frac{3}{8}\right]$	[31,228]
32	$\left[-x, \frac{7}{8}, \frac{1}{8}\right]$	[32,265]
33	$\left[x+\frac{1}{4}, \frac{3}{8}, \frac{1}{8}\right]$	[33,274]
34	$\left[x+\frac{1}{4}, \frac{7}{8}, \frac{1}{8}\right]$	[34,273]
35	$\left[\frac{5}{8}, \frac{1}{4}-x, \frac{7}{8}\right]$	[35,222]
36	$\left[\frac{5}{8}, x, \frac{7}{8}\right]$	[36,223]
37	$\left[x, \frac{3}{8}, \frac{5}{8}\right]$	[37,278]

continued ...

Table 8

No.	position	mapping
38	$\left[x, \frac{7}{8}, \frac{5}{8}\right]$	[38,277]
39	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{4} - x\right]$	[39,317]
40	$\left[\frac{7}{8}, \frac{5}{8}, x\right]$	[40,316]
41	$\left[\frac{1}{8}, -x, \frac{3}{8}\right]$	[41,240]
42	$\left[\frac{3}{8}, \frac{1}{8}, -x\right]$	[42,333]
43	$\left[\frac{7}{8}, \frac{1}{8}, x + \frac{1}{4}\right]$	[43,335]
44	$\left[\frac{1}{8}, x + \frac{1}{4}, \frac{3}{8}\right]$	[44,238]
45	$\left[\frac{7}{8}, \frac{1}{8}, -x\right]$	[45,330]
46	$\left[\frac{1}{8}, x + \frac{1}{4}, \frac{7}{8}\right]$	[46,236]
47	$\left[\frac{3}{8}, \frac{1}{8}, x + \frac{1}{4}\right]$	[47,331]
48	$\left[\frac{1}{8}, -x, \frac{7}{8}\right]$	[48,233]
49	$\left[x, \frac{1}{8}, \frac{3}{8}\right]$	[49,248]
50	$\left[x + \frac{1}{4}, \frac{5}{8}, \frac{3}{8}\right]$	[50,243]
51	$\left[x + \frac{1}{4}, \frac{5}{8}, \frac{7}{8}\right]$	[51,242]
52	$\left[\frac{1}{8}, \frac{3}{8}, \frac{1}{2} - x\right]$	[52,208]
53	$\left[\frac{1}{8}, \frac{3}{8}, x + \frac{3}{4}\right]$	[53,207]
54	$\left[\frac{3}{8}, x + \frac{3}{4}, \frac{5}{8}\right]$	[54,347]
55	$\left[\frac{7}{8}, \frac{1}{2} - x, \frac{5}{8}\right]$	[55,348]
56	$\left[x, \frac{1}{8}, \frac{7}{8}\right]$	[56,241]
57	$\left[\frac{1}{4} - x, \frac{1}{8}, \frac{7}{8}\right]$	[57,250]
58	$\left[\frac{1}{4} - x, \frac{1}{8}, \frac{3}{8}\right]$	[58,249]
59	$\left[\frac{7}{8}, x + \frac{3}{4}, \frac{5}{8}\right]$	[59,342]
60	$\left[\frac{3}{8}, \frac{1}{2} - x, \frac{5}{8}\right]$	[60,343]
61	$\left[-x, \frac{5}{8}, \frac{3}{8}\right]$	[61,254]
62	$\left[-x, \frac{5}{8}, \frac{7}{8}\right]$	[62,253]
63	$\left[\frac{1}{8}, \frac{7}{8}, x + \frac{3}{4}\right]$	[63,197]
64	$\left[\frac{1}{8}, \frac{7}{8}, \frac{1}{2} - x\right]$	[64,196]
65	$\left[\frac{7}{8}, x + \frac{1}{2}, \frac{1}{8}\right]$	[65,360]
66	$\left[\frac{5}{8}, \frac{3}{8}, x + \frac{1}{2}\right]$	[66,213]
67	$\left[\frac{5}{8}, \frac{3}{8}, \frac{3}{4} - x\right]$	[67,215]
68	$\left[\frac{3}{8}, \frac{3}{4} - x, \frac{1}{8}\right]$	[68,358]
69	$\left[\frac{5}{8}, \frac{7}{8}, x + \frac{1}{2}\right]$	[69,210]
70	$\left[\frac{7}{8}, \frac{3}{4} - x, \frac{1}{8}\right]$	[70,356]
71	$\left[\frac{5}{8}, \frac{7}{8}, \frac{3}{4} - x\right]$	[71,211]
72	$\left[\frac{3}{8}, x + \frac{1}{2}, \frac{1}{8}\right]$	[72,353]
73	$\left[-x, \frac{7}{8}, \frac{5}{8}\right]$	[73,224]
74	$\left[\frac{1}{4} - x, \frac{3}{8}, \frac{1}{8}\right]$	[74,219]
75	$\left[\frac{1}{4} - x, \frac{7}{8}, \frac{1}{8}\right]$	[75,218]
76	$\left[\frac{3}{8}, \frac{1}{8}, x + \frac{1}{2}\right]$	[76,376]
77	$\left[\frac{7}{8}, \frac{1}{8}, \frac{3}{4} - x\right]$	[77,375]
78	$\left[\frac{5}{8}, \frac{3}{4} - x, \frac{7}{8}\right]$	[78,275]
79	$\left[\frac{5}{8}, x + \frac{1}{2}, \frac{7}{8}\right]$	[79,276]
80	$\left[-x, \frac{3}{8}, \frac{5}{8}\right]$	[80,217]
81	$\left[x + \frac{1}{4}, \frac{7}{8}, \frac{5}{8}\right]$	[81,226]
82	$\left[x + \frac{1}{4}, \frac{3}{8}, \frac{5}{8}\right]$	[82,225]
83	$\left[\frac{5}{8}, \frac{3}{4} - x, \frac{3}{8}\right]$	[83,270]
84	$\left[\frac{5}{8}, x + \frac{1}{2}, \frac{3}{8}\right]$	[84,271]

continued ...

Table 8

No.	position	mapping
85	$\left[x,\ \frac{7}{8},\ \frac{1}{8}\right]$	[85,230]
86	$\left[x,\ \frac{3}{8},\ \frac{1}{8}\right]$	[86,229]
87	$\left[\frac{3}{8},\ \frac{1}{8},\ \frac{3}{4}-x\right]$	[87,365]
88	$\left[\frac{7}{8},\ \frac{1}{8},\ x+\frac{1}{2}\right]$	[88,364]
89	$\left[\frac{1}{8},\ \frac{1}{2}-x,\ \frac{7}{8}\right]$	[89,288]
90	$\left[\frac{3}{8},\ \frac{5}{8},\ \frac{1}{2}-x\right]$	[90,381]
91	$\left[\frac{7}{8},\ \frac{5}{8},\ x+\frac{3}{4}\right]$	[91,383]
92	$\left[\frac{1}{8},\ x+\frac{3}{4},\ \frac{7}{8}\right]$	[92,286]
93	$\left[\frac{7}{8},\ \frac{5}{8},\ \frac{1}{2}-x\right]$	[93,378]
94	$\left[\frac{1}{8},\ x+\frac{3}{4},\ \frac{3}{8}\right]$	[94,284]
95	$\left[\frac{3}{8},\ \frac{5}{8},\ x+\frac{3}{4}\right]$	[95,379]
96	$\left[\frac{1}{8},\ \frac{1}{2}-x,\ \frac{3}{8}\right]$	[96,281]
97	$\left[x+\frac{1}{2},\ \frac{5}{8},\ \frac{3}{8}\right]$	[97,296]
98	$\left[x+\frac{3}{4},\ \frac{1}{8},\ \frac{3}{8}\right]$	[98,291]
99	$\left[x+\frac{3}{4},\ \frac{1}{8},\ \frac{7}{8}\right]$	[99,290]
100	$\left[\frac{5}{8},\ \frac{7}{8},\ \frac{1}{2}-x\right]$	[100,352]
101	$\left[\frac{5}{8},\ \frac{7}{8},\ x+\frac{3}{4}\right]$	[101,351]
102	$\left[\frac{7}{8},\ x+\frac{1}{4},\ \frac{5}{8}\right]$	[102,203]
103	$\left[\frac{3}{8},\ -x,\ \frac{5}{8}\right]$	[103,204]
104	$\left[x+\frac{1}{2},\ \frac{5}{8},\ \frac{7}{8}\right]$	[104,289]
105	$\left[\frac{3}{4}-x,\ \frac{5}{8},\ \frac{7}{8}\right]$	[105,298]
106	$\left[\frac{3}{4}-x,\ \frac{5}{8},\ \frac{3}{8}\right]$	[106,297]
107	$\left[\frac{3}{8},\ x+\frac{1}{4},\ \frac{5}{8}\right]$	[107,198]
108	$\left[\frac{7}{8},\ -x,\ \frac{5}{8}\right]$	[108,199]
109	$\left[\frac{1}{2}-x,\ \frac{1}{8},\ \frac{3}{8}\right]$	[109,302]
110	$\left[\frac{1}{2}-x,\ \frac{1}{8},\ \frac{7}{8}\right]$	[110,301]
111	$\left[\frac{5}{8},\ \frac{3}{8},\ x+\frac{3}{4}\right]$	[111,341]
112	$\left[\frac{5}{8},\ \frac{3}{8},\ \frac{1}{2}-x\right]$	[112,340]
113	$\left[\frac{3}{8},\ x,\ \frac{1}{8}\right]$	[113,216]
114	$\left[\frac{1}{8},\ \frac{7}{8},\ x+\frac{1}{2}\right]$	[114,357]
115	$\left[\frac{1}{8},\ \frac{7}{8},\ \frac{3}{4}-x\right]$	[115,359]
116	$\left[\frac{7}{8},\ \frac{1}{4}-x,\ \frac{1}{8}\right]$	[116,214]
117	$\left[\frac{1}{8},\ \frac{3}{8},\ x+\frac{1}{2}\right]$	[117,354]
118	$\left[\frac{3}{8},\ \frac{1}{4}-x,\ \frac{1}{8}\right]$	[118,212]
119	$\left[\frac{1}{8},\ \frac{3}{8},\ \frac{3}{4}-x\right]$	[119,355]
120	$\left[\frac{7}{8},\ x,\ \frac{1}{8}\right]$	[120,209]
121	$\left[\frac{1}{2}-x,\ \frac{3}{8},\ \frac{5}{8}\right]$	[121,368]
122	$\left[\frac{3}{4}-x,\ \frac{7}{8},\ \frac{1}{8}\right]$	[122,363]
123	$\left[\frac{3}{4}-x,\ \frac{3}{8},\ \frac{1}{8}\right]$	[123,362]
124	$\left[\frac{7}{8},\ \frac{5}{8},\ x+\frac{1}{2}\right]$	[124,232]
125	$\left[\frac{3}{8},\ \frac{5}{8},\ \frac{3}{4}-x\right]$	[125,231]
126	$\left[\frac{1}{8},\ \frac{1}{4}-x,\ \frac{7}{8}\right]$	[126,323]
127	$\left[\frac{1}{8},\ x,\ \frac{7}{8}\right]$	[127,324]
128	$\left[\frac{1}{2}-x,\ \frac{7}{8},\ \frac{5}{8}\right]$	[128,361]
129	$\left[x+\frac{3}{4},\ \frac{3}{8},\ \frac{5}{8}\right]$	[129,370]
130	$\left[x+\frac{3}{4},\ \frac{7}{8},\ \frac{5}{8}\right]$	[130,369]
131	$\left[\frac{1}{8},\ \frac{1}{4}-x,\ \frac{3}{8}\right]$	[131,318]

continued ...

Table 8

No.	position	mapping
132	$\left[\frac{1}{8}, x, \frac{3}{8}\right]$	[132,319]
133	$\left[x+\frac{1}{2}, \frac{3}{8}, \frac{1}{8}\right]$	[133,374]
134	$\left[x+\frac{1}{2}, \frac{7}{8}, \frac{1}{8}\right]$	[134,373]
135	$\left[\frac{7}{8}, \frac{5}{8}, \frac{3}{4}-x\right]$	[135,221]
136	$\left[\frac{3}{8}, \frac{5}{8}, x+\frac{1}{2}\right]$	[136,220]
137	$\left[\frac{5}{8}, -x, \frac{7}{8}\right]$	[137,336]
138	$\left[\frac{7}{8}, \frac{1}{8}, \frac{1}{2}-x\right]$	[138,237]
139	$\left[\frac{3}{8}, \frac{1}{8}, x+\frac{3}{4}\right]$	[139,239]
140	$\left[\frac{5}{8}, x+\frac{1}{4}, \frac{7}{8}\right]$	[140,334]
141	$\left[\frac{3}{8}, \frac{1}{8}, \frac{1}{2}-x\right]$	[141,234]
142	$\left[\frac{5}{8}, x+\frac{1}{4}, \frac{3}{8}\right]$	[142,332]
143	$\left[\frac{7}{8}, \frac{1}{8}, x+\frac{3}{4}\right]$	[143,235]
144	$\left[\frac{5}{8}, -x, \frac{3}{8}\right]$	[144,329]
145	$\left[x+\frac{1}{2}, \frac{1}{8}, \frac{7}{8}\right]$	[145,344]
146	$\left[x+\frac{3}{4}, \frac{5}{8}, \frac{7}{8}\right]$	[146,339]
147	$\left[x+\frac{3}{4}, \frac{5}{8}, \frac{3}{8}\right]$	[147,338]
148	$\left[\frac{5}{8}, \frac{3}{8}, -x\right]$	[148,304]
149	$\left[\frac{5}{8}, \frac{3}{8}, x+\frac{1}{4}\right]$	[149,303]
150	$\left[\frac{7}{8}, x+\frac{3}{4}, \frac{1}{8}\right]$	[150,251]
151	$\left[\frac{3}{8}, \frac{1}{2}-x, \frac{1}{8}\right]$	[151,252]
152	$\left[x+\frac{1}{2}, \frac{1}{8}, \frac{3}{8}\right]$	[152,337]
153	$\left[\frac{3}{4}-x, \frac{1}{8}, \frac{3}{8}\right]$	[153,346]
154	$\left[\frac{3}{4}-x, \frac{1}{8}, \frac{7}{8}\right]$	[154,345]
155	$\left[\frac{3}{8}, x+\frac{3}{4}, \frac{1}{8}\right]$	[155,246]
156	$\left[\frac{7}{8}, \frac{1}{2}-x, \frac{1}{8}\right]$	[156,247]
157	$\left[\frac{1}{2}-x, \frac{5}{8}, \frac{7}{8}\right]$	[157,350]
158	$\left[\frac{1}{2}-x, \frac{5}{8}, \frac{3}{8}\right]$	[158,349]
159	$\left[\frac{5}{8}, \frac{7}{8}, x+\frac{1}{4}\right]$	[159,293]
160	$\left[\frac{5}{8}, \frac{7}{8}, -x\right]$	[160,292]
161	$\left[\frac{3}{8}, x+\frac{1}{2}, \frac{5}{8}\right]$	[161,264]
162	$\left[\frac{1}{8}, \frac{3}{8}, x\right]$	[162,309]
163	$\left[\frac{1}{8}, \frac{3}{8}, \frac{1}{4}-x\right]$	[163,311]
164	$\left[\frac{7}{8}, \frac{3}{4}-x, \frac{5}{8}\right]$	[164,262]
165	$\left[\frac{1}{8}, \frac{7}{8}, x\right]$	[165,306]
166	$\left[\frac{3}{8}, \frac{3}{4}-x, \frac{5}{8}\right]$	[166,260]
167	$\left[\frac{1}{8}, \frac{7}{8}, \frac{1}{4}-x\right]$	[167,307]
168	$\left[\frac{7}{8}, x+\frac{1}{2}, \frac{5}{8}\right]$	[168,257]
169	$\left[\frac{1}{2}-x, \frac{7}{8}, \frac{1}{8}\right]$	[169,320]
170	$\left[\frac{3}{4}-x, \frac{3}{8}, \frac{5}{8}\right]$	[170,315]
171	$\left[\frac{3}{4}-x, \frac{7}{8}, \frac{5}{8}\right]$	[171,314]
172	$\left[\frac{7}{8}, \frac{1}{8}, x\right]$	[172,280]
173	$\left[\frac{3}{8}, \frac{1}{8}, \frac{1}{4}-x\right]$	[173,279]
174	$\left[\frac{1}{8}, \frac{3}{4}-x, \frac{3}{8}\right]$	[174,371]
175	$\left[\frac{1}{8}, x+\frac{1}{2}, \frac{3}{8}\right]$	[175,372]
176	$\left[\frac{1}{2}-x, \frac{3}{8}, \frac{1}{8}\right]$	[176,313]
177	$\left[x+\frac{3}{4}, \frac{7}{8}, \frac{1}{8}\right]$	[177,322]
178	$\left[x+\frac{3}{4}, \frac{3}{8}, \frac{1}{8}\right]$	[178,321]

