MSG No. 228.139 $F_S d\bar{3}c$ [Type IV, cubic]

Table 1: Wyckoff site: `16a`, site symmetry: `-4'3m'`

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

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

No.	position	mapping
1	$\left[\frac{1}{4},\frac{1}{4},0\right]$	[1,23,24,96,143,169,204,205,207,279,325,372]
2	$\left[\frac{1}{2},\frac{1}{2},\frac{1}{2}\right]$	[2,5,11,77,122,179,226,283,334,346,355,358]
3	$\left[\frac{1}{2},\frac{1}{4},\frac{1}{4}\right]$	[3,7,16,88,123,175,237,273,297,305,309,377]
4	$\left[\frac{1}{4},\frac{1}{2},\frac{1}{4}\right]$	[4,6,14,76,134,174,236,248,258,260,320,378]
5	$\left[\frac{1}{4},0,\frac{1}{4}\right]$	[8,18,20,92,138,176,220,244,246,254,318,374]
6	$\left[0,\frac{1}{4},\frac{1}{4}\right]$	[9,17,21,89,141,177,219,271,291,295,304,376]
7	$[0,0,0]$	[10,19,22,94,139,178,227,266,317,338,341,347]
8	$\left[\frac{1}{4},\frac{1}{4},\frac{1}{2}\right]$	[12,13,15,87,133,180,193,215,216,288,335,361]
9	$\left[\frac{3}{4},\frac{3}{4},0\right]$	[25,95,144,145,167,168,228,277,327,348,349,351]
10	$\left[0,\frac{1}{2},0\right]$	[26,83,98,101,107,173,238,250,259,262,322,379]
11	$\left[0,\frac{1}{4},\frac{3}{4}\right]$	[27,79,99,103,112,184,201,209,213,281,333,369]
12	$\left[\frac{1}{4},0,\frac{3}{4}\right]$	[28,52,54,62,126,182,200,210,212,284,330,368]
13	$\left[\frac{1}{2},0,0\right]$	[29,50,53,59,131,170,235,274,298,307,310,382]
14	$\left[\frac{3}{4},0,\frac{1}{4}\right]$	[30,86,124,148,150,158,234,272,296,306,308,380]
15	$\left[0,\frac{3}{4},\frac{1}{4}\right]$	[31,75,136,147,151,160,233,249,257,261,321,381]
16	$\left[\frac{3}{4},\frac{1}{2},\frac{1}{4}\right]$	[32,90,140,152,162,164,230,270,292,294,302,364]
17	$\left[\frac{1}{2},\frac{3}{4},\frac{1}{4}\right]$	[33,93,137,153,161,165,232,243,247,256,319,363]
18	$\left[\frac{1}{2},\frac{1}{2},0\right]$	[34,91,142,154,163,166,194,197,203,269,314,371]
19	$\left[0,0,\frac{1}{2}\right]$	[35,74,125,146,149,155,202,211,214,286,331,370]
20	$\left[\frac{3}{4},\frac{3}{4},\frac{1}{2}\right]$	[36,85,135,156,157,159,217,287,336,337,359,360]
21	$\left[\frac{3}{4},\frac{1}{4},0\right]$	[37,84,108,109,111,183,239,265,289,311,312,384]

Table 2

No.	position	mapping
22	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[38,78,100,102,110,172,224,282,332,344,354,356]
23	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[39,60,61,63,132,181,240,241,263,264,313,383]
24	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[40,51,55,64,127,171,225,285,329,345,353,357]
25	$\left[0, \frac{3}{4}, \frac{3}{4}\right]$	[41,57,65,69,129,189,223,267,328,339,343,352]
26	$\left[\frac{3}{4}, 0, \frac{3}{4}\right]$	[42,80,104,114,116,188,222,278,316,340,342,350]
27	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[43,82,106,115,118,190,221,242,245,251,323,362]
28	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[44,56,66,68,128,186,196,198,206,268,326,366]
29	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[45,81,105,113,117,185,195,199,208,280,315,367]
30	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[46,58,67,70,130,187,218,275,290,293,299,365]
31	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[47,73,97,119,120,192,229,276,300,301,303,375]
32	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[48,49,71,72,121,191,231,252,253,255,324,373]

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

No.	position	mapping
1	$\left[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	[1,23,24,156,157,159,217,279,287,325,336,372]
2	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[2,5,10,11,19,22,226,227,266,283,317,334]
3	$\left[\frac{3}{4}, 0, 0\right]$	[3,7,16,57,65,69,223,237,267,273,328,377]
4	$\left[0, \frac{3}{4}, 0\right]$	[4,6,14,104,114,116,222,236,278,316,320,378]
5	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{2}\right]$	[8,18,20,100,102,110,220,224,282,318,332,374]
6	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}\right]$	[9,17,21,51,55,64,219,225,271,285,329,376]
7	$\left[0, 0, \frac{3}{4}\right]$	[12,13,15,145,167,168,228,277,288,327,335,361]
8	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[25,87,95,133,144,180,193,215,216,348,349,351]
9	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[26,43,82,83,173,190,242,245,250,251,259,262]
10	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	[27,33,79,93,137,184,201,209,213,243,247,256]
11	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	[28,32,90,126,140,182,200,210,212,292,294,302]
12	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[29,46,130,131,170,187,290,293,298,299,307,310]
13	$\left[0, \frac{3}{4}, \frac{1}{2}\right]$	[30,44,86,124,128,186,196,198,206,296,306,308]
14	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	[31,45,75,81,136,185,195,199,208,249,257,261]
15	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[34,35,74,91,125,142,194,197,202,203,211,214]
16	$\left[0, 0, \frac{1}{4}\right]$	[36,85,96,135,143,169,204,205,207,337,359,360]
17	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[37,48,84,121,183,191,252,253,255,289,311,312]
18	$\left[0, \frac{1}{4}, 0\right]$	[38,78,92,138,172,176,244,246,254,344,354,356]
19	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[39,47,73,132,181,192,241,263,264,300,301,303]
20	$\left[\frac{1}{4}, 0, 0\right]$	[40,89,127,141,171,177,291,295,304,345,353,357]
21	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}\right]$	[41,88,123,129,175,189,297,305,309,339,343,352]
22	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{2}\right]$	[42,76,80,134,174,188,248,258,260,340,342,350]
23	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[49,71,72,108,109,111,231,239,265,324,373,384]
24	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[50,53,58,59,67,70,218,235,274,275,365,382]
25	$\left[0, \frac{1}{4}, \frac{1}{2}\right]$	[52,54,62,152,162,164,230,270,284,330,364,368]
26	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[56,66,68,148,150,158,234,268,272,326,366,380]
27	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[60,61,63,97,119,120,229,240,276,313,375,383]
28	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[77,94,122,139,178,179,338,341,346,347,355,358]
29	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[98,101,106,107,115,118,221,238,322,323,362,379]

continued ...

Table 3

No.	position	mapping
30	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[99,103,112,153,161,165,232,281,319,333,363,369]
31	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	[105,113,117,147,151,160,233,280,315,321,367,381]
32	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[146,149,154,155,163,166,269,286,314,331,370,371]

Table 4: Wyckoff site: 48d, site symmetry: -42'.m'

No.	position	mapping
1	$\left[\frac{5}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[1,9,76,173,248,250,279,376]
2	$\left[\frac{7}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[2,13,44,185,195,206,288,334]
3	$\left[\frac{7}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[3,14,96,142,194,205,236,377]
4	$\left[\frac{7}{8}, \frac{5}{8}, \frac{7}{8}\right]$	[4,5,33,121,226,255,256,320]
5	$\left[\frac{1}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[6,12,141,187,295,299,335,378]
6	$\left[\frac{5}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[7,11,47,90,237,283,294,300]
7	$\left[\frac{5}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[8,10,39,136,220,241,249,317]
8	$\left[\frac{7}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[15,16,82,176,244,245,273,361]
9	$\left[\frac{5}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[17,20,74,133,214,216,219,374]
10	$\left[\frac{3}{8}, \frac{5}{8}, \frac{5}{8}\right]$	[18,23,131,175,307,309,318,372]
11	$\left[\frac{7}{8}, \frac{5}{8}, \frac{5}{8}\right]$	[19,21,30,84,227,271,306,311]
12	$\left[\frac{5}{8}, \frac{5}{8}, \frac{7}{8}\right]$	[22,24,27,182,209,212,266,325]
13	$\left[\frac{3}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[25,100,101,129,224,322,351,352]
14	$\left[\frac{5}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[26,65,68,181,262,264,267,326]
15	$\left[\frac{5}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[28,49,57,125,200,202,231,328]
16	$\left[\frac{1}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[29,124,145,153,232,296,298,327]
17	$\left[\frac{7}{8}, \frac{1}{8}, \frac{5}{8}\right]$	[31,83,162,167,228,259,261,270]
18	$\left[\frac{3}{8}, \frac{5}{8}, \frac{7}{8}\right]$	[32,130,159,160,217,292,293,321]
19	$\left[\frac{7}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[34,63,64,128,196,197,225,313]
20	$\left[\frac{7}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[35,79,114,119,211,213,222,276]
21	$\left[\frac{7}{8}, \frac{1}{8}, \frac{1}{8}\right]$	[36,67,69,78,223,275,354,359]
22	$\left[\frac{1}{8}, \frac{5}{8}, \frac{7}{8}\right]$	[37,113,116,170,278,310,312,315]
23	$\left[\frac{1}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[38,166,168,171,277,314,353,356]
24	$\left[\frac{1}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[40,104,106,135,221,316,337,345]
25	$\left[\frac{3}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[41,146,157,188,286,336,339,350]
26	$\left[\frac{5}{8}, \frac{3}{8}, \frac{3}{8}\right]$	[42,55,59,95,235,285,342,348]
27	$\left[\frac{5}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[43,93,150,156,234,247,251,287]
28	$\left[\frac{5}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[45,91,102,108,199,203,239,282]
29	$\left[\frac{3}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[46,99,110,192,281,290,301,332]
30	$\left[\frac{7}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[48,51,62,190,242,253,284,329]
31	$\left[\frac{7}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[50,61,92,137,240,243,254,382]
32	$\left[\frac{7}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[52,53,81,169,207,208,274,368]
33	$\left[\frac{1}{8}, \frac{3}{8}, \frac{3}{8}\right]$	[54,60,139,189,330,343,347,383]
34	$\left[\frac{5}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[56,58,87,184,193,201,268,365]
35	$\left[\frac{3}{8}, \frac{1}{8}, \frac{1}{8}\right]$	[66,71,127,179,324,355,357,366]
36	$\left[\frac{5}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[70,72,75,134,218,257,260,373]
37	$\left[\frac{3}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[73,148,149,177,272,303,304,370]

Table 4

No.	position	mapping
38	$\left[\frac{1}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[77,97,105,172,280,344,346,375]
39	$\left[\frac{3}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[80,111,112,178,265,340,341,369]
40	$\left[\frac{1}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[85,122,161,164,230,358,360,363]
41	$\left[\frac{1}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[86,118,120,123,229,305,308,362]
42	$\left[\frac{1}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[88,152,154,183,269,289,297,364]
43	$\left[\frac{3}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[89,98,109,140,238,291,302,384]
44	$\left[\frac{3}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[94,144,147,158,233,338,349,380]
45	$\left[\frac{1}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[103,107,143,186,198,204,333,379]
46	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[115,117,126,180,210,215,323,367]
47	$\left[\frac{3}{8}, \frac{1}{8}, \frac{5}{8}\right]$	[132,163,165,174,258,263,319,371]
48	$\left[\frac{1}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[138,151,155,191,246,252,331,381]

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

No.	position	mapping
1	$\left[x, x, \frac{1}{4} - x\right]$	[1,23,24,279,325,372]
2	$\left[x + \frac{1}{4}, x + \frac{1}{4}, x + \frac{1}{4}\right]$	[2,5,11,226,283,334]
3	$\left[x + \frac{1}{4}, \frac{1}{2} - x, \frac{1}{2} - x\right]$	[3,7,16,237,273,377]
4	$\left[\frac{1}{2} - x, x + \frac{1}{4}, \frac{1}{2} - x\right]$	[4,6,14,236,320,378]
5	$\left[x, \frac{1}{4} - x, x\right]$	[8,18,20,220,318,374]
6	$\left[\frac{1}{4} - x, x, x\right]$	[9,17,21,219,271,376]
7	$\left[\frac{1}{4} - x, \frac{1}{4} - x, \frac{1}{4} - x\right]$	[10,19,22,227,266,317]
8	$\left[\frac{1}{2} - x, \frac{1}{2} - x, x + \frac{1}{4}\right]$	[12,13,15,288,335,361]
9	$\left[-x, -x, x + \frac{3}{4}\right]$	[25,95,144,348,349,351]
10	$\left[\frac{1}{4} - x, \frac{3}{4} - x, \frac{1}{4} - x\right]$	[26,83,173,250,259,262]
11	$\left[\frac{1}{4} - x, x, x + \frac{1}{2}\right]$	[27,79,184,201,209,213]
12	$\left[x, \frac{1}{4} - x, x + \frac{1}{2}\right]$	[28,126,182,200,210,212]
13	$\left[\frac{3}{4} - x, \frac{1}{4} - x, \frac{1}{4} - x\right]$	[29,131,170,298,307,310]
14	$\left[x + \frac{1}{2}, \frac{1}{4} - x, x\right]$	[30,86,124,296,306,308]
15	$\left[\frac{1}{4} - x, x + \frac{1}{2}, x\right]$	[31,75,136,249,257,261]
16	$\left[-x, x + \frac{1}{4}, \frac{1}{2} - x\right]$	[32,90,140,292,294,302]
17	$\left[x + \frac{1}{4}, -x, \frac{1}{2} - x\right]$	[33,93,137,243,247,256]
18	$\left[x + \frac{1}{4}, x + \frac{1}{4}, x + \frac{3}{4}\right]$	[34,91,142,194,197,203]
19	$\left[\frac{1}{4} - x, \frac{1}{4} - x, \frac{3}{4} - x\right]$	[35,74,125,202,211,214]
20	$\left[x + \frac{1}{2}, x + \frac{1}{2}, \frac{3}{4} - x\right]$	[36,85,135,337,359,360]
21	$\left[x + \frac{1}{2}, x, \frac{1}{4} - x\right]$	[37,84,183,289,311,312]
22	$\left[x + \frac{1}{2}, \frac{3}{4} - x, x + \frac{1}{2}\right]$	[38,78,172,344,354,356]
23	$\left[x, x + \frac{1}{2}, \frac{1}{4} - x\right]$	[39,132,181,241,263,264]
24	$\left[\frac{3}{4} - x, x + \frac{1}{2}, x + \frac{1}{2}\right]$	[40,127,171,345,353,357]
25	$\left[x + \frac{3}{4}, -x, -x\right]$	[41,129,189,339,343,352]
26	$\left[-x, x + \frac{3}{4}, -x\right]$	[42,80,188,340,342,350]
27	$\left[x + \frac{1}{4}, x + \frac{3}{4}, x + \frac{1}{4}\right]$	[43,82,190,242,245,251]
28	$\left[\frac{1}{2} - x, x + \frac{1}{4}, -x\right]$	[44,128,186,196,198,206]
29	$\left[x + \frac{1}{4}, \frac{1}{2} - x, -x\right]$	[45,81,185,195,199,208]

continued ...