continued ...

Table 8

No.	position	mapping
179	$\left[\frac{1}{8},\ \frac{3}{4}-x,\ \frac{7}{8}\right]$	[179,366]
180	$\left[\frac{1}{8},\ x+\frac{1}{2},\ \frac{7}{8}\right]$	[180,367]
181	$\left[x+\frac{1}{2},\ \frac{7}{8},\ \frac{5}{8}\right]$	[181,326]
182	$\left[x+\frac{1}{2},\ \frac{3}{8},\ \frac{5}{8}\right]$	[182,325]
183	$\left[\frac{7}{8},\ \frac{1}{8},\ \frac{1}{4}-x\right]$	[183,269]
184	$\left[\frac{3}{8},\ \frac{1}{8},\ x\right]$	[184,268]
185	$\left[\frac{5}{8},\ \frac{1}{2}-x,\ \frac{3}{8}\right]$	[185,384]
186	$\left[\frac{7}{8},\ \frac{5}{8},\ -x\right]$	[186,285]
187	$\left[\frac{3}{8},\ \frac{5}{8},\ x+\frac{1}{4}\right]$	[187,287]
188	$\left[\frac{5}{8},\ x+\frac{3}{4},\ \frac{3}{8}\right]$	[188,382]
189	$\left[\frac{3}{8},\ \frac{5}{8},\ -x\right]$	[189,282]
190	$\left[\frac{5}{8},\ x+\frac{3}{4},\ \frac{7}{8}\right]$	[190,380]
191	$\left[\frac{7}{8},\ \frac{5}{8},\ x+\frac{1}{4}\right]$	[191,283]
192	$\left[\frac{5}{8},\ \frac{1}{2}-x,\ \frac{7}{8}\right]$	[192,377]

Table 9: Wyckoff site: 192i, site symmetry: ..2

No.	position	mapping
1	$\left[\frac{3}{4},\ y,\ y+\frac{1}{4}\right]$	[1,157]
2	$\left[0,\ \frac{3}{4}-y,\ y+\frac{1}{4}\right]$	[2,154]
3	$\left[0,\ y+\frac{1}{2},\ -y\right]$	[3,153]
4	$\left[y+\frac{1}{2},\ y+\frac{1}{4},\ \frac{1}{4}\right]$	[4,114]
5	$\left[\frac{3}{4}-y,\ y+\frac{1}{4},\ 0\right]$	[5,115]
6	$\left[-y,\ 0,\ y+\frac{1}{2}\right]$	[6,68]
7	$\left[y+\frac{1}{4},\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[7,65]
8	$\left[\frac{3}{4},\ \frac{1}{4}-y,\ -y\right]$	[8,158]
9	$\left[\frac{1}{2},\ y,\ -y\right]$	[9,147]
10	$\left[\frac{1}{2},\ \frac{1}{4}-y,\ y+\frac{1}{4}\right]$	[10,146]
11	$\left[y+\frac{1}{4},\ 0,\ \frac{3}{4}-y\right]$	[11,70]
12	$\left[-y,\ \frac{1}{4},\ \frac{3}{4}-y\right]$	[12,72]
13	$\left[\frac{1}{4},\ y+\frac{1}{2},\ y+\frac{1}{4}\right]$	[13,145]
14	$\left[\frac{1}{4},\ \frac{3}{4}-y,\ -y\right]$	[14,152]
15	$\left[y+\frac{1}{2},\ -y,\ 0\right]$	[15,119]
16	$\left[\frac{3}{4}-y,\ -y,\ \frac{1}{4}\right]$	[16,117]
17	$\left[y+\frac{1}{4},\ \frac{3}{4},\ y\right]$	[17,55]
18	$\left[y,\ y+\frac{1}{4},\ \frac{3}{4}\right]$	[18,100]
19	$\left[\frac{1}{4}-y,\ y+\frac{1}{4},\ \frac{1}{2}\right]$	[19,101]
20	$\left[-y,\ \frac{1}{2},\ y\right]$	[20,54]
21	$\left[\frac{1}{4}-y,\ -y,\ \frac{3}{4}\right]$	[21,112]
22	$\left[y+\frac{1}{4},\ \frac{1}{2},\ \frac{1}{4}-y\right]$	[22,59]
23	$\left[y,\ -y,\ \frac{1}{2}\right]$	[23,111]
24	$\left[-y,\ \frac{3}{4},\ \frac{1}{4}-y\right]$	[24,60]
25	$\left[\frac{1}{4},\ -y,\ \frac{3}{4}-y\right]$	[25,133]
26	$\left[\frac{1}{2},\ y+\frac{1}{4},\ \frac{1}{4}-y\right]$	[26,130]

continued ...

Table 9

No.	position	mapping
27	$\left[\frac{1}{2}, -y, y\right]$	[27,129]
28	$\left[-y, \frac{1}{4} - y, \frac{3}{4}\right]$	[28,90]
29	$\left[y + \frac{1}{4}, \frac{1}{4} - y, \frac{1}{2}\right]$	[29,91]
30	$\left[y, \frac{1}{2}, -y\right]$	[30,188]
31	$\left[\frac{1}{4} - y, \frac{3}{4}, -y\right]$	[31,185]
32	$\left[\frac{1}{4}, y + \frac{1}{4}, y + \frac{1}{2}\right]$	[32,134]
33	$\left[0, -y, y + \frac{1}{2}\right]$	[33,123]
34	$\left[0, y + \frac{1}{4}, \frac{3}{4} - y\right]$	[34,122]
35	$\left[\frac{1}{4} - y, \frac{1}{2}, y + \frac{1}{4}\right]$	[35,190]
36	$\left[y, \frac{3}{4}, y + \frac{1}{4}\right]$	[36,192]
37	$\left[\frac{3}{4}, -y, \frac{1}{4} - y\right]$	[37,121]
38	$\left[\frac{3}{4}, y + \frac{1}{4}, y\right]$	[38,128]
39	$\left[-y, y, \frac{1}{2}\right]$	[39,95]
40	$\left[y + \frac{1}{4}, y, \frac{3}{4}\right]$	[40,93]
41	$\left[\frac{3}{4} - y, \frac{1}{4}, -y\right]$	[41,175]
42	$\left[-y, \frac{3}{4} - y, \frac{1}{4}\right]$	[42,76]
43	$\left[y + \frac{1}{4}, \frac{3}{4} - y, 0\right]$	[43,77]
44	$\left[y + \frac{1}{2}, 0, -y\right]$	[44,174]
45	$\left[y + \frac{1}{4}, y + \frac{1}{2}, \frac{1}{4}\right]$	[45,88]
46	$\left[\frac{3}{4} - y, 0, y + \frac{1}{4}\right]$	[46,179]
47	$\left[-y, y + \frac{1}{2}, 0\right]$	[47,87]
48	$\left[y + \frac{1}{2}, \frac{1}{4}, y + \frac{1}{4}\right]$	[48,180]
49	$\left[\frac{3}{4}, y + \frac{1}{2}, y + \frac{3}{4}\right]$	[49,109]
50	$\left[0, \frac{1}{4} - y, y + \frac{3}{4}\right]$	[50,106]
51	$\left[0, y, \frac{1}{2} - y\right]$	[51,105]
52	$\left[y + \frac{1}{2}, y + \frac{3}{4}, \frac{3}{4}\right]$	[52,162]
53	$\left[\frac{3}{4} - y, y + \frac{3}{4}, \frac{1}{2}\right]$	[53,163]
54	$\left[\frac{3}{4}, \frac{3}{4} - y, \frac{1}{2} - y\right]$	[56,110]
55	$\left[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - y\right]$	[57,99]
56	$\left[\frac{1}{2}, \frac{3}{4} - y, y + \frac{3}{4}\right]$	[58,98]
57	$\left[\frac{1}{4}, y, y + \frac{3}{4}\right]$	[61,97]
58	$\left[\frac{1}{4}, \frac{1}{4} - y, \frac{1}{2} - y\right]$	[62,104]
59	$\left[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}\right]$	[63,167]
60	$\left[\frac{3}{4} - y, \frac{1}{2} - y, \frac{3}{4}\right]$	[64,165]
61	$\left[y, y + \frac{3}{4}, \frac{1}{4}\right]$	[66,148]
62	$\left[\frac{1}{4} - y, y + \frac{3}{4}, 0\right]$	[67,149]
63	$\left[\frac{1}{4} - y, \frac{1}{2} - y, \frac{1}{4}\right]$	[69,160]
64	$\left[y, \frac{1}{2} - y, 0\right]$	[71,159]
65	$\left[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{4} - y\right]$	[73,181]
66	$\left[\frac{1}{2}, y + \frac{3}{4}, \frac{3}{4} - y\right]$	[74,178]
67	$\left[\frac{1}{2}, \frac{1}{2} - y, y + \frac{1}{2}\right]$	[75,177]
68	$\left[y, 0, \frac{1}{2} - y\right]$	[78,140]
69	$\left[\frac{1}{4} - y, \frac{1}{4}, \frac{1}{2} - y\right]$	[79,137]
70	$\left[\frac{1}{4}, y + \frac{3}{4}, y\right]$	[80,182]
71	$\left[0, \frac{1}{2} - y, y\right]$	[81,171]
72	$\left[0, y + \frac{3}{4}, \frac{1}{4} - y\right]$	[82,170]
73	$\left[\frac{1}{4} - y, 0, y + \frac{3}{4}\right]$	[83,142]

continued ...

Table 9

No.	position	mapping
74	$\left[y,\ \frac{1}{4},\ y+\frac{3}{4}\right]$	[84,144]
75	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ \frac{3}{4}-y\right]$	[85,169]
76	$\left[\frac{3}{4},\ y+\frac{3}{4},\ y+\frac{1}{2}\right]$	[86,176]
77	$\left[\frac{3}{4}-y,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[89,127]
78	$\left[y+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[92,126]
79	$\left[\frac{3}{4}-y,\ \frac{1}{2},\ y+\frac{3}{4}\right]$	[94,131]
80	$\left[y+\frac{1}{2},\ \frac{3}{4},\ y+\frac{3}{4}\right]$	[96,132]
81	$\left[\frac{1}{2}-y,\ 0,\ y\right]$	[102,164]
82	$\left[y+\frac{3}{4},\ \frac{1}{4},\ y\right]$	[103,161]
83	$\left[y+\frac{3}{4},\ 0,\ \frac{1}{4}-y\right]$	[107,166]
84	$\left[\frac{1}{2}-y,\ \frac{1}{4},\ \frac{1}{4}-y\right]$	[108,168]
85	$\left[y+\frac{3}{4},\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[113,151]
86	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[116,150]
87	$\left[y+\frac{3}{4},\ \frac{1}{2},\ \frac{3}{4}-y\right]$	[118,155]
88	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ \frac{3}{4}-y\right]$	[120,156]
89	$\left[\frac{1}{2}-y,\ \frac{1}{4}-y,\ \frac{1}{4}\right]$	[124,186]
90	$\left[y+\frac{3}{4},\ \frac{1}{4}-y,\ 0\right]$	[125,187]
91	$\left[\frac{1}{2}-y,\ y,\ 0\right]$	[135,191]
92	$\left[y+\frac{3}{4},\ y,\ \frac{1}{4}\right]$	[136,189]
93	$\left[\frac{1}{2}-y,\ \frac{3}{4}-y,\ \frac{3}{4}\right]$	[138,172]
94	$\left[y+\frac{3}{4},\ \frac{3}{4}-y,\ \frac{1}{2}\right]$	[139,173]
95	$\left[y+\frac{3}{4},\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[141,184]
96	$\left[\frac{1}{2}-y,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[143,183]
97	$\left[\frac{3}{4},\ y,\ y+\frac{3}{4}\right]$	[193,349]
98	$\left[0,\ \frac{3}{4}-y,\ y+\frac{3}{4}\right]$	[194,346]
99	$\left[0,\ y+\frac{1}{2},\ \frac{1}{2}-y\right]$	[195,345]
100	$\left[y+\frac{1}{2},\ y+\frac{1}{4},\ \frac{3}{4}\right]$	[196,306]
101	$\left[\frac{3}{4}-y,\ y+\frac{1}{4},\ \frac{1}{2}\right]$	[197,307]
102	$[-y,\ 0,\ y]$	[198,260]
103	$\left[y+\frac{1}{4},\ \frac{1}{4},\ y\right]$	[199,257]
104	$\left[\frac{3}{4},\ \frac{1}{4}-y,\ \frac{1}{2}-y\right]$	[200,350]
105	$\left[\frac{1}{2},\ y,\ \frac{1}{2}-y\right]$	[201,339]
106	$\left[\frac{1}{2},\ \frac{1}{4}-y,\ y+\frac{3}{4}\right]$	[202,338]
107	$\left[y+\frac{1}{4},\ 0,\ \frac{1}{4}-y\right]$	[203,262]
108	$\left[-y,\ \frac{1}{4},\ \frac{1}{4}-y\right]$	[204,264]
109	$\left[\frac{1}{4},\ y+\frac{1}{2},\ y+\frac{3}{4}\right]$	[205,337]
110	$\left[\frac{1}{4},\ \frac{3}{4}-y,\ \frac{1}{2}-y\right]$	[206,344]
111	$\left[y+\frac{1}{2},\ -y,\ \frac{1}{2}\right]$	[207,311]
112	$\left[\frac{3}{4}-y,\ -y,\ \frac{3}{4}\right]$	[208,309]
113	$\left[y+\frac{1}{4},\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[209,247]
114	$\left[y,\ y+\frac{1}{4},\ \frac{1}{4}\right]$	[210,292]
115	$\left[\frac{1}{4}-y,\ y+\frac{1}{4},\ 0\right]$	[211,293]
116	$\left[-y,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[212,246]
117	$\left[\frac{1}{4}-y,\ -y,\ \frac{1}{4}\right]$	[213,304]
118	$\left[y+\frac{1}{4},\ \frac{1}{2},\ \frac{3}{4}-y\right]$	[214,251]
119	$[y,\ -y,\ 0]$	[215,303]
120	$\left[-y,\ \frac{3}{4},\ \frac{3}{4}-y\right]$	[216,252]

continued ...