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Table 5

No.	position	mapping
30	$\left[x+\frac{3}{4},\, x+\frac{1}{4},\, x+\frac{1}{4}\right]$	[46,130,187,290,293,299]
31	$\left[-x,\, \frac{1}{2}-x,\, x+\frac{1}{4}\right]$	[47,73,192,300,301,303]
32	$\left[\frac{1}{2}-x,\, -x,\, x+\frac{1}{4}\right]$	[48,121,191,252,253,255]
33	$\left[x,\, x+\frac{1}{2},\, \frac{3}{4}-x\right]$	[49,71,72,231,324,373]
34	$\left[x+\frac{1}{4},\, x+\frac{3}{4},\, x+\frac{3}{4}\right]$	[50,53,59,235,274,382]
35	$\left[x+\frac{1}{4},\, -x,\, -x\right]$	[51,55,64,225,285,329]
36	$\left[\frac{1}{2}-x,\, x+\frac{3}{4},\, -x\right]$	[52,54,62,284,330,368]
37	$\left[x,\, \frac{3}{4}-x,\, x+\frac{1}{2}\right]$	[56,66,68,268,326,366]
38	$\left[\frac{1}{4}-x,\, x+\frac{1}{2},\, x+\frac{1}{2}\right]$	[57,65,69,223,267,328]
39	$\left[\frac{1}{4}-x,\, \frac{3}{4}-x,\, \frac{3}{4}-x\right]$	[58,67,70,218,275,365]
40	$\left[\frac{1}{2}-x,\, -x,\, x+\frac{3}{4}\right]$	[60,61,63,240,313,383]
41	$\left[x,\, \frac{3}{4}-x,\, x\right]$	[76,134,174,248,258,260]
42	$\left[\frac{3}{4}-x,\, \frac{3}{4}-x,\, \frac{3}{4}-x\right]$	[77,122,179,346,355,358]
43	$\left[x,\, x,\, \frac{3}{4}-x\right]$	[87,133,180,193,215,216]
44	$\left[\frac{3}{4}-x,\, x,\, x\right]$	[88,123,175,297,305,309]
45	$\left[x+\frac{3}{4},\, \frac{1}{2}-x,\, \frac{1}{2}-x\right]$	[89,141,177,291,295,304]
46	$\left[\frac{1}{2}-x,\, x+\frac{3}{4},\, \frac{1}{2}-x\right]$	[92,138,176,244,246,254]
47	$\left[x+\frac{3}{4},\, x+\frac{3}{4},\, x+\frac{3}{4}\right]$	[94,139,178,338,341,347]
48	$\left[\frac{1}{2}-x,\, \frac{1}{2}-x,\, x+\frac{3}{4}\right]$	[96,143,169,204,205,207]
49	$\left[x+\frac{1}{2},\, x,\, \frac{3}{4}-x\right]$	[97,119,120,229,276,375]
50	$\left[x+\frac{3}{4},\, x+\frac{1}{4},\, x+\frac{3}{4}\right]$	[98,101,107,238,322,379]
51	$\left[x+\frac{3}{4},\, \frac{1}{2}-x,\, -x\right]$	[99,103,112,281,333,369]
52	$\left[-x,\, x+\frac{1}{4},\, -x\right]$	[100,102,110,224,282,332]
53	$\left[x+\frac{1}{2},\, \frac{1}{4}-x,\, x+\frac{1}{2}\right]$	[104,114,116,222,278,316]
54	$\left[\frac{3}{4}-x,\, x,\, x+\frac{1}{2}\right]$	[105,113,117,280,315,367]
55	$\left[\frac{3}{4}-x,\, \frac{1}{4}-x,\, \frac{3}{4}-x\right]$	[106,115,118,221,323,362]
56	$\left[-x,\, \frac{1}{2}-x,\, x+\frac{3}{4}\right]$	[108,109,111,239,265,384]
57	$\left[x+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{4}-x\right]$	[145,167,168,228,277,327]
58	$\left[x+\frac{3}{4},\, x+\frac{3}{4},\, x+\frac{1}{4}\right]$	[146,149,155,286,331,370]
59	$\left[x+\frac{3}{4},\, -x,\, \frac{1}{2}-x\right]$	[147,151,160,233,321,381]
60	$\left[-x,\, x+\frac{3}{4},\, \frac{1}{2}-x\right]$	[148,150,158,234,272,380]
61	$\left[x+\frac{1}{2},\, \frac{3}{4}-x,\, x\right]$	[152,162,164,230,270,364]
62	$\left[\frac{3}{4}-x,\, x+\frac{1}{2},\, x\right]$	[153,161,165,232,319,363]
63	$\left[\frac{3}{4}-x,\, \frac{3}{4}-x,\, \frac{1}{4}-x\right]$	[154,163,166,269,314,371]
64	$\left[-x,\, -x,\, x+\frac{1}{4}\right]$	[156,157,159,217,287,336]

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

No.	position	mapping
1	$\left[\frac{3}{8},\, \frac{1}{2},\, \frac{5}{8}\right]$	[1,159,297,352]
2	$\left[\frac{5}{8},\, \frac{7}{8},\, \frac{3}{4}\right]$	[2,22,264,301]
3	$\left[\frac{5}{8},\, \frac{7}{8},\, 0\right]$	[3,65,212,302]
4	$\left[\frac{7}{8},\, \frac{3}{4},\, \frac{1}{8}\right]$	[4,104,197,202]
5	$\left[\frac{7}{8},\, \frac{3}{4},\, \frac{5}{8}\right]$	[5,10,196,296]

continued ...

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Table 6

No.	position	mapping
6	$\left[0, \frac{5}{8}, \frac{7}{8}\right]$	[6,114,252,311]
7	$\left[\frac{3}{4}, \frac{1}{8}, \frac{7}{8}\right]$	[7,69,251,259]
8	$\left[\frac{3}{8}, \frac{3}{4}, \frac{5}{8}\right]$	[8,100,293,298]
9	$\left[\frac{7}{8}, \frac{1}{2}, \frac{5}{8}\right]$	[9,64,255,289]
10	$\left[\frac{3}{4}, \frac{5}{8}, \frac{7}{8}\right]$	[11,19,213,247]
11	$\left[0, \frac{1}{8}, \frac{7}{8}\right]$	[12,167,246,354]
12	$\left[\frac{1}{8}, \frac{7}{8}, \frac{3}{4}\right]$	[13,168,290,310]
13	$\left[\frac{1}{8}, \frac{7}{8}, 0\right]$	[14,116,291,353]
14	$\left[\frac{7}{8}, 0, \frac{5}{8}\right]$	[15,145,208,249]
15	$\left[\frac{7}{8}, 0, \frac{1}{8}\right]$	[16,57,207,337]
16	$\left[\frac{5}{8}, \frac{3}{8}, \frac{1}{2}\right]$	[17,51,260,350]
17	$\left[\frac{1}{2}, \frac{5}{8}, \frac{3}{8}\right]$	[18,102,215,348]
18	$\left[\frac{5}{8}, \frac{7}{8}, \frac{1}{2}\right]$	[20,110,195,257]
19	$\left[\frac{3}{4}, \frac{5}{8}, \frac{3}{8}\right]$	[21,55,203,211]
20	$\left[\frac{1}{2}, \frac{5}{8}, \frac{7}{8}\right]$	[23,156,210,294]
21	$\left[\frac{5}{8}, \frac{3}{8}, \frac{3}{4}\right]$	[24,157,242,262]
22	$\left[\frac{5}{8}, \frac{1}{2}, \frac{3}{8}\right]$	[25,87,225,376]
23	$\left[\frac{7}{8}, \frac{1}{8}, \frac{3}{4}\right]$	[26,190,277,288]
24	$\left[\frac{7}{8}, \frac{5}{8}, 0\right]$	[27,137,236,278]
25	$\left[\frac{5}{8}, \frac{3}{4}, \frac{7}{8}\right]$	[28,32,226,317]
26	$\left[\frac{1}{8}, \frac{3}{4}, \frac{7}{8}\right]$	[29,130,316,320]
27	$\left[0, \frac{7}{8}, \frac{5}{8}\right]$	[30,186,228,335]
28	$\left[\frac{3}{4}, \frac{7}{8}, \frac{5}{8}\right]$	[31,45,227,283]
29	$\left[\frac{5}{8}, \frac{1}{2}, \frac{7}{8}\right]$	[33,184,217,279]
30	$\left[\frac{5}{8}, \frac{3}{4}, \frac{3}{8}\right]$	[34,125,220,224]
31	$\left[\frac{3}{4}, \frac{7}{8}, \frac{1}{8}\right]$	[35,91,223,237]
32	$\left[0, \frac{7}{8}, \frac{1}{8}\right]$	[36,143,222,378]
33	$\left[\frac{7}{8}, \frac{5}{8}, \frac{3}{4}\right]$	[37,48,266,334]
34	$\left[\frac{7}{8}, \frac{1}{8}, 0\right]$	[38,92,267,377]
35	$\left[\frac{5}{8}, 0, \frac{7}{8}\right]$	[39,73,273,328]
36	$\left[\frac{1}{8}, 0, \frac{7}{8}\right]$	[40,177,327,361]
37	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{2}\right]$	[41,123,332,374]
38	$\left[\frac{1}{2}, \frac{3}{8}, \frac{5}{8}\right]$	[42,174,287,372]
39	$\left[\frac{3}{4}, \frac{3}{8}, \frac{5}{8}\right]$	[43,83,271,285]
40	$\left[\frac{7}{8}, \frac{5}{8}, \frac{1}{2}\right]$	[44,86,219,329]
41	$\left[\frac{3}{8}, \frac{5}{8}, \frac{3}{4}\right]$	[46,170,325,336]
42	$\left[\frac{1}{2}, \frac{7}{8}, \frac{5}{8}\right]$	[47,132,282,318]
43	$\left[\frac{3}{8}, 0, \frac{1}{8}\right]$	[49,111,304,345]
44	$\left[\frac{5}{8}, \frac{3}{8}, \frac{1}{4}\right]$	[50,70,216,349]
45	$\left[\frac{7}{8}, \frac{1}{4}, \frac{5}{8}\right]$	[52,152,245,250]
46	$\left[\frac{7}{8}, \frac{1}{4}, \frac{1}{8}\right]$	[53,58,244,344]
47	$\left[0, \frac{1}{8}, \frac{3}{8}\right]$	[54,162,204,359]
48	$\left[\frac{3}{8}, \frac{1}{4}, \frac{1}{8}\right]$	[56,148,341,346]
49	$\left[\frac{3}{4}, \frac{1}{8}, \frac{3}{8}\right]$	[59,67,199,261]
50	$\left[0, \frac{5}{8}, \frac{3}{8}\right]$	[60,119,198,306]
51	$\left[\frac{1}{8}, \frac{3}{8}, \frac{1}{4}\right]$	[61,120,338,358]
52	$\left[\frac{1}{8}, \frac{3}{8}, \frac{1}{2}\right]$	[62,164,305,339]

continued ...