Table 9

No.	position	mapping
121	$\left[\frac{1}{4},\ -y,\ \frac{1}{4}-y\right]$	[217,325]
122	$\left[\frac{1}{2},\ y+\frac{1}{4},\ \frac{3}{4}-y\right]$	[218,322]
123	$\left[\frac{1}{2},\ -y,\ y+\frac{1}{2}\right]$	[219,321]
124	$\left[-y,\ \frac{1}{4}-y,\ \frac{1}{4}\right]$	[220,282]
125	$\left[y+\frac{1}{4},\ \frac{1}{4}-y,\ 0\right]$	[221,283]
126	$\left[y,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[222,380]
127	$\left[\frac{1}{4}-y,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[223,377]
128	$\left[\frac{1}{4},\ y+\frac{1}{4},\ y\right]$	[224,326]
129	$[0,\ -y,\ y]$	[225,315]
130	$\left[0,\ y+\frac{1}{4},\ \frac{1}{4}-y\right]$	[226,314]
131	$\left[\frac{1}{4}-y,\ \frac{1}{2},\ y+\frac{3}{4}\right]$	[227,382]
132	$\left[y,\ \frac{3}{4},\ y+\frac{3}{4}\right]$	[228,384]
133	$\left[\frac{3}{4},\ -y,\ \frac{3}{4}-y\right]$	[229,313]
134	$\left[\frac{3}{4},\ y+\frac{1}{4},\ y+\frac{1}{2}\right]$	[230,320]
135	$[-y,\ y,\ 0]$	[231,287]
136	$\left[y+\frac{1}{4},\ y,\ \frac{1}{4}\right]$	[232,285]
137	$\left[\frac{3}{4}-y,\ \frac{1}{4},\ \frac{1}{2}-y\right]$	[233,367]
138	$\left[-y,\ \frac{3}{4}-y,\ \frac{3}{4}\right]$	[234,268]
139	$\left[y+\frac{1}{4},\ \frac{3}{4}-y,\ \frac{1}{2}\right]$	[235,269]
140	$\left[y+\frac{1}{2},\ 0,\ \frac{1}{2}-y\right]$	[236,366]
141	$\left[y+\frac{1}{4},\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[237,280]
142	$\left[\frac{3}{4}-y,\ 0,\ y+\frac{3}{4}\right]$	[238,371]
143	$\left[-y,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[239,279]
144	$\left[y+\frac{1}{2},\ \frac{1}{4},\ y+\frac{3}{4}\right]$	[240,372]
145	$\left[\frac{3}{4},\ y+\frac{1}{2},\ y+\frac{1}{4}\right]$	[241,301]
146	$\left[0,\ \frac{1}{4}-y,\ y+\frac{1}{4}\right]$	[242,298]
147	$[0,\ y,\ -y]$	[243,297]
148	$\left[y+\frac{1}{2},\ y+\frac{3}{4},\ \frac{1}{4}\right]$	[244,354]
149	$\left[\frac{3}{4}-y,\ y+\frac{3}{4},\ 0\right]$	[245,355]
150	$\left[\frac{3}{4},\ \frac{3}{4}-y,\ -y\right]$	[248,302]
151	$\left[\frac{1}{2},\ y+\frac{1}{2},\ -y\right]$	[249,291]
152	$\left[\frac{1}{2},\ \frac{3}{4}-y,\ y+\frac{1}{4}\right]$	[250,290]
153	$\left[\frac{1}{4},\ y,\ y+\frac{1}{4}\right]$	[253,289]
154	$\left[\frac{1}{4},\ \frac{1}{4}-y,\ -y\right]$	[254,296]
155	$\left[y+\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	[255,359]
156	$\left[\frac{3}{4}-y,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[256,357]
157	$\left[y,\ y+\frac{3}{4},\ \frac{3}{4}\right]$	[258,340]
158	$\left[\frac{1}{4}-y,\ y+\frac{3}{4},\ \frac{1}{2}\right]$	[259,341]
159	$\left[\frac{1}{4}-y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[261,352]
160	$\left[y,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[263,351]
161	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ \frac{3}{4}-y\right]$	[265,373]
162	$\left[\frac{1}{2},\ y+\frac{3}{4},\ \frac{1}{4}-y\right]$	[266,370]
163	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ y\right]$	[267,369]
164	$[y,\ 0,\ -y]$	[270,332]
165	$\left[\frac{1}{4}-y,\ \frac{1}{4},\ -y\right]$	[271,329]
166	$\left[\frac{1}{4},\ y+\frac{3}{4},\ y+\frac{1}{2}\right]$	[272,374]
167	$\left[0,\ \frac{1}{2}-y,\ y+\frac{1}{2}\right]$	[273,363]

continued ...

Table 9

No.	position	mapping
168	$\left[0,\, y+\frac{3}{4},\, \frac{3}{4}-y\right]$	[274,362]
169	$\left[\frac{1}{4}-y,\, 0,\, y+\frac{1}{4}\right]$	[275,334]
170	$\left[y,\, \frac{1}{4},\, y+\frac{1}{4}\right]$	[276,336]
171	$\left[\frac{3}{4},\, \frac{1}{2}-y,\, \frac{1}{4}-y\right]$	[277,361]
172	$\left[\frac{3}{4},\, y+\frac{3}{4},\, y\right]$	[278,368]
173	$\left[\frac{3}{4}-y,\, \frac{3}{4},\, -y\right]$	[281,319]
174	$\left[y+\frac{1}{2},\, \frac{1}{2},\, -y\right]$	[284,318]
175	$\left[\frac{3}{4}-y,\, \frac{1}{2},\, y+\frac{1}{4}\right]$	[286,323]
176	$\left[y+\frac{1}{2},\, \frac{3}{4},\, y+\frac{1}{4}\right]$	[288,324]
177	$\left[\frac{1}{2}-y,\, 0,\, y+\frac{1}{2}\right]$	[294,356]
178	$\left[y+\frac{3}{4},\, \frac{1}{4},\, y+\frac{1}{2}\right]$	[295,353]
179	$\left[y+\frac{3}{4},\, 0,\, \frac{3}{4}-y\right]$	[299,358]
180	$\left[\frac{1}{2}-y,\, \frac{1}{4},\, \frac{3}{4}-y\right]$	[300,360]
181	$\left[y+\frac{3}{4},\, \frac{3}{4},\, y\right]$	[305,343]
182	$\left[\frac{1}{2}-y,\, \frac{1}{2},\, y\right]$	[308,342]
183	$\left[y+\frac{3}{4},\, \frac{1}{2},\, \frac{1}{4}-y\right]$	[310,347]
184	$\left[\frac{1}{2}-y,\, \frac{3}{4},\, \frac{1}{4}-y\right]$	[312,348]
185	$\left[\frac{1}{2}-y,\, \frac{1}{4}-y,\, \frac{3}{4}\right]$	[316,378]
186	$\left[y+\frac{3}{4},\, \frac{1}{4}-y,\, \frac{1}{2}\right]$	[317,379]
187	$\left[\frac{1}{2}-y,\, y,\, \frac{1}{2}\right]$	[327,383]
188	$\left[y+\frac{3}{4},\, y,\, \frac{3}{4}\right]$	[328,381]
189	$\left[\frac{1}{2}-y,\, \frac{3}{4}-y,\, \frac{1}{4}\right]$	[330,364]
190	$\left[y+\frac{3}{4},\, \frac{3}{4}-y,\, 0\right]$	[331,365]
191	$\left[y+\frac{3}{4},\, y+\frac{1}{2},\, \frac{1}{4}\right]$	[333,376]
192	$\left[\frac{1}{2}-y,\, y+\frac{1}{2},\, 0\right]$	[335,375]

Table 10: Wyckoff site: 192j, site symmetry: ..2'

No.	position	mapping
1	$\left[\frac{3}{4},\, y,\, -y\right]$	[1,302]
2	$\left[0,\, y,\, y+\frac{1}{4}\right]$	[2,297]
3	$\left[0,\, \frac{1}{4}-y,\, -y\right]$	[3,298]
4	$\left[\frac{1}{4}-y,\, y+\frac{1}{4},\, \frac{1}{4}\right]$	[4,213]
5	$\left[y,\, y+\frac{1}{4},\, 0\right]$	[5,215]
6	$\left[-y,\, 0,\, \frac{1}{4}-y\right]$	[6,262]
7	$\left[y+\frac{1}{4},\, \frac{1}{4},\, \frac{1}{4}-y\right]$	[7,264]
8	$\left[\frac{3}{4},\, \frac{1}{4}-y,\, y+\frac{1}{4}\right]$	[8,301]
9	$\left[\frac{1}{2},\, y,\, y+\frac{1}{4}\right]$	[9,290]
10	$\left[\frac{1}{2},\, \frac{1}{4}-y,\, -y\right]$	[10,291]
11	$\left[y+\frac{1}{4},\, 0,\, y\right]$	[11,260]
12	$\left[-y,\, \frac{1}{4},\, y\right]$	[12,257]
13	$\left[\frac{1}{4},\, \frac{1}{4}-y,\, y+\frac{1}{4}\right]$	[13,296]
14	$\left[\frac{1}{4},\, y,\, -y\right]$	[14,289]
15	$\left[\frac{1}{4}-y,\, -y,\, 0\right]$	[15,211]

continued ...

Table 10

No.	position	mapping
16	$\left[y,\ -y,\ \frac{1}{4}\right]$	[16,210]
17	$\left[-y,\ \frac{3}{4},\ y\right]$	[17,252]
18	$\left[y,\ -y,\ \frac{3}{4}\right]$	[18,208]
19	$\left[\frac{1}{4}-y,\ -y,\ \frac{1}{2}\right]$	[19,207]
20	$\left[y+\frac{1}{4},\ \frac{1}{2},\ y\right]$	[20,251]
21	$\left[\frac{1}{4}-y,\ y+\frac{1}{4},\ \frac{3}{4}\right]$	[21,196]
22	$\left[-y,\ \frac{1}{2},\ \frac{1}{4}-y\right]$	[22,246]
23	$\left[y,\ y+\frac{1}{4},\ \frac{1}{2}\right]$	[23,197]
24	$\left[y+\frac{1}{4},\ \frac{3}{4},\ \frac{1}{4}-y\right]$	[24,247]
25	$\left[\frac{1}{4},\ -y,\ y\right]$	[25,326]
26	$\left[\frac{1}{2},\ -y,\ \frac{1}{4}-y\right]$	[26,321]
27	$\left[\frac{1}{2},\ y+\frac{1}{4},\ y\right]$	[27,322]
28	$\left[y+\frac{1}{4},\ \frac{1}{4}-y,\ \frac{3}{4}\right]$	[28,237]
29	$\left[-y,\ \frac{1}{4}-y,\ \frac{1}{2}\right]$	[29,239]
30	$\left[y,\ \frac{1}{2},\ y+\frac{1}{4}\right]$	[30,286]
31	$\left[\frac{1}{4}-y,\ \frac{3}{4},\ y+\frac{1}{4}\right]$	[31,288]
32	$\left[\frac{1}{4},\ y+\frac{1}{4},\ \frac{1}{4}-y\right]$	[32,325]
33	$\left[0,\ -y,\ \frac{1}{4}-y\right]$	[33,314]
34	$\left[0,\ y+\frac{1}{4},\ y\right]$	[34,315]
35	$\left[\frac{1}{4}-y,\ \frac{1}{2},\ -y\right]$	[35,284]
36	$\left[y,\ \frac{3}{4},\ -y\right]$	[36,281]
37	$\left[\frac{3}{4},\ y+\frac{1}{4},\ \frac{1}{4}-y\right]$	[37,320]
38	$\left[\frac{3}{4},\ -y,\ y\right]$	[38,313]
39	$\left[y+\frac{1}{4},\ y,\ \frac{1}{2}\right]$	[39,235]
40	$\left[-y,\ y,\ \frac{3}{4}\right]$	[40,234]
41	$\left[y,\ \frac{1}{4},\ -y\right]$	[41,276]
42	$\left[-y,\ y,\ \frac{1}{4}\right]$	[42,232]
43	$\left[y+\frac{1}{4},\ y,\ 0\right]$	[43,231]
44	$\left[\frac{1}{4}-y,\ 0,\ -y\right]$	[44,275]
45	$\left[y+\frac{1}{4},\ \frac{1}{4}-y,\ \frac{1}{4}\right]$	[45,220]
46	$\left[y,\ 0,\ y+\frac{1}{4}\right]$	[46,270]
47	$\left[-y,\ \frac{1}{4}-y,\ 0\right]$	[47,221]
48	$\left[\frac{1}{4}-y,\ \frac{1}{4},\ y+\frac{1}{4}\right]$	[48,271]
49	$\left[\frac{3}{4},\ y+\frac{1}{2},\ \frac{1}{2}-y\right]$	[49,350]
50	$\left[0,\ y+\frac{1}{2},\ y+\frac{3}{4}\right]$	[50,345]
51	$\left[0,\ \frac{3}{4}-y,\ \frac{1}{2}-y\right]$	[51,346]
52	$\left[\frac{1}{4}-y,\ y+\frac{3}{4},\ \frac{3}{4}\right]$	[52,261]
53	$\left[y,\ y+\frac{3}{4},\ \frac{1}{2}\right]$	[53,263]
54	$\left[-y,\ \frac{1}{2},\ \frac{3}{4}-y\right]$	[54,214]
55	$\left[y+\frac{1}{4},\ \frac{3}{4},\ \frac{3}{4}-y\right]$	[55,216]
56	$\left[\frac{3}{4},\ \frac{3}{4}-y,\ y+\frac{3}{4}\right]$	[56,349]
57	$\left[\frac{1}{2},\ y+\frac{1}{2},\ y+\frac{3}{4}\right]$	[57,338]
58	$\left[\frac{1}{2},\ \frac{3}{4}-y,\ \frac{1}{2}-y\right]$	[58,339]
59	$\left[y+\frac{1}{4},\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[59,212]
60	$\left[-y,\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[60,209]
61	$\left[\frac{1}{4},\ \frac{3}{4}-y,\ y+\frac{3}{4}\right]$	[61,344]
62	$\left[\frac{1}{4},\ y+\frac{1}{2},\ \frac{1}{2}-y\right]$	[62,337]

continued ...

Table 10

No.	position	mapping
63	$\left[\frac{1}{4}-y,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[63,259]
64	$\left[y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[64,258]
65	$\left[-y,\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[65,204]
66	$\left[y,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[66,256]
67	$\left[\frac{1}{4}-y,\ \frac{1}{2}-y,\ 0\right]$	[67,255]
68	$\left[y+\frac{1}{4},\ 0,\ y+\frac{1}{2}\right]$	[68,203]
69	$\left[\frac{1}{4}-y,\ y+\frac{3}{4},\ \frac{1}{4}\right]$	[69,244]
70	$\left[-y,\ 0,\ \frac{3}{4}-y\right]$	[70,198]
71	$\left[y,\ y+\frac{3}{4},\ 0\right]$	[71,245]
72	$\left[y+\frac{1}{4},\ \frac{1}{4},\ \frac{3}{4}-y\right]$	[72,199]
73	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ y+\frac{1}{2}\right]$	[73,374]
74	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{3}{4}-y\right]$	[74,369]
75	$\left[\frac{1}{2},\ y+\frac{3}{4},\ y+\frac{1}{2}\right]$	[75,370]
76	$\left[y+\frac{1}{4},\ \frac{3}{4}-y,\ \frac{1}{4}\right]$	[76,285]
77	$\left[-y,\ \frac{3}{4}-y,\ 0\right]$	[77,287]
78	$\left[y,\ 0,\ y+\frac{3}{4}\right]$	[78,238]
79	$\left[\frac{1}{4}-y,\ \frac{1}{4},\ y+\frac{3}{4}\right]$	[79,240]
80	$\left[\frac{1}{4},\ y+\frac{3}{4},\ \frac{3}{4}-y\right]$	[80,373]
81	$\left[0,\ \frac{1}{2}-y,\ \frac{3}{4}-y\right]$	[81,362]
82	$\left[0,\ y+\frac{3}{4},\ y+\frac{1}{2}\right]$	[82,363]
83	$\left[\frac{1}{4}-y,\ 0,\ \frac{1}{2}-y\right]$	[83,236]
84	$\left[y,\ \frac{1}{4},\ \frac{1}{2}-y\right]$	[84,233]
85	$\left[\frac{3}{4},\ y+\frac{3}{4},\ \frac{3}{4}-y\right]$	[85,368]
86	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ y+\frac{1}{2}\right]$	[86,361]
87	$\left[y+\frac{1}{4},\ y+\frac{1}{2},\ 0\right]$	[87,283]
88	$\left[-y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[88,282]
89	$\left[y,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[89,228]
90	$\left[-y,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[90,280]
91	$\left[y+\frac{1}{4},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[91,279]
92	$\left[\frac{1}{4}-y,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[92,227]
93	$\left[y+\frac{1}{4},\ \frac{3}{4}-y,\ \frac{3}{4}\right]$	[93,268]
94	$\left[y,\ \frac{1}{2},\ y+\frac{3}{4}\right]$	[94,222]
95	$\left[-y,\ \frac{3}{4}-y,\ \frac{1}{2}\right]$	[95,269]
96	$\left[\frac{1}{4}-y,\ \frac{3}{4},\ y+\frac{3}{4}\right]$	[96,223]
97	$\left[\frac{1}{4},\ y,\ \frac{1}{2}-y\right]$	[97,206]
98	$\left[\frac{1}{2},\ y,\ y+\frac{3}{4}\right]$	[98,201]
99	$\left[\frac{1}{2},\ \frac{1}{4}-y,\ \frac{1}{2}-y\right]$	[99,202]
100	$\left[\frac{3}{4}-y,\ y+\frac{1}{4},\ \frac{3}{4}\right]$	[100,309]
101	$\left[y+\frac{1}{2},\ y+\frac{1}{4},\ \frac{1}{2}\right]$	[101,311]
102	$\left[\frac{1}{2}-y,\ 0,\ \frac{3}{4}-y\right]$	[102,358]
103	$\left[y+\frac{3}{4},\ \frac{1}{4},\ \frac{3}{4}-y\right]$	[103,360]
104	$\left[\frac{1}{4},\ \frac{1}{4}-y,\ y+\frac{3}{4}\right]$	[104,205]
105	$\left[0,\ y,\ y+\frac{3}{4}\right]$	[105,194]
106	$\left[0,\ \frac{1}{4}-y,\ \frac{1}{2}-y\right]$	[106,195]
107	$\left[y+\frac{3}{4},\ 0,\ y+\frac{1}{2}\right]$	[107,356]
108	$\left[\frac{1}{2}-y,\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[108,353]
109	$\left[\frac{3}{4},\ \frac{1}{4}-y,\ y+\frac{3}{4}\right]$	[109,200]

continued ...

Table 10

No.	position	mapping
110	$\left[\frac{3}{4},\, y,\, \frac{1}{2}-y\right]$	[110,193]
111	$\left[\frac{3}{4}-y,\, -y,\, \frac{1}{2}\right]$	[111,307]
112	$\left[y+\frac{1}{2},\, -y,\, \frac{3}{4}\right]$	[112,306]
113	$\left[\frac{1}{2}-y,\, \frac{3}{4},\, y+\frac{1}{2}\right]$	[113,348]
114	$\left[y+\frac{1}{2},\, -y,\, \frac{1}{4}\right]$	[114,304]
115	$\left[\frac{3}{4}-y,\, -y,\, 0\right]$	[115,303]
116	$\left[y+\frac{3}{4},\, \frac{1}{2},\, y+\frac{1}{2}\right]$	[116,347]
117	$\left[\frac{3}{4}-y,\, y+\frac{1}{4},\, \frac{1}{4}\right]$	[117,292]
118	$\left[\frac{1}{2}-y,\, \frac{1}{2},\, \frac{3}{4}-y\right]$	[118,342]
119	$\left[y+\frac{1}{2},\, y+\frac{1}{4},\, 0\right]$	[119,293]
120	$\left[y+\frac{3}{4},\, \frac{3}{4},\, \frac{3}{4}-y\right]$	[120,343]
121	$\left[\frac{3}{4},\, -y,\, y+\frac{1}{2}\right]$	[121,230]
122	$\left[0,\, -y,\, \frac{3}{4}-y\right]$	[122,225]
123	$\left[0,\, y+\frac{1}{4},\, y+\frac{1}{2}\right]$	[123,226]
124	$\left[y+\frac{3}{4},\, \frac{1}{4}-y,\, \frac{1}{4}\right]$	[124,333]
125	$\left[\frac{1}{2}-y,\, \frac{1}{4}-y,\, 0\right]$	[125,335]
126	$\left[y+\frac{1}{2},\, \frac{1}{2},\, y+\frac{3}{4}\right]$	[126,382]
127	$\left[\frac{3}{4}-y,\, \frac{3}{4},\, y+\frac{3}{4}\right]$	[127,384]
128	$\left[\frac{3}{4},\, y+\frac{1}{4},\, \frac{3}{4}-y\right]$	[128,229]
129	$\left[\frac{1}{2},\, -y,\, \frac{3}{4}-y\right]$	[129,218]
130	$\left[\frac{1}{2},\, y+\frac{1}{4},\, y+\frac{1}{2}\right]$	[130,219]
131	$\left[\frac{3}{4}-y,\, \frac{1}{2},\, \frac{1}{2}-y\right]$	[131,380]
132	$\left[y+\frac{1}{2},\, \frac{3}{4},\, \frac{1}{2}-y\right]$	[132,377]
133	$\left[\frac{1}{4},\, y+\frac{1}{4},\, \frac{3}{4}-y\right]$	[133,224]
134	$\left[\frac{1}{4},\, -y,\, y+\frac{1}{2}\right]$	[134,217]
135	$\left[y+\frac{3}{4},\, y,\, 0\right]$	[135,331]
136	$\left[\frac{1}{2}-y,\, y,\, \frac{1}{4}\right]$	[136,330]
137	$\left[y+\frac{1}{2},\, \frac{1}{4},\, \frac{1}{2}-y\right]$	[137,372]
138	$\left[\frac{1}{2}-y,\, y,\, \frac{3}{4}\right]$	[138,328]
139	$\left[y+\frac{3}{4},\, y,\, \frac{1}{2}\right]$	[139,327]
140	$\left[\frac{3}{4}-y,\, 0,\, \frac{1}{2}-y\right]$	[140,371]
141	$\left[y+\frac{3}{4},\, \frac{1}{4}-y,\, \frac{3}{4}\right]$	[141,316]
142	$\left[y+\frac{1}{2},\, 0,\, y+\frac{3}{4}\right]$	[142,366]
143	$\left[\frac{1}{2}-y,\, \frac{1}{4}-y,\, \frac{1}{2}\right]$	[143,317]
144	$\left[\frac{3}{4}-y,\, \frac{1}{4},\, y+\frac{3}{4}\right]$	[144,367]
145	$\left[\frac{1}{4},\, y+\frac{1}{2},\, -y\right]$	[145,254]
146	$\left[\frac{1}{2},\, y+\frac{1}{2},\, y+\frac{1}{4}\right]$	[146,249]
147	$\left[\frac{1}{2},\, \frac{3}{4}-y,\, -y\right]$	[147,250]
148	$\left[\frac{3}{4}-y,\, y+\frac{3}{4},\, \frac{1}{4}\right]$	[148,357]
149	$\left[y+\frac{1}{2},\, y+\frac{3}{4},\, 0\right]$	[149,359]
150	$\left[\frac{1}{2}-y,\, \frac{1}{2},\, \frac{1}{4}-y\right]$	[150,310]
151	$\left[y+\frac{3}{4},\, \frac{3}{4},\, \frac{1}{4}-y\right]$	[151,312]
152	$\left[\frac{1}{4},\, \frac{3}{4}-y,\, y+\frac{1}{4}\right]$	[152,253]
153	$\left[0,\, y+\frac{1}{2},\, y+\frac{1}{4}\right]$	[153,242]
154	$\left[0,\, \frac{3}{4}-y,\, -y\right]$	[154,243]
155	$\left[y+\frac{3}{4},\, \frac{1}{2},\, y\right]$	[155,308]
156	$\left[\frac{1}{2}-y,\, \frac{3}{4},\, y\right]$	[156,305]

continued ...

Table 10

No.	position	mapping
157	$\left[\frac{3}{4},\ \frac{3}{4}-y,\ y+\frac{1}{4}\right]$	[157,248]
158	$\left[\frac{3}{4},\ y+\frac{1}{2},\ -y\right]$	[158,241]
159	$\left[\frac{3}{4}-y,\ \frac{1}{2}-y,\ 0\right]$	[159,355]
160	$\left[y+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[160,354]
161	$\left[\frac{1}{2}-y,\ \frac{1}{4},\ y\right]$	[161,300]
162	$\left[y+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[162,352]
163	$\left[\frac{3}{4}-y,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[163,351]
164	$\left[y+\frac{3}{4},\ 0,\ y\right]$	[164,299]
165	$\left[\frac{3}{4}-y,\ y+\frac{3}{4},\ \frac{3}{4}\right]$	[165,340]
166	$\left[\frac{1}{2}-y,\ 0,\ \frac{1}{4}-y\right]$	[166,294]
167	$\left[y+\frac{1}{2},\ y+\frac{3}{4},\ \frac{1}{2}\right]$	[167,341]
168	$\left[y+\frac{3}{4},\ \frac{1}{4},\ \frac{1}{4}-y\right]$	[168,295]
169	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ y\right]$	[169,278]
170	$\left[0,\ \frac{1}{2}-y,\ \frac{1}{4}-y\right]$	[170,273]
171	$\left[0,\ y+\frac{3}{4},\ y\right]$	[171,274]
172	$\left[y+\frac{3}{4},\ \frac{3}{4}-y,\ \frac{3}{4}\right]$	[172,381]
173	$\left[\frac{1}{2}-y,\ \frac{3}{4}-y,\ \frac{1}{2}\right]$	[173,383]
174	$\left[y+\frac{1}{2},\ 0,\ y+\frac{1}{4}\right]$	[174,334]
175	$\left[\frac{3}{4}-y,\ \frac{1}{4},\ y+\frac{1}{4}\right]$	[175,336]
176	$\left[\frac{3}{4},\ y+\frac{3}{4},\ \frac{1}{4}-y\right]$	[176,277]
177	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{4}-y\right]$	[177,266]
178	$\left[\frac{1}{2},\ y+\frac{3}{4},\ y\right]$	[178,267]
179	$\left[\frac{3}{4}-y,\ 0,\ -y\right]$	[179,332]
180	$\left[y+\frac{1}{2},\ \frac{1}{4},\ -y\right]$	[180,329]
181	$\left[\frac{1}{4},\ y+\frac{3}{4},\ \frac{1}{4}-y\right]$	[181,272]
182	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ y\right]$	[182,265]
183	$\left[y+\frac{3}{4},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[183,379]
184	$\left[\frac{1}{2}-y,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[184,378]
185	$\left[y+\frac{1}{2},\ \frac{3}{4},\ -y\right]$	[185,324]
186	$\left[\frac{1}{2}-y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[186,376]
187	$\left[y+\frac{3}{4},\ y+\frac{1}{2},\ 0\right]$	[187,375]
188	$\left[\frac{3}{4}-y,\ \frac{1}{2},\ -y\right]$	[188,323]
189	$\left[y+\frac{3}{4},\ \frac{3}{4}-y,\ \frac{1}{4}\right]$	[189,364]
190	$\left[y+\frac{1}{2},\ \frac{1}{2},\ y+\frac{1}{4}\right]$	[190,318]
191	$\left[\frac{1}{2}-y,\ \frac{3}{4}-y,\ 0\right]$	[191,365]
192	$\left[\frac{3}{4}-y,\ \frac{3}{4},\ y+\frac{1}{4}\right]$	[192,319]

Table 11: Wyckoff site: 192k, site symmetry: ..m

No.	position	mapping
1	$[x,\ x,\ z]$	[1,36]
2	$\left[x+\frac{1}{4},\ -z,\ x+\frac{1}{4}\right]$	[2,43]
3	$\left[x+\frac{1}{4},\ z+\frac{1}{4},\ -x\right]$	[3,45]
4	$\left[z+\frac{1}{4},\ x+\frac{1}{4},\ -x\right]$	[4,44]

continued ...