Table 6

No.	position	mapping
53	$\left[\frac{7}{8}, \frac{1}{2}, \frac{1}{8}\right]$	[63,97,201,256]
54	$\left[\frac{1}{2}, \frac{1}{8}, \frac{7}{8}\right]$	[66,150,263,300]
55	$\left[\frac{5}{8}, \frac{3}{8}, 0\right]$	[68,158,209,243]
56	$\left[\frac{1}{2}, \frac{1}{8}, \frac{3}{8}\right]$	[71,108,258,342]
57	$\left[\frac{5}{8}, \frac{7}{8}, \frac{1}{4}\right]$	[72,109,194,214]
58	$\left[\frac{7}{8}, \frac{5}{8}, \frac{1}{4}\right]$	[74,142,229,240]
59	$\left[\frac{7}{8}, \frac{1}{8}, \frac{1}{2}\right]$	[75,185,230,284]
60	$\left[\frac{5}{8}, \frac{1}{4}, \frac{3}{8}\right]$	[76,80,274,365]
61	$\left[\frac{1}{8}, \frac{1}{4}, \frac{3}{8}\right]$	[77,178,364,368]
62	$\left[0, \frac{3}{8}, \frac{1}{8}\right]$	[78,138,276,383]
63	$\left[\frac{3}{4}, \frac{3}{8}, \frac{1}{8}\right]$	[79,93,235,275]
64	$\left[\frac{5}{8}, 0, \frac{3}{8}\right]$	[81,136,231,265]
65	$\left[\frac{5}{8}, \frac{1}{4}, \frac{7}{8}\right]$	[82,173,268,272]
66	$\left[0, \frac{3}{8}, \frac{5}{8}\right]$	[84,191,270,330]
67	$\left[\frac{7}{8}, \frac{1}{8}, \frac{1}{4}\right]$	[85,96,218,382]
68	$\left[\frac{1}{8}, \frac{1}{2}, \frac{3}{8}\right]$	[88,129,313,375]
69	$\left[\frac{3}{8}, \frac{1}{8}, 0\right]$	[89,171,326,380]
70	$\left[\frac{1}{2}, \frac{7}{8}, \frac{1}{8}\right]$	[90,126,239,324]
71	$\left[\frac{3}{8}, \frac{1}{8}, \frac{1}{4}\right]$	[94,122,373,384]
72	$\left[\frac{1}{2}, \frac{3}{8}, \frac{1}{8}\right]$	[95,180,234,366]
73	$\left[\frac{1}{8}, \frac{7}{8}, \frac{1}{4}\right]$	[98,118,205,360]
74	$\left[\frac{1}{8}, \frac{7}{8}, \frac{1}{2}\right]$	[99,161,206,308]
75	$\left[\frac{3}{8}, \frac{3}{4}, \frac{1}{8}\right]$	[101,106,200,292]
76	$\left[\frac{1}{4}, \frac{1}{8}, \frac{3}{8}\right]$	[103,165,347,355]
77	$\left[\frac{3}{8}, \frac{1}{2}, \frac{1}{8}\right]$	[105,160,193,351]
78	$\left[\frac{1}{4}, \frac{5}{8}, \frac{3}{8}\right]$	[107,115,309,343]
79	$\left[\frac{3}{8}, 0, \frac{5}{8}\right]$	[112,153,241,303]
80	$\left[\frac{1}{8}, \frac{3}{8}, 0\right]$	[113,147,254,356]
81	$\left[\frac{1}{4}, \frac{5}{8}, \frac{7}{8}\right]$	[117,151,299,307]
82	$\left[\frac{1}{8}, \frac{1}{2}, \frac{7}{8}\right]$	[121,183,280,321]
83	$\left[\frac{1}{8}, \frac{3}{4}, \frac{3}{8}\right]$	[124,128,221,322]
84	$\left[\frac{1}{4}, \frac{7}{8}, \frac{1}{8}\right]$	[127,141,323,379]
85	$\left[\frac{1}{4}, \frac{7}{8}, \frac{5}{8}\right]$	[131,187,319,333]
86	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{4}\right]$	[133,144,238,362]
87	$\left[\frac{3}{8}, \frac{1}{8}, \frac{1}{2}\right]$	[134,188,281,363]
88	$\left[\frac{1}{8}, 0, \frac{3}{8}\right]$	[135,169,232,369]
89	$\left[\frac{1}{4}, \frac{3}{8}, \frac{1}{8}\right]$	[139,179,367,381]
90	$\left[\frac{3}{8}, \frac{5}{8}, 0\right]$	[140,182,233,315]
91	$\left[\frac{1}{8}, \frac{3}{8}, \frac{3}{4}\right]$	[146,166,253,312]
92	$\left[\frac{3}{8}, \frac{1}{4}, \frac{5}{8}\right]$	[149,154,248,340]
93	$\left[\frac{1}{4}, \frac{1}{8}, \frac{7}{8}\right]$	[155,163,295,357]
94	$\left[\frac{1}{8}, \frac{1}{4}, \frac{7}{8}\right]$	[172,176,269,370]
95	$\left[\frac{1}{4}, \frac{3}{8}, \frac{5}{8}\right]$	[175,189,331,371]
96	$\left[\frac{3}{8}, \frac{1}{8}, \frac{3}{4}\right]$	[181,192,286,314]

Table 7: Wyckoff site: 96g, site symmetry: 2.m'm'

No.	position	mapping
1	$\left[\frac{3}{8}, y, \frac{7}{8}\right]$	[1,105,279,280]
2	$\left[\frac{5}{8}, \frac{5}{8}, y+\frac{1}{4}\right]$	[2,157,334,336]
3	$\left[\frac{5}{8}, \frac{1}{8}, \frac{1}{2}-y\right]$	[3,158,377,380]
4	$\left[\frac{1}{8}, y+\frac{1}{4}, \frac{1}{8}\right]$	[4,101,320,322]
5	$\left[\frac{5}{8}, y+\frac{1}{4}, \frac{5}{8}\right]$	[5,100,224,226]
6	$\left[\frac{1}{2}-y, \frac{5}{8}, \frac{1}{8}\right]$	[6,60,378,383]
7	$\left[y+\frac{1}{4}, \frac{1}{8}, \frac{1}{8}\right]$	[7,59,235,237]
8	$\left[\frac{3}{8}, \frac{1}{4}-y, \frac{3}{8}\right]$	[8,106,220,221]
9	$\left[\frac{7}{8}, y, \frac{3}{8}\right]$	[9,97,375,376]
10	$\left[\frac{7}{8}, \frac{1}{4}-y, \frac{7}{8}\right]$	[10,104,316,317]
11	$\left[y+\frac{1}{4}, \frac{5}{8}, \frac{5}{8}\right]$	[11,55,283,285]
12	$\left[\frac{1}{2}-y, \frac{1}{8}, \frac{5}{8}\right]$	[12,54,330,335]
13	$\left[\frac{1}{8}, \frac{1}{8}, y+\frac{1}{4}\right]$	[13,146,286,288]
14	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{2}-y\right]$	[14,147,233,236]
15	$\left[\frac{1}{8}, \frac{1}{2}-y, \frac{5}{8}\right]$	[15,112,361,369]
16	$\left[\frac{5}{8}, \frac{1}{2}-y, \frac{1}{8}\right]$	[16,111,265,273]
17	$\left[\frac{7}{8}, \frac{3}{8}, y\right]$	[17,164,219,230]
18	$\left[y, \frac{7}{8}, \frac{3}{8}\right]$	[18,71,318,324]
19	$\left[\frac{1}{4}-y, \frac{7}{8}, \frac{7}{8}\right]$	[19,69,223,227]
20	$\left[\frac{3}{8}, \frac{7}{8}, y\right]$	[20,161,363,374]
21	$\left[\frac{1}{4}-y, \frac{3}{8}, \frac{3}{8}\right]$	[21,67,271,275]
22	$\left[\frac{7}{8}, \frac{7}{8}, \frac{1}{4}-y\right]$	[22,168,266,277]
23	$\left[y, \frac{3}{8}, \frac{7}{8}\right]$	[23,66,366,372]
24	$\left[\frac{3}{8}, \frac{3}{8}, \frac{1}{4}-y\right]$	[24,166,314,325]
25	$\left[\frac{5}{8}, -y, \frac{1}{8}\right]$	[25,33,256,351]
26	$\left[\frac{7}{8}, \frac{3}{8}, \frac{1}{4}-y\right]$	[26,37,262,312]
27	$\left[\frac{7}{8}, \frac{3}{8}, y+\frac{1}{2}\right]$	[27,38,209,356]
28	$\left[\frac{3}{8}, \frac{1}{4}-y, \frac{7}{8}\right]$	[28,29,200,298]
29	$\left[y+\frac{1}{2}, \frac{7}{8}, \frac{3}{8}\right]$	[30,36,306,359]
30	$\left[\frac{1}{4}-y, \frac{7}{8}, \frac{3}{8}\right]$	[31,35,211,261]
31	$\left[\frac{5}{8}, y+\frac{1}{4}, \frac{1}{8}\right]$	[32,34,197,292]
32	$\left[\frac{3}{8}, y+\frac{1}{2}, \frac{7}{8}\right]$	[39,40,241,345]
33	$\left[\frac{1}{8}, \frac{5}{8}, -y\right]$	[41,44,206,339]
34	$\left[-y, \frac{1}{8}, \frac{5}{8}\right]$	[42,47,300,342]
35	$\left[y+\frac{1}{4}, \frac{1}{8}, \frac{5}{8}\right]$	[43,45,199,251]
36	$\left[\frac{1}{8}, \frac{5}{8}, y+\frac{1}{4}\right]$	[46,48,253,290]
37	$\left[\frac{3}{8}, y+\frac{1}{2}, \frac{3}{8}\right]$	[49,153,231,232]
38	$\left[\frac{5}{8}, \frac{1}{8}, y+\frac{3}{4}\right]$	[50,109,382,384]
39	$\left[\frac{5}{8}, \frac{5}{8}, -y\right]$	[51,110,329,332]
40	$\left[\frac{1}{8}, y+\frac{3}{4}, \frac{5}{8}\right]$	[52,149,368,370]
41	$\left[\frac{5}{8}, y+\frac{3}{4}, \frac{1}{8}\right]$	[53,148,272,274]
42	$\left[\frac{3}{8}, \frac{3}{4}-y, \frac{7}{8}\right]$	[56,154,268,269]
43	$\left[\frac{7}{8}, y+\frac{1}{2}, \frac{7}{8}\right]$	[57,145,327,328]
44	$\left[\frac{7}{8}, \frac{3}{4}-y, \frac{3}{8}\right]$	[58,152,364,365]
45	$\left[\frac{1}{8}, \frac{5}{8}, y+\frac{3}{4}\right]$	[61,98,238,240]
46	$\left[\frac{1}{8}, \frac{1}{8}, -y\right]$	[62,99,281,284]

continued ...

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Table 7

No.	position	mapping
47	$\left[\frac{1}{8}, -y, \frac{1}{8}\right]$	[63,160,313,321]
48	$\left[\frac{5}{8}, -y, \frac{5}{8}\right]$	[64,159,217,225]
49	$\left[\frac{7}{8}, \frac{7}{8}, y+\frac{1}{2}\right]$	[65,116,267,278]
50	$\left[\frac{3}{8}, \frac{3}{8}, y+\frac{1}{2}\right]$	[68,113,315,326]
51	$\left[\frac{7}{8}, \frac{3}{8}, \frac{3}{4}-y\right]$	[70,120,218,229]
52	$\left[\frac{3}{8}, \frac{7}{8}, \frac{3}{4}-y\right]$	[72,118,362,373]
53	$\left[\frac{5}{8}, \frac{1}{2}-y, \frac{5}{8}\right]$	[73,81,208,303]
54	$\left[\frac{7}{8}, \frac{7}{8}, \frac{3}{4}-y\right]$	[74,85,214,360]
55	$\left[\frac{7}{8}, \frac{7}{8}, y\right]$	[75,86,257,308]
56	$\left[\frac{3}{8}, \frac{3}{4}-y, \frac{3}{8}\right]$	[76,77,248,346]
57	$\left[y+\frac{1}{2}, \frac{3}{8}, \frac{7}{8}\right]$	[78,84,311,354]
58	$\left[\frac{1}{4}-y, \frac{3}{8}, \frac{7}{8}\right]$	[79,83,213,259]
59	$\left[\frac{5}{8}, y+\frac{3}{4}, \frac{5}{8}\right]$	[80,82,245,340]
60	$\left[\frac{3}{8}, y, \frac{3}{8}\right]$	[87,88,193,297]
61	$\left[\frac{1}{8}, \frac{1}{8}, \frac{1}{2}-y\right]$	[89,92,254,291]
62	$\left[-y, \frac{5}{8}, \frac{1}{8}\right]$	[90,95,294,348]
63	$\left[y+\frac{1}{4}, \frac{5}{8}, \frac{1}{8}\right]$	[91,93,203,247]
64	$\left[\frac{1}{8}, \frac{1}{8}, y+\frac{3}{4}\right]$	[94,96,205,338]
65	$\left[-y, \frac{5}{8}, \frac{5}{8}\right]$	[102,156,282,287]
66	$\left[y+\frac{3}{4}, \frac{1}{8}, \frac{5}{8}\right]$	[103,155,331,333]
67	$\left[y+\frac{3}{4}, \frac{5}{8}, \frac{1}{8}\right]$	[107,151,379,381]
68	$\left[-y, \frac{1}{8}, \frac{1}{8}\right]$	[108,150,234,239]
69	$\left[y+\frac{1}{2}, \frac{7}{8}, \frac{7}{8}\right]$	[114,167,222,228]
70	$\left[\frac{3}{4}-y, \frac{7}{8}, \frac{3}{8}\right]$	[115,165,319,323]
71	$\left[\frac{3}{4}-y, \frac{3}{8}, \frac{7}{8}\right]$	[117,163,367,371]
72	$\left[y+\frac{1}{2}, \frac{3}{8}, \frac{3}{8}\right]$	[119,162,270,276]
73	$\left[\frac{1}{8}, -y, \frac{5}{8}\right]$	[121,129,255,352]
74	$\left[\frac{3}{8}, \frac{3}{8}, \frac{3}{4}-y\right]$	[122,133,216,358]
75	$\left[\frac{3}{8}, \frac{3}{8}, y\right]$	[123,134,260,305]
76	$\left[\frac{7}{8}, \frac{1}{4}-y, \frac{3}{8}\right]$	[124,125,202,296]
77	$\left[y, \frac{7}{8}, \frac{7}{8}\right]$	[126,132,210,263]
78	$\left[\frac{3}{4}-y, \frac{7}{8}, \frac{7}{8}\right]$	[127,131,307,357]
79	$\left[\frac{1}{8}, y+\frac{1}{4}, \frac{5}{8}\right]$	[128,130,196,293]
80	$\left[\frac{7}{8}, y+\frac{1}{2}, \frac{3}{8}\right]$	[135,136,249,337]
81	$\left[\frac{5}{8}, \frac{5}{8}, \frac{1}{2}-y\right]$	[137,140,243,302]
82	$\left[\frac{1}{2}-y, \frac{1}{8}, \frac{1}{8}\right]$	[138,143,204,246]
83	$\left[y+\frac{3}{4}, \frac{1}{8}, \frac{1}{8}\right]$	[139,141,295,347]
84	$\left[\frac{5}{8}, \frac{5}{8}, y+\frac{3}{4}\right]$	[142,144,194,349]
85	$\left[\frac{1}{8}, \frac{1}{2}-y, \frac{1}{8}\right]$	[169,177,207,304]
86	$\left[\frac{3}{8}, \frac{7}{8}, \frac{1}{4}-y\right]$	[170,181,264,310]
87	$\left[\frac{3}{8}, \frac{7}{8}, y+\frac{1}{2}\right]$	[171,182,212,353]
88	$\left[\frac{7}{8}, \frac{3}{4}-y, \frac{7}{8}\right]$	[172,173,250,344]
89	$\left[y, \frac{3}{8}, \frac{3}{8}\right]$	[174,180,215,258]
90	$\left[\frac{3}{4}-y, \frac{3}{8}, \frac{3}{8}\right]$	[175,179,309,355]
91	$\left[\frac{1}{8}, y+\frac{3}{4}, \frac{1}{8}\right]$	[176,178,244,341]
92	$\left[\frac{7}{8}, y, \frac{7}{8}\right]$	[183,184,201,289]
93	$\left[\frac{5}{8}, \frac{1}{8}, -y\right]$	[185,188,195,350]

continued ...

Table 7

No.	position	mapping
94	$\left[\frac{1}{2}-y, \frac{5}{8}, \frac{5}{8}\right]$	[186,191,198,252]
95	$\left[y+\frac{3}{4}, \frac{5}{8}, \frac{5}{8}\right]$	[187,189,299,343]
96	$\left[\frac{5}{8}, \frac{1}{8}, y+\frac{1}{4}\right]$	[190,192,242,301]

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

No.	position	mapping
1	$\left[\frac{3}{8}, y, \frac{5}{8}\right]$	[1,297]
2	$\left[\frac{5}{8}, \frac{7}{8}, y+\frac{1}{4}\right]$	[2,301]
3	$\left[\frac{5}{8}, \frac{7}{8}, \frac{1}{2}-y\right]$	[3,302]
4	$\left[\frac{7}{8}, y+\frac{1}{4}, \frac{1}{8}\right]$	[4,197]
5	$\left[\frac{7}{8}, y+\frac{1}{4}, \frac{5}{8}\right]$	[5,196]
6	$\left[\frac{1}{2}-y, \frac{5}{8}, \frac{7}{8}\right]$	[6,252]
7	$\left[y+\frac{1}{4}, \frac{1}{8}, \frac{7}{8}\right]$	[7,251]
8	$\left[\frac{3}{8}, \frac{1}{4}-y, \frac{5}{8}\right]$	[8,298]
9	$\left[\frac{7}{8}, y, \frac{5}{8}\right]$	[9,289]
10	$\left[\frac{7}{8}, \frac{1}{4}-y, \frac{5}{8}\right]$	[10,296]
11	$\left[y+\frac{1}{4}, \frac{5}{8}, \frac{7}{8}\right]$	[11,247]
12	$\left[\frac{1}{2}-y, \frac{1}{8}, \frac{7}{8}\right]$	[12,246]
13	$\left[\frac{1}{8}, \frac{7}{8}, y+\frac{1}{4}\right]$	[13,290]
14	$\left[\frac{1}{8}, \frac{7}{8}, \frac{1}{2}-y\right]$	[14,291]
15	$\left[\frac{7}{8}, \frac{1}{2}-y, \frac{5}{8}\right]$	[15,208]
16	$\left[\frac{7}{8}, \frac{1}{2}-y, \frac{1}{8}\right]$	[16,207]
17	$\left[\frac{5}{8}, \frac{3}{8}, y\right]$	[17,260]
18	$\left[y, \frac{5}{8}, \frac{3}{8}\right]$	[18,215]
19	$\left[\frac{1}{4}-y, \frac{5}{8}, \frac{7}{8}\right]$	[19,213]
20	$\left[\frac{5}{8}, \frac{7}{8}, y\right]$	[20,257]
21	$\left[\frac{1}{4}-y, \frac{5}{8}, \frac{3}{8}\right]$	[21,211]
22	$\left[\frac{5}{8}, \frac{7}{8}, \frac{1}{4}-y\right]$	[22,264]
23	$\left[y, \frac{5}{8}, \frac{7}{8}\right]$	[23,210]
24	$\left[\frac{5}{8}, \frac{3}{8}, \frac{1}{4}-y\right]$	[24,262]
25	$\left[\frac{5}{8}, -y, \frac{3}{8}\right]$	[25,225]
26	$\left[\frac{7}{8}, \frac{1}{8}, \frac{1}{4}-y\right]$	[26,277]
27	$\left[\frac{7}{8}, \frac{5}{8}, y+\frac{1}{2}\right]$	[27,278]
28	$\left[\frac{5}{8}, \frac{1}{4}-y, \frac{7}{8}\right]$	[28,317]
29	$\left[\frac{1}{8}, \frac{1}{4}-y, \frac{7}{8}\right]$	[29,316]
30	$\left[y+\frac{1}{2}, \frac{7}{8}, \frac{5}{8}\right]$	[30,228]
31	$\left[\frac{1}{4}-y, \frac{7}{8}, \frac{5}{8}\right]$	[31,227]
32	$\left[\frac{5}{8}, y+\frac{1}{4}, \frac{7}{8}\right]$	[32,226]
33	$\left[\frac{5}{8}, -y, \frac{7}{8}\right]$	[33,217]
34	$\left[\frac{5}{8}, y+\frac{1}{4}, \frac{3}{8}\right]$	[34,224]
35	$\left[\frac{1}{4}-y, \frac{7}{8}, \frac{1}{8}\right]$	[35,223]
36	$\left[y+\frac{1}{2}, \frac{7}{8}, \frac{1}{8}\right]$	[36,222]
37	$\left[\frac{7}{8}, \frac{5}{8}, \frac{1}{4}-y\right]$	[37,266]

continued ...

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Table 8

No.	position	mapping
38	$\left[\frac{7}{8}, \frac{1}{8}, y+\frac{1}{2}\right]$	[38,267]
39	$\left[\frac{5}{8}, y+\frac{1}{2}, \frac{7}{8}\right]$	[39,328]
40	$\left[\frac{1}{8}, y+\frac{1}{2}, \frac{7}{8}\right]$	[40,327]
41	$\left[\frac{3}{8}, \frac{5}{8}, -y\right]$	[41,332]
42	$\left[-y, \frac{3}{8}, \frac{5}{8}\right]$	[42,287]
43	$\left[y+\frac{1}{4}, \frac{3}{8}, \frac{5}{8}\right]$	[43,285]
44	$\left[\frac{7}{8}, \frac{5}{8}, -y\right]$	[44,329]
45	$\left[y+\frac{1}{4}, \frac{7}{8}, \frac{5}{8}\right]$	[45,283]
46	$\left[\frac{3}{8}, \frac{5}{8}, y+\frac{1}{4}\right]$	[46,336]
47	$\left[-y, \frac{7}{8}, \frac{5}{8}\right]$	[47,282]
48	$\left[\frac{7}{8}, \frac{5}{8}, y+\frac{1}{4}\right]$	[48,334]
49	$\left[\frac{3}{8}, y+\frac{1}{2}, \frac{1}{8}\right]$	[49,345]
50	$\left[\frac{5}{8}, \frac{3}{8}, y+\frac{3}{4}\right]$	[50,349]
51	$\left[\frac{5}{8}, \frac{3}{8}, -y\right]$	[51,350]
52	$\left[\frac{7}{8}, y+\frac{3}{4}, \frac{5}{8}\right]$	[52,245]
53	$\left[\frac{7}{8}, y+\frac{3}{4}, \frac{1}{8}\right]$	[53,244]
54	$\left[\frac{1}{2}-y, \frac{1}{8}, \frac{3}{8}\right]$	[54,204]
55	$\left[y+\frac{1}{4}, \frac{5}{8}, \frac{3}{8}\right]$	[55,203]
56	$\left[\frac{3}{8}, \frac{3}{4}-y, \frac{1}{8}\right]$	[56,346]
57	$\left[\frac{7}{8}, y+\frac{1}{2}, \frac{1}{8}\right]$	[57,337]
58	$\left[\frac{7}{8}, \frac{3}{4}-y, \frac{1}{8}\right]$	[58,344]
59	$\left[y+\frac{1}{4}, \frac{1}{8}, \frac{3}{8}\right]$	[59,199]
60	$\left[\frac{1}{2}-y, \frac{5}{8}, \frac{3}{8}\right]$	[60,198]
61	$\left[\frac{1}{8}, \frac{3}{8}, y+\frac{3}{4}\right]$	[61,338]
62	$\left[\frac{1}{8}, \frac{3}{8}, -y\right]$	[62,339]
63	$\left[\frac{7}{8}, -y, \frac{1}{8}\right]$	[63,256]
64	$\left[\frac{7}{8}, -y, \frac{5}{8}\right]$	[64,255]
65	$\left[\frac{5}{8}, \frac{7}{8}, y+\frac{1}{2}\right]$	[65,212]
66	$\left[y, \frac{1}{8}, \frac{7}{8}\right]$	[66,263]
67	$\left[\frac{1}{4}-y, \frac{1}{8}, \frac{3}{8}\right]$	[67,261]
68	$\left[\frac{5}{8}, \frac{3}{8}, y+\frac{1}{2}\right]$	[68,209]
69	$\left[\frac{1}{4}-y, \frac{1}{8}, \frac{7}{8}\right]$	[69,259]
70	$\left[\frac{5}{8}, \frac{3}{8}, \frac{3}{4}-y\right]$	[70,216]
71	$\left[y, \frac{1}{8}, \frac{3}{8}\right]$	[71,258]
72	$\left[\frac{5}{8}, \frac{7}{8}, \frac{3}{4}-y\right]$	[72,214]
73	$\left[\frac{5}{8}, \frac{1}{2}-y, \frac{7}{8}\right]$	[73,273]
74	$\left[\frac{7}{8}, \frac{5}{8}, \frac{3}{4}-y\right]$	[74,229]
75	$\left[\frac{7}{8}, \frac{1}{8}, y\right]$	[75,230]
76	$\left[\frac{5}{8}, \frac{3}{4}-y, \frac{3}{8}\right]$	[76,365]
77	$\left[\frac{1}{8}, \frac{3}{4}-y, \frac{3}{8}\right]$	[77,364]
78	$\left[y+\frac{1}{2}, \frac{3}{8}, \frac{1}{8}\right]$	[78,276]
79	$\left[\frac{1}{4}-y, \frac{3}{8}, \frac{1}{8}\right]$	[79,275]
80	$\left[\frac{5}{8}, y+\frac{3}{4}, \frac{3}{8}\right]$	[80,274]
81	$\left[\frac{5}{8}, \frac{1}{2}-y, \frac{3}{8}\right]$	[81,265]
82	$\left[\frac{5}{8}, y+\frac{3}{4}, \frac{7}{8}\right]$	[82,272]
83	$\left[\frac{1}{4}-y, \frac{3}{8}, \frac{5}{8}\right]$	[83,271]
84	$\left[y+\frac{1}{2}, \frac{3}{8}, \frac{5}{8}\right]$	[84,270]

continued ...