Table 11

No.	position	mapping
5	$\left[-z,\, x+\frac{1}{4},\, x+\frac{1}{4}\right]$	[5,46]
6	$\left[-x,\, x+\frac{1}{4},\, z+\frac{1}{4}\right]$	[6,32]
7	$\left[x+\frac{1}{4},\, -x,\, z+\frac{1}{4}\right]$	[7,33]
8	$\left[x,\, \frac{1}{4}-x,\, \frac{1}{4}-z\right]$	[8,30]
9	$\left[\frac{1}{4}-x,\, x,\, \frac{1}{4}-z\right]$	[9,31]
10	$\left[\frac{1}{4}-x,\, \frac{1}{4}-x,\, z\right]$	[10,35]
11	$\left[x+\frac{1}{4},\, x+\frac{1}{4},\, -z\right]$	[11,34]
12	$[-x,\, -x,\, -z]$	[12,25]
13	$\left[-x,\, z+\frac{1}{4},\, x+\frac{1}{4}\right]$	[13,47]
14	$[-x,\, -z,\, -x]$	[14,42]
15	$\left[z+\frac{1}{4},\, -x,\, x+\frac{1}{4}\right]$	[15,48]
16	$[-z,\, -x,\, -x]$	[16,41]
17	$[z,\, x,\, x]$	[17,40]
18	$[x,\, z,\, x]$	[18,38]
19	$\left[\frac{1}{4}-x,\, z,\, \frac{1}{4}-x\right]$	[19,26]
20	$\left[\frac{1}{4}-z,\, \frac{1}{4}-x,\, x\right]$	[20,28]
21	$\left[\frac{1}{4}-x,\, \frac{1}{4}-z,\, x\right]$	[21,27]
22	$\left[z,\, \frac{1}{4}-x,\, \frac{1}{4}-x\right]$	[22,29]
23	$\left[x,\, \frac{1}{4}-z,\, \frac{1}{4}-x\right]$	[23,37]
24	$\left[\frac{1}{4}-z,\, x,\, \frac{1}{4}-x\right]$	[24,39]
25	$\left[x,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[49,84]
26	$\left[x+\frac{1}{4},\, \frac{1}{2}-z,\, x+\frac{3}{4}\right]$	[50,91]
27	$\left[x+\frac{1}{4},\, z+\frac{3}{4},\, \frac{1}{2}-x\right]$	[51,93]
28	$\left[z+\frac{1}{4},\, x+\frac{3}{4},\, \frac{1}{2}-x\right]$	[52,92]
29	$\left[-z,\, x+\frac{3}{4},\, x+\frac{3}{4}\right]$	[53,94]
30	$\left[-x,\, x+\frac{3}{4},\, z+\frac{3}{4}\right]$	[54,80]
31	$\left[x+\frac{1}{4},\, \frac{1}{2}-x,\, z+\frac{3}{4}\right]$	[55,81]
32	$\left[x,\, \frac{3}{4}-x,\, \frac{3}{4}-z\right]$	[56,78]
33	$\left[\frac{1}{4}-x,\, x+\frac{1}{2},\, \frac{3}{4}-z\right]$	[57,79]
34	$\left[\frac{1}{4}-x,\, \frac{3}{4}-x,\, z+\frac{1}{2}\right]$	[58,83]
35	$\left[x+\frac{1}{4},\, x+\frac{3}{4},\, \frac{1}{2}-z\right]$	[59,82]
36	$\left[-x,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[60,73]
37	$\left[-x,\, z+\frac{3}{4},\, x+\frac{3}{4}\right]$	[61,95]
38	$\left[-x,\, \frac{1}{2}-z,\, \frac{1}{2}-x\right]$	[62,90]
39	$\left[z+\frac{1}{4},\, \frac{1}{2}-x,\, x+\frac{3}{4}\right]$	[63,96]
40	$\left[-z,\, \frac{1}{2}-x,\, \frac{1}{2}-x\right]$	[64,89]
41	$\left[z,\, x+\frac{1}{2},\, x+\frac{1}{2}\right]$	[65,88]
42	$\left[x,\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[66,86]
43	$\left[\frac{1}{4}-x,\, z+\frac{1}{2},\, \frac{3}{4}-x\right]$	[67,74]
44	$\left[\frac{1}{4}-z,\, \frac{3}{4}-x,\, x+\frac{1}{2}\right]$	[68,76]
45	$\left[\frac{1}{4}-x,\, \frac{3}{4}-z,\, x+\frac{1}{2}\right]$	[69,75]
46	$\left[z,\, \frac{3}{4}-x,\, \frac{3}{4}-x\right]$	[70,77]
47	$\left[x,\, \frac{3}{4}-z,\, \frac{3}{4}-x\right]$	[71,85]
48	$\left[\frac{1}{4}-z,\, x+\frac{1}{2},\, \frac{3}{4}-x\right]$	[72,87]
49	$\left[x+\frac{1}{2},\, x,\, z+\frac{1}{2}\right]$	[97,132]
50	$\left[x+\frac{3}{4},\, -z,\, x+\frac{3}{4}\right]$	[98,139]
51	$\left[x+\frac{3}{4},\, z+\frac{1}{4},\, \frac{1}{2}-x\right]$	[99,141]

continued ...

Table 11

No.	position	mapping
52	$\left[z+\frac{3}{4},\, x+\frac{1}{4},\, \frac{1}{2}-x\right]$	[100,140]
53	$\left[\frac{1}{2}-z,\, x+\frac{1}{4},\, x+\frac{3}{4}\right]$	[101,142]
54	$\left[\frac{1}{2}-x,\, x+\frac{1}{4},\, z+\frac{3}{4}\right]$	[102,128]
55	$\left[x+\frac{3}{4},\, -x,\, z+\frac{3}{4}\right]$	[103,129]
56	$\left[x+\frac{1}{2},\, \frac{1}{4}-x,\, \frac{3}{4}-z\right]$	[104,126]
57	$\left[\frac{3}{4}-x,\, x,\, \frac{3}{4}-z\right]$	[105,127]
58	$\left[\frac{3}{4}-x,\, \frac{1}{4}-x,\, z+\frac{1}{2}\right]$	[106,131]
59	$\left[x+\frac{3}{4},\, x+\frac{1}{4},\, \frac{1}{2}-z\right]$	[107,130]
60	$\left[\frac{1}{2}-x,\, -x,\, \frac{1}{2}-z\right]$	[108,121]
61	$\left[\frac{1}{2}-x,\, z+\frac{1}{4},\, x+\frac{3}{4}\right]$	[109,143]
62	$\left[\frac{1}{2}-x,\, -z,\, \frac{1}{2}-x\right]$	[110,138]
63	$\left[z+\frac{3}{4},\, -x,\, x+\frac{3}{4}\right]$	[111,144]
64	$\left[\frac{1}{2}-z,\, -x,\, \frac{1}{2}-x\right]$	[112,137]
65	$\left[z+\frac{1}{2},\, x,\, x+\frac{1}{2}\right]$	[113,136]
66	$\left[x+\frac{1}{2},\, z,\, x+\frac{1}{2}\right]$	[114,134]
67	$\left[\frac{3}{4}-x,\, z,\, \frac{3}{4}-x\right]$	[115,122]
68	$\left[\frac{3}{4}-z,\, \frac{1}{4}-x,\, x+\frac{1}{2}\right]$	[116,124]
69	$\left[\frac{3}{4}-x,\, \frac{1}{4}-z,\, x+\frac{1}{2}\right]$	[117,123]
70	$\left[z+\frac{1}{2},\, \frac{1}{4}-x,\, \frac{3}{4}-x\right]$	[118,125]
71	$\left[x+\frac{1}{2},\, \frac{1}{4}-z,\, \frac{3}{4}-x\right]$	[119,133]
72	$\left[\frac{3}{4}-z,\, x,\, \frac{3}{4}-x\right]$	[120,135]
73	$\left[x+\frac{1}{2},\, x+\frac{1}{2},\, z\right]$	[145,180]
74	$\left[x+\frac{3}{4},\, \frac{1}{2}-z,\, x+\frac{1}{4}\right]$	[146,187]
75	$\left[x+\frac{3}{4},\, z+\frac{3}{4},\, -x\right]$	[147,189]
76	$\left[z+\frac{3}{4},\, x+\frac{3}{4},\, -x\right]$	[148,188]
77	$\left[\frac{1}{2}-z,\, x+\frac{3}{4},\, x+\frac{1}{4}\right]$	[149,190]
78	$\left[\frac{1}{2}-x,\, x+\frac{3}{4},\, z+\frac{1}{4}\right]$	[150,176]
79	$\left[x+\frac{3}{4},\, \frac{1}{2}-x,\, z+\frac{1}{4}\right]$	[151,177]
80	$\left[x+\frac{1}{2},\, \frac{3}{4}-x,\, \frac{1}{4}-z\right]$	[152,174]
81	$\left[\frac{3}{4}-x,\, x+\frac{1}{2},\, \frac{1}{4}-z\right]$	[153,175]
82	$\left[\frac{3}{4}-x,\, \frac{3}{4}-x,\, z\right]$	[154,179]
83	$\left[x+\frac{3}{4},\, x+\frac{3}{4},\, -z\right]$	[155,178]
84	$\left[\frac{1}{2}-x,\, \frac{1}{2}-x,\, -z\right]$	[156,169]
85	$\left[\frac{1}{2}-x,\, z+\frac{3}{4},\, x+\frac{1}{4}\right]$	[157,191]
86	$\left[\frac{1}{2}-x,\, \frac{1}{2}-z,\, -x\right]$	[158,186]
87	$\left[z+\frac{3}{4},\, \frac{1}{2}-x,\, x+\frac{1}{4}\right]$	[159,192]
88	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, -x\right]$	[160,185]
89	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, x\right]$	[161,184]
90	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, x\right]$	[162,182]
91	$\left[\frac{3}{4}-x,\, z+\frac{1}{2},\, \frac{1}{4}-x\right]$	[163,170]
92	$\left[\frac{3}{4}-z,\, \frac{3}{4}-x,\, x\right]$	[164,172]
93	$\left[\frac{3}{4}-x,\, \frac{3}{4}-z,\, x\right]$	[165,171]
94	$\left[z+\frac{1}{2},\, \frac{3}{4}-x,\, \frac{1}{4}-x\right]$	[166,173]
95	$\left[x+\frac{1}{2},\, \frac{3}{4}-z,\, \frac{1}{4}-x\right]$	[167,181]
96	$\left[\frac{3}{4}-z,\, x+\frac{1}{2},\, \frac{1}{4}-x\right]$	[168,183]
97	$\left[x,\, x,\, z+\frac{1}{2}\right]$	[193,228]
98	$\left[x+\frac{1}{4},\, -z,\, x+\frac{3}{4}\right]$	[194,235]

continued ...

Table 11

No.	position	mapping
99	$\left[x+\frac{1}{4},\, z+\frac{1}{4},\, \frac{1}{2}-x\right]$	[195,237]
100	$\left[z+\frac{1}{4},\, x+\frac{1}{4},\, \frac{1}{2}-x\right]$	[196,236]
101	$\left[-z,\, x+\frac{1}{4},\, x+\frac{3}{4}\right]$	[197,238]
102	$\left[-x,\, x+\frac{1}{4},\, z+\frac{3}{4}\right]$	[198,224]
103	$\left[x+\frac{1}{4},\, -x,\, z+\frac{3}{4}\right]$	[199,225]
104	$\left[x,\, \frac{1}{4}-x,\, \frac{3}{4}-z\right]$	[200,222]
105	$\left[\frac{1}{4}-x,\, x,\, \frac{3}{4}-z\right]$	[201,223]
106	$\left[\frac{1}{4}-x,\, \frac{1}{4}-x,\, z+\frac{1}{2}\right]$	[202,227]
107	$\left[x+\frac{1}{4},\, x+\frac{1}{4},\, \frac{1}{2}-z\right]$	[203,226]
108	$\left[-x,\, -x,\, \frac{1}{2}-z\right]$	[204,217]
109	$\left[-x,\, z+\frac{1}{4},\, x+\frac{3}{4}\right]$	[205,239]
110	$\left[-x,\, -z,\, \frac{1}{2}-x\right]$	[206,234]
111	$\left[z+\frac{1}{4},\, -x,\, x+\frac{3}{4}\right]$	[207,240]
112	$\left[-z,\, -x,\, \frac{1}{2}-x\right]$	[208,233]
113	$\left[z,\, x,\, x+\frac{1}{2}\right]$	[209,232]
114	$\left[x,\, z,\, x+\frac{1}{2}\right]$	[210,230]
115	$\left[\frac{1}{4}-x,\, z,\, \frac{3}{4}-x\right]$	[211,218]
116	$\left[\frac{1}{4}-z,\, \frac{1}{4}-x,\, x+\frac{1}{2}\right]$	[212,220]
117	$\left[\frac{1}{4}-x,\, \frac{1}{4}-z,\, x+\frac{1}{2}\right]$	[213,219]
118	$\left[z,\, \frac{1}{4}-x,\, \frac{3}{4}-x\right]$	[214,221]
119	$\left[x,\, \frac{1}{4}-z,\, \frac{3}{4}-x\right]$	[215,229]
120	$\left[\frac{1}{4}-z,\, x,\, \frac{3}{4}-x\right]$	[216,231]
121	$\left[x,\, x+\frac{1}{2},\, z\right]$	[241,276]
122	$\left[x+\frac{1}{4},\, \frac{1}{2}-z,\, x+\frac{1}{4}\right]$	[242,283]
123	$\left[x+\frac{1}{4},\, z+\frac{3}{4},\, -x\right]$	[243,285]
124	$\left[z+\frac{1}{4},\, x+\frac{3}{4},\, -x\right]$	[244,284]
125	$\left[-z,\, x+\frac{3}{4},\, x+\frac{1}{4}\right]$	[245,286]
126	$\left[-x,\, x+\frac{3}{4},\, z+\frac{1}{4}\right]$	[246,272]
127	$\left[x+\frac{1}{4},\, \frac{1}{2}-x,\, z+\frac{1}{4}\right]$	[247,273]
128	$\left[x,\, \frac{3}{4}-x,\, \frac{1}{4}-z\right]$	[248,270]
129	$\left[\frac{1}{4}-x,\, x+\frac{1}{2},\, \frac{1}{4}-z\right]$	[249,271]
130	$\left[\frac{1}{4}-x,\, \frac{3}{4}-x,\, z\right]$	[250,275]
131	$\left[x+\frac{1}{4},\, x+\frac{3}{4},\, -z\right]$	[251,274]
132	$\left[-x,\, \frac{1}{2}-x,\, -z\right]$	[252,265]
133	$\left[-x,\, z+\frac{3}{4},\, x+\frac{1}{4}\right]$	[253,287]
134	$\left[-x,\, \frac{1}{2}-z,\, -x\right]$	[254,282]
135	$\left[z+\frac{1}{4},\, \frac{1}{2}-x,\, x+\frac{1}{4}\right]$	[255,288]
136	$\left[-z,\, \frac{1}{2}-x,\, -x\right]$	[256,281]
137	$\left[z,\, x+\frac{1}{2},\, x\right]$	[257,280]
138	$\left[x,\, z+\frac{1}{2},\, x\right]$	[258,278]
139	$\left[\frac{1}{4}-x,\, z+\frac{1}{2},\, \frac{1}{4}-x\right]$	[259,266]
140	$\left[\frac{1}{4}-z,\, \frac{3}{4}-x,\, x\right]$	[260,268]
141	$\left[\frac{1}{4}-x,\, \frac{3}{4}-z,\, x\right]$	[261,267]
142	$\left[z,\, \frac{3}{4}-x,\, \frac{1}{4}-x\right]$	[262,269]
143	$\left[x,\, \frac{3}{4}-z,\, \frac{1}{4}-x\right]$	[263,277]
144	$\left[\frac{1}{4}-z,\, x+\frac{1}{2},\, \frac{1}{4}-x\right]$	[264,279]
145	$\left[x+\frac{1}{2},\, x,\, z\right]$	[289,324]

continued ...