Table 8

No.	position	mapping
85	$\left[\frac{7}{8}, \frac{1}{8}, \frac{3}{4} - y\right]$	[85,218]
86	$\left[\frac{7}{8}, \frac{5}{8}, y\right]$	[86,219]
87	$\left[\frac{5}{8}, y, \frac{3}{8}\right]$	[87,376]
88	$\left[\frac{1}{8}, y, \frac{3}{8}\right]$	[88,375]
89	$\left[\frac{3}{8}, \frac{1}{8}, \frac{1}{2} - y\right]$	[89,380]
90	$\left[-y, \frac{7}{8}, \frac{1}{8}\right]$	[90,239]
91	$\left[y + \frac{1}{4}, \frac{7}{8}, \frac{1}{8}\right]$	[91,237]
92	$\left[\frac{7}{8}, \frac{1}{8}, \frac{1}{2} - y\right]$	[92,377]
93	$\left[y + \frac{1}{4}, \frac{3}{8}, \frac{1}{8}\right]$	[93,235]
94	$\left[\frac{3}{8}, \frac{1}{8}, y + \frac{3}{4}\right]$	[94,384]
95	$\left[-y, \frac{3}{8}, \frac{1}{8}\right]$	[95,234]
96	$\left[\frac{7}{8}, \frac{1}{8}, y + \frac{3}{4}\right]$	[96,382]
97	$\left[\frac{7}{8}, y, \frac{1}{8}\right]$	[97,201]
98	$\left[\frac{1}{8}, \frac{7}{8}, y + \frac{3}{4}\right]$	[98,205]
99	$\left[\frac{1}{8}, \frac{7}{8}, -y\right]$	[99,206]
100	$\left[\frac{3}{8}, y + \frac{1}{4}, \frac{5}{8}\right]$	[100,293]
101	$\left[\frac{3}{8}, y + \frac{1}{4}, \frac{1}{8}\right]$	[101,292]
102	$\left[-y, \frac{5}{8}, \frac{3}{8}\right]$	[102,348]
103	$\left[y + \frac{3}{4}, \frac{1}{8}, \frac{3}{8}\right]$	[103,347]
104	$\left[\frac{7}{8}, \frac{1}{4} - y, \frac{1}{8}\right]$	[104,202]
105	$\left[\frac{3}{8}, y, \frac{1}{8}\right]$	[105,193]
106	$\left[\frac{3}{8}, \frac{1}{4} - y, \frac{1}{8}\right]$	[106,200]
107	$\left[y + \frac{3}{4}, \frac{5}{8}, \frac{3}{8}\right]$	[107,343]
108	$\left[-y, \frac{1}{8}, \frac{3}{8}\right]$	[108,342]
109	$\left[\frac{5}{8}, \frac{7}{8}, y + \frac{3}{4}\right]$	[109,194]
110	$\left[\frac{5}{8}, \frac{7}{8}, -y\right]$	[110,195]
111	$\left[\frac{3}{8}, \frac{1}{2} - y, \frac{1}{8}\right]$	[111,304]
112	$\left[\frac{3}{8}, \frac{1}{2} - y, \frac{5}{8}\right]$	[112,303]
113	$\left[\frac{1}{8}, \frac{3}{8}, y + \frac{1}{2}\right]$	[113,356]
114	$\left[y + \frac{1}{2}, \frac{5}{8}, \frac{7}{8}\right]$	[114,311]
115	$\left[\frac{3}{4} - y, \frac{5}{8}, \frac{3}{8}\right]$	[115,309]
116	$\left[\frac{1}{8}, \frac{7}{8}, y + \frac{1}{2}\right]$	[116,353]
117	$\left[\frac{3}{4} - y, \frac{5}{8}, \frac{7}{8}\right]$	[117,307]
118	$\left[\frac{1}{8}, \frac{7}{8}, \frac{3}{4} - y\right]$	[118,360]
119	$\left[y + \frac{1}{2}, \frac{5}{8}, \frac{3}{8}\right]$	[119,306]
120	$\left[\frac{1}{8}, \frac{3}{8}, \frac{3}{4} - y\right]$	[120,358]
121	$\left[\frac{1}{8}, -y, \frac{7}{8}\right]$	[121,321]
122	$\left[\frac{3}{8}, \frac{1}{8}, \frac{3}{4} - y\right]$	[122,373]
123	$\left[\frac{3}{8}, \frac{5}{8}, y\right]$	[123,374]
124	$\left[\frac{1}{8}, \frac{1}{4} - y, \frac{3}{8}\right]$	[124,221]
125	$\left[\frac{5}{8}, \frac{1}{4} - y, \frac{3}{8}\right]$	[125,220]
126	$\left[y, \frac{7}{8}, \frac{1}{8}\right]$	[126,324]
127	$\left[\frac{3}{4} - y, \frac{7}{8}, \frac{1}{8}\right]$	[127,323]
128	$\left[\frac{1}{8}, y + \frac{1}{4}, \frac{3}{8}\right]$	[128,322]
129	$\left[\frac{1}{8}, -y, \frac{3}{8}\right]$	[129,313]
130	$\left[\frac{1}{8}, y + \frac{1}{4}, \frac{7}{8}\right]$	[130,320]
131	$\left[\frac{3}{4} - y, \frac{7}{8}, \frac{5}{8}\right]$	[131,319]

continued ...

Table 8

No.	position	mapping
132	$\left[y, \frac{7}{8}, \frac{5}{8}\right]$	[132,318]
133	$\left[\frac{3}{8}, \frac{5}{8}, \frac{3}{4} - y\right]$	[133,362]
134	$\left[\frac{3}{8}, \frac{1}{8}, y\right]$	[134,363]
135	$\left[\frac{1}{8}, y + \frac{1}{2}, \frac{3}{8}\right]$	[135,232]
136	$\left[\frac{5}{8}, y + \frac{1}{2}, \frac{3}{8}\right]$	[136,231]
137	$\left[\frac{7}{8}, \frac{5}{8}, \frac{1}{2} - y\right]$	[137,236]
138	$\left[\frac{1}{2} - y, \frac{3}{8}, \frac{1}{8}\right]$	[138,383]
139	$\left[y + \frac{3}{4}, \frac{3}{8}, \frac{1}{8}\right]$	[139,381]
140	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{2} - y\right]$	[140,233]
141	$\left[y + \frac{3}{4}, \frac{7}{8}, \frac{1}{8}\right]$	[141,379]
142	$\left[\frac{7}{8}, \frac{5}{8}, y + \frac{3}{4}\right]$	[142,240]
143	$\left[\frac{1}{2} - y, \frac{7}{8}, \frac{1}{8}\right]$	[143,378]
144	$\left[\frac{3}{8}, \frac{5}{8}, y + \frac{3}{4}\right]$	[144,238]
145	$\left[\frac{7}{8}, y + \frac{1}{2}, \frac{5}{8}\right]$	[145,249]
146	$\left[\frac{1}{8}, \frac{3}{8}, y + \frac{1}{4}\right]$	[146,253]
147	$\left[\frac{1}{8}, \frac{3}{8}, \frac{1}{2} - y\right]$	[147,254]
148	$\left[\frac{3}{8}, y + \frac{3}{4}, \frac{1}{8}\right]$	[148,341]
149	$\left[\frac{3}{8}, y + \frac{3}{4}, \frac{5}{8}\right]$	[149,340]
150	$\left[-y, \frac{1}{8}, \frac{7}{8}\right]$	[150,300]
151	$\left[y + \frac{3}{4}, \frac{5}{8}, \frac{7}{8}\right]$	[151,299]
152	$\left[\frac{7}{8}, \frac{3}{4} - y, \frac{5}{8}\right]$	[152,250]
153	$\left[\frac{3}{8}, y + \frac{1}{2}, \frac{5}{8}\right]$	[153,241]
154	$\left[\frac{3}{8}, \frac{3}{4} - y, \frac{5}{8}\right]$	[154,248]
155	$\left[y + \frac{3}{4}, \frac{1}{8}, \frac{7}{8}\right]$	[155,295]
156	$\left[-y, \frac{5}{8}, \frac{7}{8}\right]$	[156,294]
157	$\left[\frac{5}{8}, \frac{3}{8}, y + \frac{1}{4}\right]$	[157,242]
158	$\left[\frac{5}{8}, \frac{3}{8}, \frac{1}{2} - y\right]$	[158,243]
159	$\left[\frac{3}{8}, -y, \frac{5}{8}\right]$	[159,352]
160	$\left[\frac{3}{8}, -y, \frac{1}{8}\right]$	[160,351]
161	$\left[\frac{1}{8}, \frac{7}{8}, y\right]$	[161,308]
162	$\left[y + \frac{1}{2}, \frac{1}{8}, \frac{3}{8}\right]$	[162,359]
163	$\left[\frac{3}{4} - y, \frac{1}{8}, \frac{7}{8}\right]$	[163,357]
164	$\left[\frac{1}{8}, \frac{3}{8}, y\right]$	[164,305]
165	$\left[\frac{3}{4} - y, \frac{1}{8}, \frac{3}{8}\right]$	[165,355]
166	$\left[\frac{1}{8}, \frac{3}{8}, \frac{1}{4} - y\right]$	[166,312]
167	$\left[y + \frac{1}{2}, \frac{1}{8}, \frac{7}{8}\right]$	[167,354]
168	$\left[\frac{1}{8}, \frac{7}{8}, \frac{1}{4} - y\right]$	[168,310]
169	$\left[\frac{1}{8}, \frac{1}{2} - y, \frac{3}{8}\right]$	[169,369]
170	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{4} - y\right]$	[170,325]
171	$\left[\frac{3}{8}, \frac{1}{8}, y + \frac{1}{2}\right]$	[171,326]
172	$\left[\frac{1}{8}, \frac{3}{4} - y, \frac{7}{8}\right]$	[172,269]
173	$\left[\frac{5}{8}, \frac{3}{4} - y, \frac{7}{8}\right]$	[173,268]
174	$\left[y, \frac{3}{8}, \frac{5}{8}\right]$	[174,372]
175	$\left[\frac{3}{4} - y, \frac{3}{8}, \frac{5}{8}\right]$	[175,371]
176	$\left[\frac{1}{8}, y + \frac{3}{4}, \frac{7}{8}\right]$	[176,370]
177	$\left[\frac{1}{8}, \frac{1}{2} - y, \frac{7}{8}\right]$	[177,361]
178	$\left[\frac{1}{8}, y + \frac{3}{4}, \frac{3}{8}\right]$	[178,368]

continued ...

Table 8

No.	position	mapping
179	$\left[\frac{3}{4} - y, \frac{3}{8}, \frac{1}{8}\right]$	[179,367]
180	$\left[y, \frac{3}{8}, \frac{1}{8}\right]$	[180,366]
181	$\left[\frac{3}{8}, \frac{1}{8}, \frac{1}{4} - y\right]$	[181,314]
182	$\left[\frac{3}{8}, \frac{5}{8}, y + \frac{1}{2}\right]$	[182,315]
183	$\left[\frac{1}{8}, y, \frac{7}{8}\right]$	[183,280]
184	$\left[\frac{5}{8}, y, \frac{7}{8}\right]$	[184,279]
185	$\left[\frac{7}{8}, \frac{1}{8}, -y\right]$	[185,284]
186	$\left[\frac{1}{2} - y, \frac{7}{8}, \frac{5}{8}\right]$	[186,335]
187	$\left[y + \frac{3}{4}, \frac{7}{8}, \frac{5}{8}\right]$	[187,333]
188	$\left[\frac{3}{8}, \frac{1}{8}, -y\right]$	[188,281]
189	$\left[y + \frac{3}{4}, \frac{3}{8}, \frac{5}{8}\right]$	[189,331]
190	$\left[\frac{7}{8}, \frac{1}{8}, y + \frac{1}{4}\right]$	[190,288]
191	$\left[\frac{1}{2} - y, \frac{3}{8}, \frac{5}{8}\right]$	[191,330]
192	$\left[\frac{3}{8}, \frac{1}{8}, y + \frac{1}{4}\right]$	[192,286]

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

No.	position	mapping
1	$\left[x, \frac{1}{2}, -x\right]$	[1,352]
2	$\left[x + \frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}\right]$	[2,264]
3	$\left[x + \frac{1}{4}, \frac{1}{4} - x, 0\right]$	[3,212]
4	$\left[\frac{1}{4} - x, \frac{3}{4}, \frac{1}{2} - x\right]$	[4,202]
5	$\left[x + \frac{1}{2}, \frac{3}{4}, x + \frac{1}{4}\right]$	[5,296]
6	$\left[0, x + \frac{1}{4}, \frac{1}{4} - x\right]$	[6,311]
7	$\left[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{4} - x\right]$	[7,259]
8	$\left[x, \frac{3}{4}, x + \frac{1}{4}\right]$	[8,293]
9	$\left[\frac{1}{4} - x, \frac{1}{2}, x + \frac{1}{4}\right]$	[9,255]
10	$\left[\frac{1}{4} - x, \frac{3}{4}, -x\right]$	[10,196]
11	$\left[\frac{3}{4}, x + \frac{1}{4}, x + \frac{1}{2}\right]$	[11,213]
12	$\left[0, \frac{1}{2} - x, x + \frac{1}{2}\right]$	[12,354]
13	$\left[\frac{1}{2} - x, \frac{1}{4} - x, \frac{3}{4}\right]$	[13,310]
14	$\left[\frac{1}{2} - x, x + \frac{1}{2}, 0\right]$	[14,353]
15	$\left[\frac{1}{4} - x, 0, x + \frac{1}{4}\right]$	[15,249]
16	$\left[x + \frac{1}{2}, 0, \frac{1}{2} - x\right]$	[16,337]
17	$\left[-x, x, \frac{1}{2}\right]$	[17,350]
18	$\left[\frac{1}{2}, -x, x\right]$	[18,348]
19	$\left[\frac{3}{4}, -x, \frac{1}{4} - x\right]$	[19,247]
20	$\left[x + \frac{1}{4}, \frac{1}{4} - x, \frac{1}{2}\right]$	[20,195]
21	$\left[\frac{3}{4}, x + \frac{1}{4}, x\right]$	[21,203]
22	$\left[-x, \frac{1}{4} - x, \frac{3}{4}\right]$	[22,301]
23	$\left[\frac{1}{2}, x + \frac{1}{4}, \frac{1}{4} - x\right]$	[23,294]
24	$\left[x + \frac{1}{4}, x, \frac{3}{4}\right]$	[24,242]
25	$\left[-x, \frac{1}{2}, x\right]$	[25,376]
26	$\left[\frac{1}{4} - x, \frac{1}{2} - x, \frac{3}{4}\right]$	[26,288]

Table 9

No.	position	mapping
27	$\left[\frac{1}{4} - x,\, x + \frac{1}{4},\, 0\right]$	[27,236]
28	$\left[x + \frac{1}{4},\, \frac{3}{4},\, x + \frac{1}{2}\right]$	[28,226]
29	$\left[\frac{1}{2} - x,\, \frac{3}{4},\, \frac{1}{4} - x\right]$	[29,320]
30	$\left[0,\, \frac{1}{4} - x,\, x + \frac{1}{4}\right]$	[30,335]
31	$\left[\frac{3}{4},\, x + \frac{1}{2},\, x + \frac{1}{4}\right]$	[31,283]
32	$\left[-x,\, \frac{3}{4},\, \frac{1}{4} - x\right]$	[32,317]
33	$\left[x + \frac{1}{4},\, \frac{1}{2},\, \frac{1}{4} - x\right]$	[33,279]
34	$\left[x + \frac{1}{4},\, \frac{3}{4},\, x\right]$	[34,220]
35	$\left[\frac{3}{4},\, \frac{1}{4} - x,\, \frac{1}{2} - x\right]$	[35,237]
36	$\left[0,\, x + \frac{1}{2},\, \frac{1}{2} - x\right]$	[36,378]
37	$\left[x + \frac{1}{2},\, x + \frac{1}{4},\, \frac{3}{4}\right]$	[37,334]
38	$\left[x + \frac{1}{2},\, \frac{1}{2} - x,\, 0\right]$	[38,377]
39	$\left[x + \frac{1}{4},\, 0,\, \frac{1}{4} - x\right]$	[39,273]
40	$\left[\frac{1}{2} - x,\, 0,\, x + \frac{1}{2}\right]$	[40,361]
41	$\left[x,\, -x,\, \frac{1}{2}\right]$	[41,374]
42	$\left[\frac{1}{2},\, x,\, -x\right]$	[42,372]
43	$\left[\frac{3}{4},\, x,\, x + \frac{1}{4}\right]$	[43,271]
44	$\left[\frac{1}{4} - x,\, x + \frac{1}{4},\, \frac{1}{2}\right]$	[44,219]
45	$\left[\frac{3}{4},\, \frac{1}{4} - x,\, -x\right]$	[45,227]
46	$\left[x,\, x + \frac{1}{4},\, \frac{3}{4}\right]$	[46,325]
47	$\left[\frac{1}{2},\, \frac{1}{4} - x,\, x + \frac{1}{4}\right]$	[47,318]
48	$\left[\frac{1}{4} - x,\, -x,\, \frac{3}{4}\right]$	[48,266]
49	$\left[x,\, 0,\, \frac{1}{2} - x\right]$	[49,304]
50	$\left[x + \frac{1}{4},\, x,\, \frac{1}{4}\right]$	[50,216]
51	$\left[x + \frac{1}{4},\, \frac{3}{4} - x,\, \frac{1}{2}\right]$	[51,260]
52	$\left[\frac{1}{4} - x,\, \frac{1}{4},\, -x\right]$	[52,250]
53	$\left[x + \frac{1}{2},\, \frac{1}{4},\, x + \frac{3}{4}\right]$	[53,344]
54	$\left[0,\, x + \frac{3}{4},\, \frac{3}{4} - x\right]$	[54,359]
55	$\left[\frac{3}{4},\, -x,\, \frac{3}{4} - x\right]$	[55,211]
56	$\left[x,\, \frac{1}{4},\, x + \frac{3}{4}\right]$	[56,341]
57	$\left[\frac{1}{4} - x,\, 0,\, x + \frac{3}{4}\right]$	[57,207]
58	$\left[\frac{1}{4} - x,\, \frac{1}{4},\, \frac{1}{2} - x\right]$	[58,244]
59	$\left[\frac{3}{4},\, x + \frac{3}{4},\, x\right]$	[59,261]
60	$\left[0,\, -x,\, x\right]$	[60,306]
61	$\left[\frac{1}{2} - x,\, \frac{3}{4} - x,\, \frac{1}{4}\right]$	[61,358]
62	$\left[\frac{1}{2} - x,\, x,\, \frac{1}{2}\right]$	[62,305]
63	$\left[\frac{1}{4} - x,\, \frac{1}{2},\, x + \frac{3}{4}\right]$	[63,201]
64	$\left[x + \frac{1}{2},\, \frac{1}{2},\, -x\right]$	[64,289]
65	$\left[-x,\, x + \frac{1}{2},\, 0\right]$	[65,302]
66	$\left[\frac{1}{2},\, \frac{1}{2} - x,\, x + \frac{1}{2}\right]$	[66,300]
67	$\left[\frac{3}{4},\, \frac{1}{2} - x,\, \frac{3}{4} - x\right]$	[67,199]
68	$\left[x + \frac{1}{4},\, \frac{3}{4} - x,\, 0\right]$	[68,243]
69	$\left[\frac{3}{4},\, x + \frac{3}{4},\, x + \frac{1}{2}\right]$	[69,251]
70	$\left[-x,\, \frac{3}{4} - x,\, \frac{1}{4}\right]$	[70,349]
71	$\left[\frac{1}{2},\, x + \frac{3}{4},\, \frac{3}{4} - x\right]$	[71,342]
72	$\left[x + \frac{1}{4},\, x + \frac{1}{2},\, \frac{1}{4}\right]$	[72,194]
73	$\left[-x,\, 0,\, x + \frac{1}{2}\right]$	[73,328]

Table 9

No.	position	mapping
74	$\left[\frac{1}{4} - x, -x, \frac{1}{4}\right]$	[74,240]
75	$\left[\frac{1}{4} - x, x + \frac{3}{4}, \frac{1}{2}\right]$	[75,284]
76	$\left[x + \frac{1}{4}, \frac{1}{4}, x\right]$	[76,274]
77	$\left[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4} - x\right]$	[77,368]
78	$\left[0, \frac{3}{4} - x, x + \frac{3}{4}\right]$	[78,383]
79	$\left[\frac{3}{4}, x, x + \frac{3}{4}\right]$	[79,235]
80	$\left[-x, \frac{1}{4}, \frac{3}{4} - x\right]$	[80,365]
81	$\left[x + \frac{1}{4}, 0, \frac{3}{4} - x\right]$	[81,231]
82	$\left[x + \frac{1}{4}, \frac{1}{4}, x + \frac{1}{2}\right]$	[82,268]
83	$\left[\frac{3}{4}, \frac{3}{4} - x, -x\right]$	[83,285]
84	$[0, x, -x]$	[84,330]
85	$\left[x + \frac{1}{2}, x + \frac{3}{4}, \frac{1}{4}\right]$	[85,382]
86	$\left[x + \frac{1}{2}, -x, \frac{1}{2}\right]$	[86,329]
87	$\left[x + \frac{1}{4}, \frac{1}{2}, \frac{3}{4} - x\right]$	[87,225]
88	$\left[\frac{1}{2} - x, \frac{1}{2}, x\right]$	[88,313]
89	$\left[x, \frac{1}{2} - x, 0\right]$	[89,326]
90	$\left[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - x\right]$	[90,324]
91	$\left[\frac{3}{4}, x + \frac{1}{2}, x + \frac{3}{4}\right]$	[91,223]
92	$\left[\frac{1}{4} - x, x + \frac{3}{4}, 0\right]$	[92,267]
93	$\left[\frac{3}{4}, \frac{3}{4} - x, \frac{1}{2} - x\right]$	[93,275]
94	$\left[x, x + \frac{3}{4}, \frac{1}{4}\right]$	[94,373]
95	$\left[\frac{1}{2}, \frac{3}{4} - x, x + \frac{3}{4}\right]$	[95,366]
96	$\left[\frac{1}{4} - x, \frac{1}{2} - x, \frac{1}{4}\right]$	[96,218]
97	$\left[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x\right]$	[97,256]
98	$\left[x + \frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}\right]$	[98,360]
99	$\left[x + \frac{3}{4}, \frac{1}{4} - x, \frac{1}{2}\right]$	[99,308]
100	$\left[\frac{3}{4} - x, \frac{3}{4}, -x\right]$	[100,298]
101	$\left[x, \frac{3}{4}, x + \frac{3}{4}\right]$	[101,200]
102	$\left[\frac{1}{2}, x + \frac{1}{4}, \frac{3}{4} - x\right]$	[102,215]
103	$\left[\frac{1}{4}, \frac{1}{2} - x, \frac{3}{4} - x\right]$	[103,355]
104	$\left[x + \frac{1}{2}, \frac{3}{4}, x + \frac{3}{4}\right]$	[104,197]
105	$\left[\frac{3}{4} - x, \frac{1}{2}, x + \frac{3}{4}\right]$	[105,351]
106	$\left[\frac{3}{4} - x, \frac{3}{4}, \frac{1}{2} - x\right]$	[106,292]
107	$\left[\frac{1}{4}, x + \frac{1}{4}, x\right]$	[107,309]
108	$\left[\frac{1}{2}, \frac{1}{2} - x, x\right]$	[108,258]
109	$\left[-x, \frac{1}{4} - x, \frac{1}{4}\right]$	[109,214]
110	$\left[-x, x + \frac{1}{2}, \frac{1}{2}\right]$	[110,257]
111	$\left[\frac{3}{4} - x, 0, x + \frac{3}{4}\right]$	[111,345]
112	$[x, 0, -x]$	[112,241]
113	$\left[\frac{1}{2} - x, x, 0\right]$	[113,254]
114	$\left[0, -x, x + \frac{1}{2}\right]$	[114,252]
115	$\left[\frac{1}{4}, -x, \frac{3}{4} - x\right]$	[115,343]
116	$\left[x + \frac{3}{4}, \frac{1}{4} - x, 0\right]$	[116,291]
117	$\left[\frac{1}{4}, x + \frac{1}{4}, x + \frac{1}{2}\right]$	[117,299]
118	$\left[\frac{1}{2} - x, \frac{1}{4} - x, \frac{1}{4}\right]$	[118,205]
119	$\left[0, x + \frac{1}{4}, \frac{3}{4} - x\right]$	[119,198]
120	$\left[x + \frac{3}{4}, x, \frac{1}{4}\right]$	[120,338]

continued ...

Table 9

No.	position	mapping
121	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ x+\frac{1}{2}\right]$	[121,280]
122	$\left[\frac{3}{4}-x,\ \frac{1}{2}-x,\ \frac{1}{4}\right]$	[122,384]
123	$\left[\frac{3}{4}-x,\ x+\frac{1}{4},\ \frac{1}{2}\right]$	[123,332]
124	$\left[x+\frac{3}{4},\ \frac{3}{4},\ x\right]$	[124,322]
125	$\left[-x,\ \frac{3}{4},\ \frac{3}{4}-x\right]$	[125,224]
126	$\left[\frac{1}{2},\ \frac{1}{4}-x,\ x+\frac{3}{4}\right]$	[126,239]
127	$\left[\frac{1}{4},\ x+\frac{1}{2},\ x+\frac{3}{4}\right]$	[127,379]
128	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ \frac{3}{4}-x\right]$	[128,221]
129	$\left[x+\frac{3}{4},\ \frac{1}{2},\ \frac{3}{4}-x\right]$	[129,375]
130	$\left[x+\frac{3}{4},\ \frac{3}{4},\ x+\frac{1}{2}\right]$	[130,316]
131	$\left[\frac{1}{4},\ \frac{1}{4}-x,\ -x\right]$	[131,333]
132	$\left[\frac{1}{2},\ x+\frac{1}{2},\ -x\right]$	[132,282]
133	$\left[x,\ x+\frac{1}{4},\ \frac{1}{4}\right]$	[133,238]
134	$\left[x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[134,281]
135	$\left[x+\frac{3}{4},\ 0,\ \frac{3}{4}-x\right]$	[135,369]
136	$\left[-x,\ 0,\ x\right]$	[136,265]
137	$\left[x+\frac{1}{2},\ -x,\ 0\right]$	[137,278]
138	$\left[0,\ x,\ \frac{1}{2}-x\right]$	[138,276]
139	$\left[\frac{1}{4},\ x,\ x+\frac{3}{4}\right]$	[139,367]
140	$\left[\frac{3}{4}-x,\ x+\frac{1}{4},\ 0\right]$	[140,315]
141	$\left[\frac{1}{4},\ \frac{1}{4}-x,\ \frac{1}{2}-x\right]$	[141,323]
142	$\left[x+\frac{1}{2},\ x+\frac{1}{4},\ \frac{1}{4}\right]$	[142,229]
143	$\left[0,\ \frac{1}{4}-x,\ x+\frac{3}{4}\right]$	[143,222]
144	$\left[\frac{3}{4}-x,\ -x,\ \frac{1}{4}\right]$	[144,362]
145	$\left[x+\frac{1}{2},\ 0,\ -x\right]$	[145,208]
146	$\left[x+\frac{3}{4},\ x,\ \frac{3}{4}\right]$	[146,312]
147	$\left[x+\frac{3}{4},\ \frac{3}{4}-x,\ 0\right]$	[147,356]
148	$\left[\frac{3}{4}-x,\ \frac{1}{4},\ \frac{1}{2}-x\right]$	[148,346]
149	$\left[x,\ \frac{1}{4},\ x+\frac{1}{4}\right]$	[149,248]
150	$\left[\frac{1}{2},\ x+\frac{3}{4},\ \frac{1}{4}-x\right]$	[150,263]
151	$\left[\frac{1}{4},\ -x,\ \frac{1}{4}-x\right]$	[151,307]
152	$\left[x+\frac{1}{2},\ \frac{1}{4},\ x+\frac{1}{4}\right]$	[152,245]
153	$\left[\frac{3}{4}-x,\ 0,\ x+\frac{1}{4}\right]$	[153,303]
154	$\left[\frac{3}{4}-x,\ \frac{1}{4},\ -x\right]$	[154,340]
155	$\left[\frac{1}{4},\ x+\frac{3}{4},\ x+\frac{1}{2}\right]$	[155,357]
156	$\left[\frac{1}{2},\ -x,\ x+\frac{1}{2}\right]$	[156,210]
157	$\left[-x,\ \frac{3}{4}-x,\ \frac{3}{4}\right]$	[157,262]
158	$\left[-x,\ x,\ 0\right]$	[158,209]
159	$\left[\frac{3}{4}-x,\ \frac{1}{2},\ x+\frac{1}{4}\right]$	[159,297]
160	$\left[x,\ \frac{1}{2},\ \frac{1}{2}-x\right]$	[160,193]
161	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[161,206]
162	$\left[0,\ \frac{1}{2}-x,\ x\right]$	[162,204]
163	$\left[\frac{1}{4},\ \frac{1}{2}-x,\ \frac{1}{4}-x\right]$	[163,295]
164	$\left[x+\frac{3}{4},\ \frac{3}{4}-x,\ \frac{1}{2}\right]$	[164,339]
165	$\left[\frac{1}{4},\ x+\frac{3}{4},\ x\right]$	[165,347]
166	$\left[\frac{1}{2}-x,\ \frac{3}{4}-x,\ \frac{3}{4}\right]$	[166,253]
167	$\left[0,\ x+\frac{3}{4},\ \frac{1}{4}-x\right]$	[167,246]

continued ...