Table 11

No.	position	mapping
146	$\left[x+\frac{3}{4},\ -z,\ x+\frac{1}{4}\right]$	[290,331]
147	$\left[x+\frac{3}{4},\ z+\frac{1}{4},\ -x\right]$	[291,333]
148	$\left[z+\frac{3}{4},\ x+\frac{1}{4},\ -x\right]$	[292,332]
149	$\left[\frac{1}{2}-z,\ x+\frac{1}{4},\ x+\frac{1}{4}\right]$	[293,334]
150	$\left[\frac{1}{2}-x,\ x+\frac{1}{4},\ z+\frac{1}{4}\right]$	[294,320]
151	$\left[x+\frac{3}{4},\ -x,\ z+\frac{1}{4}\right]$	[295,321]
152	$\left[x+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{1}{4}-z\right]$	[296,318]
153	$\left[\frac{3}{4}-x,\ x,\ \frac{1}{4}-z\right]$	[297,319]
154	$\left[\frac{3}{4}-x,\ \frac{1}{4}-x,\ z\right]$	[298,323]
155	$\left[x+\frac{3}{4},\ x+\frac{1}{4},\ -z\right]$	[299,322]
156	$\left[\frac{1}{2}-x,\ -x,\ -z\right]$	[300,313]
157	$\left[\frac{1}{2}-x,\ z+\frac{1}{4},\ x+\frac{1}{4}\right]$	[301,335]
158	$\left[\frac{1}{2}-x,\ -z,\ -x\right]$	[302,330]
159	$\left[z+\frac{3}{4},\ -x,\ x+\frac{1}{4}\right]$	[303,336]
160	$\left[\frac{1}{2}-z,\ -x,\ -x\right]$	[304,329]
161	$\left[z+\frac{1}{2},\ x,\ x\right]$	[305,328]
162	$\left[x+\frac{1}{2},\ z,\ x\right]$	[306,326]
163	$\left[\frac{3}{4}-x,\ z,\ \frac{1}{4}-x\right]$	[307,314]
164	$\left[\frac{3}{4}-z,\ \frac{1}{4}-x,\ x\right]$	[308,316]
165	$\left[\frac{3}{4}-x,\ \frac{1}{4}-z,\ x\right]$	[309,315]
166	$\left[z+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{1}{4}-x\right]$	[310,317]
167	$\left[x+\frac{1}{2},\ \frac{1}{4}-z,\ \frac{1}{4}-x\right]$	[311,325]
168	$\left[\frac{3}{4}-z,\ x,\ \frac{1}{4}-x\right]$	[312,327]
169	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[337,372]
170	$\left[x+\frac{3}{4},\ \frac{1}{2}-z,\ x+\frac{3}{4}\right]$	[338,379]
171	$\left[x+\frac{3}{4},\ z+\frac{3}{4},\ \frac{1}{2}-x\right]$	[339,381]
172	$\left[z+\frac{3}{4},\ x+\frac{3}{4},\ \frac{1}{2}-x\right]$	[340,380]
173	$\left[\frac{1}{2}-z,\ x+\frac{3}{4},\ x+\frac{3}{4}\right]$	[341,382]
174	$\left[\frac{1}{2}-x,\ x+\frac{3}{4},\ z+\frac{3}{4}\right]$	[342,368]
175	$\left[x+\frac{3}{4},\ \frac{1}{2}-x,\ z+\frac{3}{4}\right]$	[343,369]
176	$\left[x+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{3}{4}-z\right]$	[344,366]
177	$\left[\frac{3}{4}-x,\ x+\frac{1}{2},\ \frac{3}{4}-z\right]$	[345,367]
178	$\left[\frac{3}{4}-x,\ \frac{3}{4}-x,\ z+\frac{1}{2}\right]$	[346,371]
179	$\left[x+\frac{3}{4},\ x+\frac{3}{4},\ \frac{1}{2}-z\right]$	[347,370]
180	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[348,361]
181	$\left[\frac{1}{2}-x,\ z+\frac{3}{4},\ x+\frac{3}{4}\right]$	[349,383]
182	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[350,378]
183	$\left[z+\frac{3}{4},\ \frac{1}{2}-x,\ x+\frac{3}{4}\right]$	[351,384]
184	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	[352,377]
185	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ x+\frac{1}{2}\right]$	[353,376]
186	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$	[354,374]
187	$\left[\frac{3}{4}-x,\ z+\frac{1}{2},\ \frac{3}{4}-x\right]$	[355,362]
188	$\left[\frac{3}{4}-z,\ \frac{3}{4}-x,\ x+\frac{1}{2}\right]$	[356,364]
189	$\left[\frac{3}{4}-x,\ \frac{3}{4}-z,\ x+\frac{1}{2}\right]$	[357,363]
190	$\left[z+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{3}{4}-x\right]$	[358,365]
191	$\left[x+\frac{1}{2},\ \frac{3}{4}-z,\ \frac{3}{4}-x\right]$	[359,373]
192	$\left[\frac{3}{4}-z,\ x+\frac{1}{2},\ \frac{3}{4}-x\right]$	[360,375]

Table 12: Wyckoff site: 3841, site symmetry: 1

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

continued ...

Table 12

No.	position	mapping
45	$\left[y+\frac{1}{4},\, z+\frac{1}{4},\, -x\right]$	[45]
46	$\left[-z,\, x+\frac{1}{4},\, y+\frac{1}{4}\right]$	[46]
47	$\left[-y,\, z+\frac{1}{4},\, x+\frac{1}{4}\right]$	[47]
48	$\left[z+\frac{1}{4},\, -x,\, y+\frac{1}{4}\right]$	[48]
49	$\left[x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[49]
50	$\left[x+\frac{1}{4},\, \frac{1}{2}-z,\, y+\frac{3}{4}\right]$	[50]
51	$\left[x+\frac{1}{4},\, z+\frac{3}{4},\, \frac{1}{2}-y\right]$	[51]
52	$\left[z+\frac{1}{4},\, y+\frac{3}{4},\, \frac{1}{2}-x\right]$	[52]
53	$\left[-z,\, y+\frac{3}{4},\, x+\frac{3}{4}\right]$	[53]
54	$\left[-y,\, x+\frac{3}{4},\, z+\frac{3}{4}\right]$	[54]
55	$\left[y+\frac{1}{4},\, \frac{1}{2}-x,\, z+\frac{3}{4}\right]$	[55]
56	$\left[x,\, \frac{3}{4}-y,\, \frac{3}{4}-z\right]$	[56]
57	$\left[\frac{1}{4}-x,\, y+\frac{1}{2},\, \frac{3}{4}-z\right]$	[57]
58	$\left[\frac{1}{4}-x,\, \frac{3}{4}-y,\, z+\frac{1}{2}\right]$	[58]
59	$\left[y+\frac{1}{4},\, x+\frac{3}{4},\, \frac{1}{2}-z\right]$	[59]
60	$\left[-y,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[60]
61	$\left[-x,\, z+\frac{3}{4},\, y+\frac{3}{4}\right]$	[61]
62	$\left[-x,\, \frac{1}{2}-z,\, \frac{1}{2}-y\right]$	[62]
63	$\left[z+\frac{1}{4},\, \frac{1}{2}-y,\, x+\frac{3}{4}\right]$	[63]
64	$\left[-z,\, \frac{1}{2}-y,\, \frac{1}{2}-x\right]$	[64]
65	$\left[z,\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[65]
66	$\left[y,\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[66]
67	$\left[\frac{1}{4}-y,\, z+\frac{1}{2},\, \frac{3}{4}-x\right]$	[67]
68	$\left[\frac{1}{4}-z,\, \frac{3}{4}-x,\, y+\frac{1}{2}\right]$	[68]
69	$\left[\frac{1}{4}-y,\, \frac{3}{4}-z,\, x+\frac{1}{2}\right]$	[69]
70	$\left[z,\, \frac{3}{4}-x,\, \frac{3}{4}-y\right]$	[70]
71	$\left[y,\, \frac{3}{4}-z,\, \frac{3}{4}-x\right]$	[71]
72	$\left[\frac{1}{4}-z,\, x+\frac{1}{2},\, \frac{3}{4}-y\right]$	[72]
73	$\left[-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[73]
74	$\left[\frac{1}{4}-x,\, z+\frac{1}{2},\, \frac{3}{4}-y\right]$	[74]
75	$\left[\frac{1}{4}-x,\, \frac{3}{4}-z,\, y+\frac{1}{2}\right]$	[75]
76	$\left[\frac{1}{4}-z,\, \frac{3}{4}-y,\, x+\frac{1}{2}\right]$	[76]
77	$\left[z,\, \frac{3}{4}-y,\, \frac{3}{4}-x\right]$	[77]
78	$\left[y,\, \frac{3}{4}-x,\, \frac{3}{4}-z\right]$	[78]
79	$\left[\frac{1}{4}-y,\, x+\frac{1}{2},\, \frac{3}{4}-z\right]$	[79]
80	$\left[-x,\, y+\frac{3}{4},\, z+\frac{3}{4}\right]$	[80]
81	$\left[x+\frac{1}{4},\, \frac{1}{2}-y,\, z+\frac{3}{4}\right]$	[81]
82	$\left[x+\frac{1}{4},\, y+\frac{3}{4},\, \frac{1}{2}-z\right]$	[82]
83	$\left[\frac{1}{4}-y,\, \frac{3}{4}-x,\, z+\frac{1}{2}\right]$	[83]
84	$\left[y,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[84]
85	$\left[x,\, \frac{3}{4}-z,\, \frac{3}{4}-y\right]$	[85]
86	$\left[x,\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[86]
87	$\left[\frac{1}{4}-z,\, y+\frac{1}{2},\, \frac{3}{4}-x\right]$	[87]
88	$\left[z,\, y+\frac{1}{2},\, x+\frac{1}{2}\right]$	[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	$\left[y+\frac{1}{4},\, \frac{1}{2}-z,\, x+\frac{3}{4}\right]$	[91]

continued ...