Table 9

No.	position	mapping
168	$\left[x+\frac{3}{4},\, x+\frac{1}{2},\, \frac{3}{4}\right]$	[168,290]
169	$\left[\frac{1}{2}-x,\, 0,\, x\right]$	[169,232]
170	$\left[\frac{3}{4}-x,\, -x,\, \frac{3}{4}\right]$	[170,336]
171	$\left[\frac{3}{4}-x,\, x+\frac{3}{4},\, 0\right]$	[171,380]
172	$\left[x+\frac{3}{4},\, \frac{1}{4},\, x+\frac{1}{2}\right]$	[172,370]
173	$\left[-x,\, \frac{1}{4},\, \frac{1}{4}-x\right]$	[173,272]
174	$\left[\frac{1}{2},\, \frac{3}{4}-x,\, x+\frac{1}{4}\right]$	[174,287]
175	$\left[\frac{1}{4},\, x,\, x+\frac{1}{4}\right]$	[175,331]
176	$\left[\frac{1}{2}-x,\, \frac{1}{4},\, \frac{1}{4}-x\right]$	[176,269]
177	$\left[x+\frac{3}{4},\, 0,\, \frac{1}{4}-x\right]$	[177,327]
178	$\left[x+\frac{3}{4},\, \frac{1}{4},\, x\right]$	[178,364]
179	$\left[\frac{1}{4},\, \frac{3}{4}-x,\, \frac{1}{2}-x\right]$	[179,381]
180	$\left[\frac{1}{2},\, x,\, \frac{1}{2}-x\right]$	[180,234]
181	$\left[x,\, x+\frac{3}{4},\, \frac{3}{4}\right]$	[181,286]
182	$\left[x,\, -x,\, 0\right]$	[182,233]
183	$\left[x+\frac{3}{4},\, \frac{1}{2},\, \frac{1}{4}-x\right]$	[183,321]
184	$\left[-x,\, \frac{1}{2},\, x+\frac{1}{2}\right]$	[184,217]
185	$\left[x+\frac{1}{2},\, \frac{1}{2}-x,\, \frac{1}{2}\right]$	[185,230]
186	$\left[0,\, x+\frac{1}{2},\, -x\right]$	[186,228]
187	$\left[\frac{1}{4},\, x+\frac{1}{2},\, x+\frac{1}{4}\right]$	[187,319]
188	$\left[\frac{3}{4}-x,\, x+\frac{3}{4},\, \frac{1}{2}\right]$	[188,363]
189	$\left[\frac{1}{4},\, \frac{3}{4}-x,\, -x\right]$	[189,371]
190	$\left[x+\frac{1}{2},\, x+\frac{3}{4},\, \frac{3}{4}\right]$	[190,277]
191	$\left[0,\, \frac{3}{4}-x,\, x+\frac{1}{4}\right]$	[191,270]
192	$\left[\frac{3}{4}-x,\, \frac{1}{2}-x,\, \frac{3}{4}\right]$	[192,314]

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

No.	position	mapping
1	$\left[x,\, \frac{1}{2},\, x+\frac{3}{4}\right]$	[1,63]
2	$\left[x+\frac{1}{4},\, \frac{3}{4}-x,\, \frac{3}{4}\right]$	[2,166]
3	$\left[x+\frac{1}{4},\, x,\, 0\right]$	[3,113]
4	$\left[x,\, \frac{3}{4},\, \frac{1}{2}-x\right]$	[4,8]
5	$\left[\frac{3}{4}-x,\, \frac{3}{4},\, x+\frac{1}{4}\right]$	[5,106]
6	$\left[0,\, x+\frac{1}{4},\, x\right]$	[6,162]
7	$\left[\frac{3}{4},\, \frac{1}{2}-x,\, x\right]$	[7,21]
8	$\left[\frac{1}{4}-x,\, \frac{1}{2},\, \frac{1}{2}-x\right]$	[9,160]
9	$\left[\frac{1}{4}-x,\, \frac{3}{4},\, x+\frac{3}{4}\right]$	[10,101]
10	$\left[\frac{3}{4},\, x+\frac{1}{4},\, \frac{3}{4}-x\right]$	[11,67]
11	$\left[0,\, \frac{1}{2}-x,\, \frac{3}{4}-x\right]$	[12,119]
12	$\left[\frac{1}{2}-x,\, x,\, \frac{3}{4}\right]$	[13,24]
13	$\left[\frac{1}{2}-x,\, \frac{3}{4}-x,\, 0\right]$	[14,68]
14	$\left[x,\, 0,\, x+\frac{1}{4}\right]$	[15,49]
15	$\left[\frac{3}{4}-x,\, 0,\, \frac{1}{2}-x\right]$	[16,153]

continued ...

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Table 10

No.	position	mapping
16	$\left[x + \frac{3}{4}, x, \frac{1}{2}\right]$	[17,99]
17	$\left[\frac{1}{2}, x + \frac{3}{4}, x\right]$	[18,150]
18	$\left[\frac{3}{4}, x + \frac{3}{4}, \frac{1}{4} - x\right]$	[19,59]
19	$\left[\frac{1}{2} - x, \frac{1}{4} - x, \frac{1}{2}\right]$	[20,62]
20	$\left[x + \frac{3}{4}, \frac{1}{4} - x, \frac{3}{4}\right]$	[22,146]
21	$\left[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{4} - x\right]$	[23,108]
22	$\left[-x, \frac{1}{2}, \frac{1}{4} - x\right]$	[25,183]
23	$\left[\frac{1}{4} - x, x + \frac{1}{4}, \frac{3}{4}\right]$	[26,46]
24	$\left[\frac{1}{4} - x, \frac{1}{2} - x, 0\right]$	[27,89]
25	$\left[\frac{1}{2} - x, \frac{3}{4}, x + \frac{1}{2}\right]$	[28,128]
26	$\left[x + \frac{1}{4}, \frac{3}{4}, \frac{1}{4} - x\right]$	[29,34]
27	$\left[0, \frac{1}{4} - x, \frac{1}{2} - x\right]$	[30,138]
28	$\left[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{2} - x\right]$	[31,93]
29	$\left[-x, \frac{3}{4}, x\right]$	[32,124]
30	$\left[x + \frac{1}{4}, \frac{1}{2}, x\right]$	[33,88]
31	$\left[\frac{3}{4}, \frac{1}{4} - x, x + \frac{1}{4}\right]$	[35,43]
32	$\left[0, x + \frac{1}{2}, x + \frac{1}{4}\right]$	[36,191]
33	$\left[x + \frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}\right]$	[37,192]
34	$\left[x + \frac{1}{2}, x + \frac{1}{4}, 0\right]$	[38,140]
35	$\left[\frac{1}{2} - x, 0, \frac{1}{4} - x\right]$	[39,169]
36	$\left[x + \frac{1}{4}, 0, x + \frac{1}{2}\right]$	[40,81]
37	$\left[\frac{1}{4} - x, -x, \frac{1}{2}\right]$	[41,75]
38	$\left[\frac{1}{2}, \frac{1}{4} - x, -x\right]$	[42,126]
39	$\left[x, x + \frac{1}{4}, \frac{1}{2}\right]$	[44,134]
40	$\left[\frac{3}{4}, x, -x\right]$	[45,79]
41	$\left[\frac{1}{2}, x, x + \frac{1}{4}\right]$	[47,180]
42	$\left[x, -x, \frac{3}{4}\right]$	[48,181]
43	$\left[x + \frac{1}{4}, \frac{1}{4} - x, \frac{1}{4}\right]$	[50,118]
44	$\left[x + \frac{1}{4}, x + \frac{1}{2}, \frac{1}{2}\right]$	[51,161]
45	$\left[x, \frac{1}{4}, -x\right]$	[52,56]
46	$\left[\frac{3}{4} - x, \frac{1}{4}, x + \frac{3}{4}\right]$	[53,154]
47	$\left[0, x + \frac{3}{4}, x + \frac{1}{2}\right]$	[54,114]
48	$\left[\frac{3}{4}, -x, x + \frac{1}{2}\right]$	[55,69]
49	$\left[\frac{1}{4} - x, 0, -x\right]$	[57,112]
50	$\left[\frac{1}{4} - x, \frac{1}{4}, x + \frac{1}{4}\right]$	[58,149]
51	$\left[0, -x, \frac{1}{4} - x\right]$	[60,167]
52	$\left[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{4}\right]$	[61,72]
53	$\left[\frac{3}{4} - x, \frac{1}{2}, -x\right]$	[64,105]
54	$\left[x + \frac{3}{4}, x + \frac{1}{2}, 0\right]$	[65,147]
55	$\left[\frac{1}{2}, x + \frac{1}{4}, x + \frac{1}{2}\right]$	[66,102]
56	$\left[x + \frac{3}{4}, \frac{3}{4} - x, \frac{1}{4}\right]$	[70,98]
57	$\left[\frac{1}{2}, -x, \frac{3}{4} - x\right]$	[71,156]
58	$\left[-x, 0, \frac{3}{4} - x\right]$	[73,135]
59	$\left[\frac{1}{4} - x, x + \frac{3}{4}, \frac{1}{4}\right]$	[74,94]
60	$\left[\frac{1}{2} - x, \frac{1}{4}, x\right]$	[76,176]
61	$\left[x + \frac{1}{4}, \frac{1}{4}, \frac{3}{4} - x\right]$	[77,82]
62	$\left[0, \frac{3}{4} - x, -x\right]$	[78,186]

continued ...