Table 12

No.	position	mapping
92	$\left[z+\frac{1}{4},\, x+\frac{3}{4},\, \frac{1}{2}-y\right]$	[92]
93	$\left[y+\frac{1}{4},\, z+\frac{3}{4},\, \frac{1}{2}-x\right]$	[93]
94	$\left[-z,\, x+\frac{3}{4},\, y+\frac{3}{4}\right]$	[94]
95	$\left[-y,\, z+\frac{3}{4},\, x+\frac{3}{4}\right]$	[95]
96	$\left[z+\frac{1}{4},\, \frac{1}{2}-x,\, y+\frac{3}{4}\right]$	[96]
97	$\left[x+\frac{1}{2},\, y,\, z+\frac{1}{2}\right]$	[97]
98	$\left[x+\frac{3}{4},\, -z,\, y+\frac{3}{4}\right]$	[98]
99	$\left[x+\frac{3}{4},\, z+\frac{1}{4},\, \frac{1}{2}-y\right]$	[99]
100	$\left[z+\frac{3}{4},\, y+\frac{1}{4},\, \frac{1}{2}-x\right]$	[100]
101	$\left[\frac{1}{2}-z,\, y+\frac{1}{4},\, x+\frac{3}{4}\right]$	[101]
102	$\left[\frac{1}{2}-y,\, x+\frac{1}{4},\, z+\frac{3}{4}\right]$	[102]
103	$\left[y+\frac{3}{4},\, -x,\, z+\frac{3}{4}\right]$	[103]
104	$\left[x+\frac{1}{2},\, \frac{1}{4}-y,\, \frac{3}{4}-z\right]$	[104]
105	$\left[\frac{3}{4}-x,\, y,\, \frac{3}{4}-z\right]$	[105]
106	$\left[\frac{3}{4}-x,\, \frac{1}{4}-y,\, z+\frac{1}{2}\right]$	[106]
107	$\left[y+\frac{3}{4},\, x+\frac{1}{4},\, \frac{1}{2}-z\right]$	[107]
108	$\left[\frac{1}{2}-y,\, -x,\, \frac{1}{2}-z\right]$	[108]
109	$\left[\frac{1}{2}-x,\, z+\frac{1}{4},\, y+\frac{3}{4}\right]$	[109]
110	$\left[\frac{1}{2}-x,\, -z,\, \frac{1}{2}-y\right]$	[110]
111	$\left[z+\frac{3}{4},\, -y,\, x+\frac{3}{4}\right]$	[111]
112	$\left[\frac{1}{2}-z,\, -y,\, \frac{1}{2}-x\right]$	[112]
113	$\left[z+\frac{1}{2},\, x,\, y+\frac{1}{2}\right]$	[113]
114	$\left[y+\frac{1}{2},\, z,\, x+\frac{1}{2}\right]$	[114]
115	$\left[\frac{3}{4}-y,\, z,\, \frac{3}{4}-x\right]$	[115]
116	$\left[\frac{3}{4}-z,\, \frac{1}{4}-x,\, y+\frac{1}{2}\right]$	[116]
117	$\left[\frac{3}{4}-y,\, \frac{1}{4}-z,\, x+\frac{1}{2}\right]$	[117]
118	$\left[z+\frac{1}{2},\, \frac{1}{4}-x,\, \frac{3}{4}-y\right]$	[118]
119	$\left[y+\frac{1}{2},\, \frac{1}{4}-z,\, \frac{3}{4}-x\right]$	[119]
120	$\left[\frac{3}{4}-z,\, x,\, \frac{3}{4}-y\right]$	[120]
121	$\left[\frac{1}{2}-x,\, -y,\, \frac{1}{2}-z\right]$	[121]
122	$\left[\frac{3}{4}-x,\, z,\, \frac{3}{4}-y\right]$	[122]
123	$\left[\frac{3}{4}-x,\, \frac{1}{4}-z,\, y+\frac{1}{2}\right]$	[123]
124	$\left[\frac{3}{4}-z,\, \frac{1}{4}-y,\, x+\frac{1}{2}\right]$	[124]
125	$\left[z+\frac{1}{2},\, \frac{1}{4}-y,\, \frac{3}{4}-x\right]$	[125]
126	$\left[y+\frac{1}{2},\, \frac{1}{4}-x,\, \frac{3}{4}-z\right]$	[126]
127	$\left[\frac{3}{4}-y,\, x,\, \frac{3}{4}-z\right]$	[127]
128	$\left[\frac{1}{2}-x,\, y+\frac{1}{4},\, z+\frac{3}{4}\right]$	[128]
129	$\left[x+\frac{3}{4},\, -y,\, z+\frac{3}{4}\right]$	[129]
130	$\left[x+\frac{3}{4},\, y+\frac{1}{4},\, \frac{1}{2}-z\right]$	[130]
131	$\left[\frac{3}{4}-y,\, \frac{1}{4}-x,\, z+\frac{1}{2}\right]$	[131]
132	$\left[y+\frac{1}{2},\, x,\, z+\frac{1}{2}\right]$	[132]
133	$\left[x+\frac{1}{2},\, \frac{1}{4}-z,\, \frac{3}{4}-y\right]$	[133]
134	$\left[x+\frac{1}{2},\, z,\, y+\frac{1}{2}\right]$	[134]
135	$\left[\frac{3}{4}-z,\, y,\, \frac{3}{4}-x\right]$	[135]
136	$\left[z+\frac{1}{2},\, y,\, x+\frac{1}{2}\right]$	[136]
137	$\left[\frac{1}{2}-z,\, -x,\, \frac{1}{2}-y\right]$	[137]
138	$\left[\frac{1}{2}-y,\, -z,\, \frac{1}{2}-x\right]$	[138]

continued ...

Table 12

No.	position	mapping
139	$\left[y+\frac{3}{4},\ -z,\ x+\frac{3}{4}\right]$	[139]
140	$\left[z+\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{2}-y\right]$	[140]
141	$\left[y+\frac{3}{4},\ z+\frac{1}{4},\ \frac{1}{2}-x\right]$	[141]
142	$\left[\frac{1}{2}-z,\ x+\frac{1}{4},\ y+\frac{3}{4}\right]$	[142]
143	$\left[\frac{1}{2}-y,\ z+\frac{1}{4},\ x+\frac{3}{4}\right]$	[143]
144	$\left[z+\frac{3}{4},\ -x,\ y+\frac{3}{4}\right]$	[144]
145	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[145]
146	$\left[x+\frac{3}{4},\ \frac{1}{2}-z,\ y+\frac{1}{4}\right]$	[146]
147	$\left[x+\frac{3}{4},\ z+\frac{3}{4},\ -y\right]$	[147]
148	$\left[z+\frac{3}{4},\ y+\frac{3}{4},\ -x\right]$	[148]
149	$\left[\frac{1}{2}-z,\ y+\frac{3}{4},\ x+\frac{1}{4}\right]$	[149]
150	$\left[\frac{1}{2}-y,\ x+\frac{3}{4},\ z+\frac{1}{4}\right]$	[150]
151	$\left[y+\frac{3}{4},\ \frac{1}{2}-x,\ z+\frac{1}{4}\right]$	[151]
152	$\left[x+\frac{1}{2},\ \frac{3}{4}-y,\ \frac{1}{4}-z\right]$	[152]
153	$\left[\frac{3}{4}-x,\ y+\frac{1}{2},\ \frac{1}{4}-z\right]$	[153]
154	$\left[\frac{3}{4}-x,\ \frac{3}{4}-y,\ z\right]$	[154]
155	$\left[y+\frac{3}{4},\ x+\frac{3}{4},\ -z\right]$	[155]
156	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ -z\right]$	[156]
157	$\left[\frac{1}{2}-x,\ z+\frac{3}{4},\ y+\frac{1}{4}\right]$	[157]
158	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ -y\right]$	[158]
159	$\left[z+\frac{3}{4},\ \frac{1}{2}-y,\ x+\frac{1}{4}\right]$	[159]
160	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ -x\right]$	[160]
161	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ y\right]$	[161]
162	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ x\right]$	[162]
163	$\left[\frac{3}{4}-y,\ z+\frac{1}{2},\ \frac{1}{4}-x\right]$	[163]
164	$\left[\frac{3}{4}-z,\ \frac{3}{4}-x,\ y\right]$	[164]
165	$\left[\frac{3}{4}-y,\ \frac{3}{4}-z,\ x\right]$	[165]
166	$\left[z+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{1}{4}-y\right]$	[166]
167	$\left[y+\frac{1}{2},\ \frac{3}{4}-z,\ \frac{1}{4}-x\right]$	[167]
168	$\left[\frac{3}{4}-z,\ x+\frac{1}{2},\ \frac{1}{4}-y\right]$	[168]
169	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ -z\right]$	[169]
170	$\left[\frac{3}{4}-x,\ z+\frac{1}{2},\ \frac{1}{4}-y\right]$	[170]
171	$\left[\frac{3}{4}-x,\ \frac{3}{4}-z,\ y\right]$	[171]
172	$\left[\frac{3}{4}-z,\ \frac{3}{4}-y,\ x\right]$	[172]
173	$\left[z+\frac{1}{2},\ \frac{3}{4}-y,\ \frac{1}{4}-x\right]$	[173]
174	$\left[y+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{1}{4}-z\right]$	[174]
175	$\left[\frac{3}{4}-y,\ x+\frac{1}{2},\ \frac{1}{4}-z\right]$	[175]
176	$\left[\frac{1}{2}-x,\ y+\frac{3}{4},\ z+\frac{1}{4}\right]$	[176]
177	$\left[x+\frac{3}{4},\ \frac{1}{2}-y,\ z+\frac{1}{4}\right]$	[177]
178	$\left[x+\frac{3}{4},\ y+\frac{3}{4},\ -z\right]$	[178]
179	$\left[\frac{3}{4}-y,\ \frac{3}{4}-x,\ z\right]$	[179]
180	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z\right]$	[180]
181	$\left[x+\frac{1}{2},\ \frac{3}{4}-z,\ \frac{1}{4}-y\right]$	[181]
182	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ y\right]$	[182]
183	$\left[\frac{3}{4}-z,\ y+\frac{1}{2},\ \frac{1}{4}-x\right]$	[183]
184	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ x\right]$	[184]
185	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ -y\right]$	[185]

continued ...

Table 12

No.	position	mapping
186	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ -x\right]$	[186]
187	$\left[y+\frac{3}{4},\ \frac{1}{2}-z,\ x+\frac{1}{4}\right]$	[187]
188	$\left[z+\frac{3}{4},\ x+\frac{3}{4},\ -y\right]$	[188]
189	$\left[y+\frac{3}{4},\ z+\frac{3}{4},\ -x\right]$	[189]
190	$\left[\frac{1}{2}-z,\ x+\frac{3}{4},\ y+\frac{1}{4}\right]$	[190]
191	$\left[\frac{1}{2}-y,\ z+\frac{3}{4},\ x+\frac{1}{4}\right]$	[191]
192	$\left[z+\frac{3}{4},\ \frac{1}{2}-x,\ y+\frac{1}{4}\right]$	[192]
193	$\left[x,\ y,\ z+\frac{1}{2}\right]$	[193]
194	$\left[x+\frac{1}{4},\ -z,\ y+\frac{3}{4}\right]$	[194]
195	$\left[x+\frac{1}{4},\ z+\frac{1}{4},\ \frac{1}{2}-y\right]$	[195]
196	$\left[z+\frac{1}{4},\ y+\frac{1}{4},\ \frac{1}{2}-x\right]$	[196]
197	$\left[-z,\ y+\frac{1}{4},\ x+\frac{3}{4}\right]$	[197]
198	$\left[-y,\ x+\frac{1}{4},\ z+\frac{3}{4}\right]$	[198]
199	$\left[y+\frac{1}{4},\ -x,\ z+\frac{3}{4}\right]$	[199]
200	$\left[x,\ \frac{1}{4}-y,\ \frac{3}{4}-z\right]$	[200]
201	$\left[\frac{1}{4}-x,\ y,\ \frac{3}{4}-z\right]$	[201]
202	$\left[\frac{1}{4}-x,\ \frac{1}{4}-y,\ z+\frac{1}{2}\right]$	[202]
203	$\left[y+\frac{1}{4},\ x+\frac{1}{4},\ \frac{1}{2}-z\right]$	[203]
204	$\left[-y,\ -x,\ \frac{1}{2}-z\right]$	[204]
205	$\left[-x,\ z+\frac{1}{4},\ y+\frac{3}{4}\right]$	[205]
206	$\left[-x,\ -z,\ \frac{1}{2}-y\right]$	[206]
207	$\left[z+\frac{1}{4},\ -y,\ x+\frac{3}{4}\right]$	[207]
208	$\left[-z,\ -y,\ \frac{1}{2}-x\right]$	[208]
209	$\left[z,\ x,\ y+\frac{1}{2}\right]$	[209]
210	$\left[y,\ z,\ x+\frac{1}{2}\right]$	[210]
211	$\left[\frac{1}{4}-y,\ z,\ \frac{3}{4}-x\right]$	[211]
212	$\left[\frac{1}{4}-z,\ \frac{1}{4}-x,\ y+\frac{1}{2}\right]$	[212]
213	$\left[\frac{1}{4}-y,\ \frac{1}{4}-z,\ x+\frac{1}{2}\right]$	[213]
214	$\left[z,\ \frac{1}{4}-x,\ \frac{3}{4}-y\right]$	[214]
215	$\left[y,\ \frac{1}{4}-z,\ \frac{3}{4}-x\right]$	[215]
216	$\left[\frac{1}{4}-z,\ x,\ \frac{3}{4}-y\right]$	[216]
217	$\left[-x,\ -y,\ \frac{1}{2}-z\right]$	[217]
218	$\left[\frac{1}{4}-x,\ z,\ \frac{3}{4}-y\right]$	[218]
219	$\left[\frac{1}{4}-x,\ \frac{1}{4}-z,\ y+\frac{1}{2}\right]$	[219]
220	$\left[\frac{1}{4}-z,\ \frac{1}{4}-y,\ x+\frac{1}{2}\right]$	[220]
221	$\left[z,\ \frac{1}{4}-y,\ \frac{3}{4}-x\right]$	[221]
222	$\left[y,\ \frac{1}{4}-x,\ \frac{3}{4}-z\right]$	[222]
223	$\left[\frac{1}{4}-y,\ x,\ \frac{3}{4}-z\right]$	[223]
224	$\left[-x,\ y+\frac{1}{4},\ z+\frac{3}{4}\right]$	[224]
225	$\left[x+\frac{1}{4},\ -y,\ z+\frac{3}{4}\right]$	[225]
226	$\left[x+\frac{1}{4},\ y+\frac{1}{4},\ \frac{1}{2}-z\right]$	[226]
227	$\left[\frac{1}{4}-y,\ \frac{1}{4}-x,\ z+\frac{1}{2}\right]$	[227]
228	$\left[y,\ x,\ z+\frac{1}{2}\right]$	[228]
229	$\left[x,\ \frac{1}{4}-z,\ \frac{3}{4}-y\right]$	[229]
230	$\left[x,\ z,\ y+\frac{1}{2}\right]$	[230]
231	$\left[\frac{1}{4}-z,\ y,\ \frac{3}{4}-x\right]$	[231]
232	$\left[z,\ y,\ x+\frac{1}{2}\right]$	[232]

continued ...

Table 12

No.	position	mapping
233	$\left[-z,\, -x,\, \frac{1}{2}-y\right]$	[233]
234	$\left[-y,\, -z,\, \frac{1}{2}-x\right]$	[234]
235	$\left[y+\frac{1}{4},\, -z,\, x+\frac{3}{4}\right]$	[235]
236	$\left[z+\frac{1}{4},\, x+\frac{1}{4},\, \frac{1}{2}-y\right]$	[236]
237	$\left[y+\frac{1}{4},\, z+\frac{1}{4},\, \frac{1}{2}-x\right]$	[237]
238	$\left[-z,\, x+\frac{1}{4},\, y+\frac{3}{4}\right]$	[238]
239	$\left[-y,\, z+\frac{1}{4},\, x+\frac{3}{4}\right]$	[239]
240	$\left[z+\frac{1}{4},\, -x,\, y+\frac{3}{4}\right]$	[240]
241	$\left[x,\, y+\frac{1}{2},\, z\right]$	[241]
242	$\left[x+\frac{1}{4},\, \frac{1}{2}-z,\, y+\frac{1}{4}\right]$	[242]
243	$\left[x+\frac{1}{4},\, z+\frac{3}{4},\, -y\right]$	[243]
244	$\left[z+\frac{1}{4},\, y+\frac{3}{4},\, -x\right]$	[244]
245	$\left[-z,\, y+\frac{3}{4},\, x+\frac{1}{4}\right]$	[245]
246	$\left[-y,\, x+\frac{3}{4},\, z+\frac{1}{4}\right]$	[246]
247	$\left[y+\frac{1}{4},\, \frac{1}{2}-x,\, z+\frac{1}{4}\right]$	[247]
248	$\left[x,\, \frac{3}{4}-y,\, \frac{1}{4}-z\right]$	[248]
249	$\left[\frac{1}{4}-x,\, y+\frac{1}{2},\, \frac{1}{4}-z\right]$	[249]
250	$\left[\frac{1}{4}-x,\, \frac{3}{4}-y,\, z\right]$	[250]
251	$\left[y+\frac{1}{4},\, x+\frac{3}{4},\, -z\right]$	[251]
252	$\left[-y,\, \frac{1}{2}-x,\, -z\right]$	[252]
253	$\left[-x,\, z+\frac{3}{4},\, y+\frac{1}{4}\right]$	[253]
254	$\left[-x,\, \frac{1}{2}-z,\, -y\right]$	[254]
255	$\left[z+\frac{1}{4},\, \frac{1}{2}-y,\, x+\frac{1}{4}\right]$	[255]
256	$\left[-z,\, \frac{1}{2}-y,\, -x\right]$	[256]
257	$\left[z,\, x+\frac{1}{2},\, y\right]$	[257]
258	$\left[y,\, z+\frac{1}{2},\, x\right]$	[258]
259	$\left[\frac{1}{4}-y,\, z+\frac{1}{2},\, \frac{1}{4}-x\right]$	[259]
260	$\left[\frac{1}{4}-z,\, \frac{3}{4}-x,\, y\right]$	[260]
261	$\left[\frac{1}{4}-y,\, \frac{3}{4}-z,\, x\right]$	[261]
262	$\left[z,\, \frac{3}{4}-x,\, \frac{1}{4}-y\right]$	[262]
263	$\left[y,\, \frac{3}{4}-z,\, \frac{1}{4}-x\right]$	[263]
264	$\left[\frac{1}{4}-z,\, x+\frac{1}{2},\, \frac{1}{4}-y\right]$	[264]
265	$\left[-x,\, \frac{1}{2}-y,\, -z\right]$	[265]
266	$\left[\frac{1}{4}-x,\, z+\frac{1}{2},\, \frac{1}{4}-y\right]$	[266]
267	$\left[\frac{1}{4}-x,\, \frac{3}{4}-z,\, y\right]$	[267]
268	$\left[\frac{1}{4}-z,\, \frac{3}{4}-y,\, x\right]$	[268]
269	$\left[z,\, \frac{3}{4}-y,\, \frac{1}{4}-x\right]$	[269]
270	$\left[y,\, \frac{3}{4}-x,\, \frac{1}{4}-z\right]$	[270]
271	$\left[\frac{1}{4}-y,\, x+\frac{1}{2},\, \frac{1}{4}-z\right]$	[271]
272	$\left[-x,\, y+\frac{3}{4},\, z+\frac{1}{4}\right]$	[272]
273	$\left[x+\frac{1}{4},\, \frac{1}{2}-y,\, z+\frac{1}{4}\right]$	[273]
274	$\left[x+\frac{1}{4},\, y+\frac{3}{4},\, -z\right]$	[274]
275	$\left[\frac{1}{4}-y,\, \frac{3}{4}-x,\, z\right]$	[275]
276	$\left[y,\, x+\frac{1}{2},\, z\right]$	[276]
277	$\left[x,\, \frac{3}{4}-z,\, \frac{1}{4}-y\right]$	[277]
278	$\left[x,\, z+\frac{1}{2},\, y\right]$	[278]
279	$\left[\frac{1}{4}-z,\, y+\frac{1}{2},\, \frac{1}{4}-x\right]$	[279]

continued ...

Table 12

No.	position	mapping
280	$\left[z,\, y+\frac{1}{2},\, x\right]$	[280]
281	$\left[-z,\, \frac{1}{2}-x,\, -y\right]$	[281]
282	$\left[-y,\, \frac{1}{2}-z,\, -x\right]$	[282]
283	$\left[y+\frac{1}{4},\, \frac{1}{2}-z,\, x+\frac{1}{4}\right]$	[283]
284	$\left[z+\frac{1}{4},\, x+\frac{3}{4},\, -y\right]$	[284]
285	$\left[y+\frac{1}{4},\, z+\frac{3}{4},\, -x\right]$	[285]
286	$\left[-z,\, x+\frac{3}{4},\, y+\frac{1}{4}\right]$	[286]
287	$\left[-y,\, z+\frac{3}{4},\, x+\frac{1}{4}\right]$	[287]
288	$\left[z+\frac{1}{4},\, \frac{1}{2}-x,\, y+\frac{1}{4}\right]$	[288]
289	$\left[x+\frac{1}{2},\, y,\, z\right]$	[289]
290	$\left[x+\frac{3}{4},\, -z,\, y+\frac{1}{4}\right]$	[290]
291	$\left[x+\frac{3}{4},\, z+\frac{1}{4},\, -y\right]$	[291]
292	$\left[z+\frac{3}{4},\, y+\frac{1}{4},\, -x\right]$	[292]
293	$\left[\frac{1}{2}-z,\, y+\frac{1}{4},\, x+\frac{1}{4}\right]$	[293]
294	$\left[\frac{1}{2}-y,\, x+\frac{1}{4},\, z+\frac{1}{4}\right]$	[294]
295	$\left[y+\frac{3}{4},\, -x,\, z+\frac{1}{4}\right]$	[295]
296	$\left[x+\frac{1}{2},\, \frac{1}{4}-y,\, \frac{1}{4}-z\right]$	[296]
297	$\left[\frac{3}{4}-x,\, y,\, \frac{1}{4}-z\right]$	[297]
298	$\left[\frac{3}{4}-x,\, \frac{1}{4}-y,\, z\right]$	[298]
299	$\left[y+\frac{3}{4},\, x+\frac{1}{4},\, -z\right]$	[299]
300	$\left[\frac{1}{2}-y,\, -x,\, -z\right]$	[300]
301	$\left[\frac{1}{2}-x,\, z+\frac{1}{4},\, y+\frac{1}{4}\right]$	[301]
302	$\left[\frac{1}{2}-x,\, -z,\, -y\right]$	[302]
303	$\left[z+\frac{3}{4},\, -y,\, x+\frac{1}{4}\right]$	[303]
304	$\left[\frac{1}{2}-z,\, -y,\, -x\right]$	[304]
305	$\left[z+\frac{1}{2},\, x,\, y\right]$	[305]
306	$\left[y+\frac{1}{2},\, z,\, x\right]$	[306]
307	$\left[\frac{3}{4}-y,\, z,\, \frac{1}{4}-x\right]$	[307]
308	$\left[\frac{3}{4}-z,\, \frac{1}{4}-x,\, y\right]$	[308]
309	$\left[\frac{3}{4}-y,\, \frac{1}{4}-z,\, x\right]$	[309]
310	$\left[z+\frac{1}{2},\, \frac{1}{4}-x,\, \frac{1}{4}-y\right]$	[310]
311	$\left[y+\frac{1}{2},\, \frac{1}{4}-z,\, \frac{1}{4}-x\right]$	[311]
312	$\left[\frac{3}{4}-z,\, x,\, \frac{1}{4}-y\right]$	[312]
313	$\left[\frac{1}{2}-x,\, -y,\, -z\right]$	[313]
314	$\left[\frac{3}{4}-x,\, z,\, \frac{1}{4}-y\right]$	[314]
315	$\left[\frac{3}{4}-x,\, \frac{1}{4}-z,\, y\right]$	[315]
316	$\left[\frac{3}{4}-z,\, \frac{1}{4}-y,\, x\right]$	[316]
317	$\left[z+\frac{1}{2},\, \frac{1}{4}-y,\, \frac{1}{4}-x\right]$	[317]
318	$\left[y+\frac{1}{2},\, \frac{1}{4}-x,\, \frac{1}{4}-z\right]$	[318]
319	$\left[\frac{3}{4}-y,\, x,\, \frac{1}{4}-z\right]$	[319]
320	$\left[\frac{1}{2}-x,\, y+\frac{1}{4},\, z+\frac{1}{4}\right]$	[320]
321	$\left[x+\frac{3}{4},\, -y,\, z+\frac{1}{4}\right]$	[321]
322	$\left[x+\frac{3}{4},\, y+\frac{1}{4},\, -z\right]$	[322]
323	$\left[\frac{3}{4}-y,\, \frac{1}{4}-x,\, z\right]$	[323]
324	$\left[y+\frac{1}{2},\, x,\, z\right]$	[324]
325	$\left[x+\frac{1}{2},\, \frac{1}{4}-z,\, \frac{1}{4}-y\right]$	[325]
326	$\left[x+\frac{1}{2},\, z,\, y\right]$	[326]

continued ...

Table 12

No.	position	mapping
327	$\left[\frac{3}{4}-z,\, y,\, \frac{1}{4}-x\right]$	[327]
328	$\left[z+\frac{1}{2},\, y,\, x\right]$	[328]
329	$\left[\frac{1}{2}-z,\, -x,\, -y\right]$	[329]
330	$\left[\frac{1}{2}-y,\, -z,\, -x\right]$	[330]
331	$\left[y+\frac{3}{4},\, -z,\, x+\frac{1}{4}\right]$	[331]
332	$\left[z+\frac{3}{4},\, x+\frac{1}{4},\, -y\right]$	[332]
333	$\left[y+\frac{3}{4},\, z+\frac{1}{4},\, -x\right]$	[333]
334	$\left[\frac{1}{2}-z,\, x+\frac{1}{4},\, y+\frac{1}{4}\right]$	[334]
335	$\left[\frac{1}{2}-y,\, z+\frac{1}{4},\, x+\frac{1}{4}\right]$	[335]
336	$\left[z+\frac{3}{4},\, -x,\, y+\frac{1}{4}\right]$	[336]
337	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[337]
338	$\left[x+\frac{3}{4},\, \frac{1}{2}-z,\, y+\frac{3}{4}\right]$	[338]
339	$\left[x+\frac{3}{4},\, z+\frac{3}{4},\, \frac{1}{2}-y\right]$	[339]
340	$\left[z+\frac{3}{4},\, y+\frac{3}{4},\, \frac{1}{2}-x\right]$	[340]
341	$\left[\frac{1}{2}-z,\, y+\frac{3}{4},\, x+\frac{3}{4}\right]$	[341]
342	$\left[\frac{1}{2}-y,\, x+\frac{3}{4},\, z+\frac{3}{4}\right]$	[342]
343	$\left[y+\frac{3}{4},\, \frac{1}{2}-x,\, z+\frac{3}{4}\right]$	[343]
344	$\left[x+\frac{1}{2},\, \frac{3}{4}-y,\, \frac{3}{4}-z\right]$	[344]
345	$\left[\frac{3}{4}-x,\, y+\frac{1}{2},\, \frac{3}{4}-z\right]$	[345]
346	$\left[\frac{3}{4}-x,\, \frac{3}{4}-y,\, z+\frac{1}{2}\right]$	[346]
347	$\left[y+\frac{3}{4},\, x+\frac{3}{4},\, \frac{1}{2}-z\right]$	[347]
348	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[348]
349	$\left[\frac{1}{2}-x,\, z+\frac{3}{4},\, y+\frac{3}{4}\right]$	[349]
350	$\left[\frac{1}{2}-x,\, \frac{1}{2}-z,\, \frac{1}{2}-y\right]$	[350]
351	$\left[z+\frac{3}{4},\, \frac{1}{2}-y,\, x+\frac{3}{4}\right]$	[351]
352	$\left[\frac{1}{2}-z,\, \frac{1}{2}-y,\, \frac{1}{2}-x\right]$	[352]
353	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[353]
354	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[354]
355	$\left[\frac{3}{4}-y,\, z+\frac{1}{2},\, \frac{3}{4}-x\right]$	[355]
356	$\left[\frac{3}{4}-z,\, \frac{3}{4}-x,\, y+\frac{1}{2}\right]$	[356]
357	$\left[\frac{3}{4}-y,\, \frac{3}{4}-z,\, x+\frac{1}{2}\right]$	[357]
358	$\left[z+\frac{1}{2},\, \frac{3}{4}-x,\, \frac{3}{4}-y\right]$	[358]
359	$\left[y+\frac{1}{2},\, \frac{3}{4}-z,\, \frac{3}{4}-x\right]$	[359]
360	$\left[\frac{3}{4}-z,\, x+\frac{1}{2},\, \frac{3}{4}-y\right]$	[360]
361	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[361]
362	$\left[\frac{3}{4}-x,\, z+\frac{1}{2},\, \frac{3}{4}-y\right]$	[362]
363	$\left[\frac{3}{4}-x,\, \frac{3}{4}-z,\, y+\frac{1}{2}\right]$	[363]
364	$\left[\frac{3}{4}-z,\, \frac{3}{4}-y,\, x+\frac{1}{2}\right]$	[364]
365	$\left[z+\frac{1}{2},\, \frac{3}{4}-y,\, \frac{3}{4}-x\right]$	[365]
366	$\left[y+\frac{1}{2},\, \frac{3}{4}-x,\, \frac{3}{4}-z\right]$	[366]
367	$\left[\frac{3}{4}-y,\, x+\frac{1}{2},\, \frac{3}{4}-z\right]$	[367]
368	$\left[\frac{1}{2}-x,\, y+\frac{3}{4},\, z+\frac{3}{4}\right]$	[368]
369	$\left[x+\frac{3}{4},\, \frac{1}{2}-y,\, z+\frac{3}{4}\right]$	[369]
370	$\left[x+\frac{3}{4},\, y+\frac{3}{4},\, \frac{1}{2}-z\right]$	[370]
371	$\left[\frac{3}{4}-y,\, \frac{3}{4}-x,\, z+\frac{1}{2}\right]$	[371]
372	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[372]
373	$\left[x+\frac{1}{2},\, \frac{3}{4}-z,\, \frac{3}{4}-y\right]$	[373]

continued ...

Table 12

No.	position	mapping
374	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[374]
375	$\left[\frac{3}{4}-z,\, y+\frac{1}{2},\, \frac{3}{4}-x\right]$	[375]
376	$\left[z+\frac{1}{2},\, y+\frac{1}{2},\, x+\frac{1}{2}\right]$	[376]
377	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, \frac{1}{2}-y\right]$	[377]
378	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, \frac{1}{2}-x\right]$	[378]
379	$\left[y+\frac{3}{4},\, \frac{1}{2}-z,\, x+\frac{3}{4}\right]$	[379]
380	$\left[z+\frac{3}{4},\, x+\frac{3}{4},\, \frac{1}{2}-y\right]$	[380]
381	$\left[y+\frac{3}{4},\, z+\frac{3}{4},\, \frac{1}{2}-x\right]$	[381]
382	$\left[\frac{1}{2}-z,\, x+\frac{3}{4},\, y+\frac{3}{4}\right]$	[382]
383	$\left[\frac{1}{2}-y,\, z+\frac{3}{4},\, x+\frac{3}{4}\right]$	[383]
384	$\left[z+\frac{3}{4},\, \frac{1}{2}-x,\, y+\frac{3}{4}\right]$	[384]