Table 10

No.	position	mapping
63	$\left[-x,\ \frac{1}{4},\ x+\frac{1}{2}\right]$	[80,172]
64	$\left[\frac{3}{4},\ \frac{3}{4}-x,\ x+\frac{3}{4}\right]$	[83,91]
65	$\left[0,\ x,\ x+\frac{3}{4}\right]$	[84,143]
66	$\left[x+\frac{1}{2},\ -x,\ \frac{1}{4}\right]$	[85,144]
67	$\left[x+\frac{1}{2},\ x+\frac{3}{4},\ \frac{1}{2}\right]$	[86,188]
68	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{3}{4}-x\right]$	[87,121]
69	$\left[\frac{1}{2},\ \frac{3}{4}-x,\ \frac{1}{2}-x\right]$	[90,174]
70	$\left[x,\ x+\frac{3}{4},\ 0\right]$	[92,182]
71	$\left[\frac{1}{2},\ x+\frac{1}{2},\ x+\frac{3}{4}\right]$	[95,132]
72	$\left[x,\ \frac{1}{2}-x,\ \frac{1}{4}\right]$	[96,133]
73	$\left[x+\frac{1}{2},\ \frac{1}{2},\ x+\frac{1}{4}\right]$	[97,159]
74	$\left[x+\frac{1}{2},\ \frac{3}{4},\ -x\right]$	[100,104]
75	$\left[\frac{1}{4},\ \frac{1}{2}-x,\ x+\frac{1}{2}\right]$	[103,117]
76	$\left[\frac{1}{4},\ x+\frac{1}{4},\ \frac{1}{4}-x\right]$	[107,163]
77	$\left[-x,\ x,\ \frac{1}{4}\right]$	[109,120]
78	$\left[-x,\ \frac{3}{4}-x,\ \frac{1}{2}\right]$	[110,164]
79	$\left[x+\frac{1}{2},\ 0,\ x+\frac{3}{4}\right]$	[111,145]
80	$\left[\frac{1}{4},\ x+\frac{3}{4},\ \frac{3}{4}-x\right]$	[115,155]
81	$\left[-x,\ \frac{1}{4}-x,\ 0\right]$	[116,158]
82	$\left[\frac{3}{4}-x,\ x+\frac{1}{4},\ \frac{1}{4}\right]$	[122,142]
83	$\left[\frac{3}{4}-x,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[123,185]
84	$\left[x+\frac{3}{4},\ \frac{3}{4},\ \frac{3}{4}-x\right]$	[125,130]
85	$\left[\frac{1}{4},\ x+\frac{1}{2},\ -x\right]$	[127,189]
86	$\left[x+\frac{3}{4},\ \frac{1}{2},\ x+\frac{1}{2}\right]$	[129,184]
87	$\left[\frac{1}{4},\ \frac{1}{4}-x,\ x+\frac{3}{4}\right]$	[131,139]
88	$\left[x+\frac{3}{4},\ 0,\ x\right]$	[136,177]
89	$\left[\frac{3}{4}-x,\ -x,\ 0\right]$	[137,171]
90	$\left[\frac{1}{4},\ x,\ \frac{1}{2}-x\right]$	[141,175]
91	$\left[x+\frac{1}{2},\ \frac{1}{4},\ \frac{1}{2}-x\right]$	[148,152]
92	$\left[\frac{1}{4},\ -x,\ x\right]$	[151,165]
93	$\left[-x,\ x+\frac{1}{2},\ \frac{3}{4}\right]$	[157,168]
94	$\left[\frac{3}{4}-x,\ x+\frac{3}{4},\ \frac{3}{4}\right]$	[170,190]
95	$\left[x+\frac{3}{4},\ \frac{1}{4},\ \frac{1}{4}-x\right]$	[173,178]
96	$\left[\frac{1}{4},\ \frac{3}{4}-x,\ x+\frac{1}{4}\right]$	[179,187]
97	$\left[x,\ \frac{1}{2},\ x+\frac{1}{4}\right]$	[193,255]
98	$\left[x+\frac{1}{4},\ \frac{3}{4}-x,\ \frac{1}{4}\right]$	[194,358]
99	$\left[x+\frac{1}{4},\ x,\ \frac{1}{2}\right]$	[195,305]
100	$\left[x,\ \frac{3}{4},\ -x\right]$	[196,200]
101	$\left[\frac{3}{4}-x,\ \frac{3}{4},\ x+\frac{3}{4}\right]$	[197,298]
102	$\left[0,\ x+\frac{1}{4},\ x+\frac{1}{2}\right]$	[198,354]
103	$\left[\frac{3}{4},\ \frac{1}{2}-x,\ x+\frac{1}{2}\right]$	[199,213]
104	$\left[\frac{1}{4}-x,\ \frac{1}{2},\ -x\right]$	[201,352]
105	$\left[\frac{1}{4}-x,\ \frac{3}{4},\ x+\frac{1}{4}\right]$	[202,293]
106	$\left[\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{4}-x\right]$	[203,259]
107	$\left[0,\ \frac{1}{2}-x,\ \frac{1}{4}-x\right]$	[204,311]
108	$\left[\frac{1}{2}-x,\ x,\ \frac{1}{4}\right]$	[205,216]
109	$\left[\frac{1}{2}-x,\ \frac{3}{4}-x,\ \frac{1}{2}\right]$	[206,260]

continued ...

Table 10

No.	position	mapping
110	$\left[x,\, 0,\, x+\frac{3}{4}\right]$	[207,241]
111	$\left[\frac{3}{4}-x,\, 0,\, -x\right]$	[208,345]
112	$\left[x+\frac{3}{4},\, x,\, 0\right]$	[209,291]
113	$\left[\frac{1}{2},\, x+\frac{3}{4},\, x+\frac{1}{2}\right]$	[210,342]
114	$\left[\frac{3}{4},\, x+\frac{3}{4},\, \frac{3}{4}-x\right]$	[211,251]
115	$\left[\frac{1}{2}-x,\, \frac{1}{4}-x,\, 0\right]$	[212,254]
116	$\left[x+\frac{3}{4},\, \frac{1}{4}-x,\, \frac{1}{4}\right]$	[214,338]
117	$\left[\frac{1}{2},\, \frac{1}{2}-x,\, \frac{3}{4}-x\right]$	[215,300]
118	$\left[-x,\, \frac{1}{2},\, \frac{3}{4}-x\right]$	[217,375]
119	$\left[\frac{1}{4}-x,\, x+\frac{1}{4},\, \frac{1}{4}\right]$	[218,238]
120	$\left[\frac{1}{4}-x,\, \frac{1}{2}-x,\, \frac{1}{2}\right]$	[219,281]
121	$\left[\frac{1}{2}-x,\, \frac{3}{4},\, x\right]$	[220,320]
122	$\left[x+\frac{1}{4},\, \frac{3}{4},\, \frac{3}{4}-x\right]$	[221,226]
123	$\left[0,\, \frac{1}{4}-x,\, -x\right]$	[222,330]
124	$\left[\frac{3}{4},\, x+\frac{1}{2},\, -x\right]$	[223,285]
125	$\left[-x,\, \frac{3}{4},\, x+\frac{1}{2}\right]$	[224,316]
126	$\left[x+\frac{1}{4},\, \frac{1}{2},\, x+\frac{1}{2}\right]$	[225,280]
127	$\left[\frac{3}{4},\, \frac{1}{4}-x,\, x+\frac{3}{4}\right]$	[227,235]
128	$\left[0,\, x+\frac{1}{2},\, x+\frac{3}{4}\right]$	[228,383]
129	$\left[x+\frac{1}{2},\, \frac{1}{2}-x,\, \frac{1}{4}\right]$	[229,384]
130	$\left[x+\frac{1}{2},\, x+\frac{1}{4},\, \frac{1}{2}\right]$	[230,332]
131	$\left[\frac{1}{2}-x,\, 0,\, \frac{3}{4}-x\right]$	[231,361]
132	$\left[x+\frac{1}{4},\, 0,\, x\right]$	[232,273]
133	$\left[\frac{1}{4}-x,\, -x,\, 0\right]$	[233,267]
134	$\left[\frac{1}{2},\, \frac{1}{4}-x,\, \frac{1}{2}-x\right]$	[234,318]
135	$\left[x,\, x+\frac{1}{4},\, 0\right]$	[236,326]
136	$\left[\frac{3}{4},\, x,\, \frac{1}{2}-x\right]$	[237,271]
137	$\left[\frac{1}{2},\, x,\, x+\frac{3}{4}\right]$	[239,372]
138	$\left[x,\, -x,\, \frac{1}{4}\right]$	[240,373]
139	$\left[x+\frac{1}{4},\, \frac{1}{4}-x,\, \frac{3}{4}\right]$	[242,310]
140	$\left[x+\frac{1}{4},\, x+\frac{1}{2},\, 0\right]$	[243,353]
141	$\left[x,\, \frac{1}{4},\, \frac{1}{2}-x\right]$	[244,248]
142	$\left[\frac{3}{4}-x,\, \frac{1}{4},\, x+\frac{1}{4}\right]$	[245,346]
143	$\left[0,\, x+\frac{3}{4},\, x\right]$	[246,306]
144	$\left[\frac{3}{4},\, -x,\, x\right]$	[247,261]
145	$\left[\frac{1}{4}-x,\, 0,\, \frac{1}{2}-x\right]$	[249,304]
146	$\left[\frac{1}{4}-x,\, \frac{1}{4},\, x+\frac{3}{4}\right]$	[250,341]
147	$\left[0,\, -x,\, \frac{3}{4}-x\right]$	[252,359]
148	$\left[\frac{1}{2}-x,\, x+\frac{1}{2},\, \frac{3}{4}\right]$	[253,264]
149	$\left[\frac{3}{4}-x,\, \frac{1}{2},\, \frac{1}{2}-x\right]$	[256,297]
150	$\left[x+\frac{3}{4},\, x+\frac{1}{2},\, \frac{1}{2}\right]$	[257,339]
151	$\left[\frac{1}{2},\, x+\frac{1}{4},\, x\right]$	[258,294]
152	$\left[x+\frac{3}{4},\, \frac{3}{4}-x,\, \frac{3}{4}\right]$	[262,290]
153	$\left[\frac{1}{2},\, -x,\, \frac{1}{4}-x\right]$	[263,348]
154	$\left[-x,\, 0,\, \frac{1}{4}-x\right]$	[265,327]
155	$\left[\frac{1}{4}-x,\, x+\frac{3}{4},\, \frac{3}{4}\right]$	[266,286]
156	$\left[\frac{1}{2}-x,\, \frac{1}{4},\, x+\frac{1}{2}\right]$	[268,368]

continued ...

Table 10

No.	position	mapping
157	$\left[x+\frac{1}{4},\,\frac{1}{4},\,\frac{1}{4}-x\right]$	[269,274]
158	$\left[0,\,\frac{3}{4}-x,\,\frac{1}{2}-x\right]$	[270,378]
159	$\left[-x,\,\frac{1}{4},\,x\right]$	[272,364]
160	$\left[\frac{3}{4},\,\frac{3}{4}-x,\,x+\frac{1}{4}\right]$	[275,283]
161	$\left[0,\,x,\,x+\frac{1}{4}\right]$	[276,335]
162	$\left[x+\frac{1}{2},\,-x,\,\frac{3}{4}\right]$	[277,336]
163	$\left[x+\frac{1}{2},\,x+\frac{3}{4},\,0\right]$	[278,380]
164	$\left[\frac{1}{2}-x,\,\frac{1}{2},\,\frac{1}{4}-x\right]$	[279,313]
165	$\left[\frac{1}{2},\,\frac{3}{4}-x,\,-x\right]$	[282,366]
166	$\left[x,\,x+\frac{3}{4},\,\frac{1}{2}\right]$	[284,374]
167	$\left[\frac{1}{2},\,x+\frac{1}{2},\,x+\frac{1}{4}\right]$	[287,324]
168	$\left[x,\,\frac{1}{2}-x,\,\frac{3}{4}\right]$	[288,325]
169	$\left[x+\frac{1}{2},\,\frac{1}{2},\,x+\frac{3}{4}\right]$	[289,351]
170	$\left[x+\frac{1}{2},\,\frac{3}{4},\,\frac{1}{2}-x\right]$	[292,296]
171	$\left[\frac{1}{4},\,\frac{1}{2}-x,\,x\right]$	[295,309]
172	$\left[\frac{1}{4},\,x+\frac{1}{4},\,\frac{3}{4}-x\right]$	[299,355]
173	$\left[-x,\,x,\,\frac{3}{4}\right]$	[301,312]
174	$\left[-x,\,\frac{3}{4}-x,\,0\right]$	[302,356]
175	$\left[x+\frac{1}{2},\,0,\,x+\frac{1}{4}\right]$	[303,337]
176	$\left[\frac{1}{4},\,x+\frac{3}{4},\,\frac{1}{4}-x\right]$	[307,347]
177	$\left[-x,\,\frac{1}{4}-x,\,\frac{1}{2}\right]$	[308,350]
178	$\left[\frac{3}{4}-x,\,x+\frac{1}{4},\,\frac{3}{4}\right]$	[314,334]
179	$\left[\frac{3}{4}-x,\,\frac{1}{2}-x,\,0\right]$	[315,377]
180	$\left[x+\frac{3}{4},\,\frac{3}{4},\,\frac{1}{4}-x\right]$	[317,322]
181	$\left[\frac{1}{4},\,x+\frac{1}{2},\,\frac{1}{2}-x\right]$	[319,381]
182	$\left[x+\frac{3}{4},\,\frac{1}{2},\,x\right]$	[321,376]
183	$\left[\frac{1}{4},\,\frac{1}{4}-x,\,x+\frac{1}{4}\right]$	[323,331]
184	$\left[x+\frac{3}{4},\,0,\,x+\frac{1}{2}\right]$	[328,369]
185	$\left[\frac{3}{4}-x,\,-x,\,\frac{1}{2}\right]$	[329,363]
186	$\left[\frac{1}{4},\,x,\,-x\right]$	[333,367]
187	$\left[x+\frac{1}{2},\,\frac{1}{4},\,-x\right]$	[340,344]
188	$\left[\frac{1}{4},\,-x,\,x+\frac{1}{2}\right]$	[343,357]
189	$\left[-x,\,x+\frac{1}{2},\,\frac{1}{4}\right]$	[349,360]
190	$\left[\frac{3}{4}-x,\,x+\frac{3}{4},\,\frac{1}{4}\right]$	[362,382]
191	$\left[x+\frac{3}{4},\,\frac{1}{4},\,\frac{3}{4}-x\right]$	[365,370]
192	$\left[\frac{1}{4},\,\frac{3}{4}-x,\,x+\frac{3}{4}\right]$	[371,379]

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

No.	position	mapping
1	$[x,\,x,\,z]$	[1,372]
2	$\left[x+\frac{1}{4},\,\frac{1}{2}-z,\,x+\frac{1}{4}\right]$	[2,283]
3	$\left[x+\frac{1}{4},\,z+\frac{1}{4},\,\frac{1}{2}-x\right]$	[3,237]
4	$\left[z+\frac{1}{4},\,x+\frac{1}{4},\,\frac{1}{2}-x\right]$	[4,236]

continued ...

Table 11

No.	position	mapping
5	$\left[\frac{1}{2}-z,\ x+\frac{1}{4},\ x+\frac{1}{4}\right]$	[5,334]
6	$\left[\frac{1}{2}-x,\ x+\frac{1}{4},\ z+\frac{1}{4}\right]$	[6,320]
7	$\left[x+\frac{1}{4},\ \frac{1}{2}-x,\ z+\frac{1}{4}\right]$	[7,273]
8	$\left[x,\ \frac{1}{4}-x,\ \frac{1}{4}-z\right]$	[8,318]
9	$\left[\frac{1}{4}-x,\ x,\ \frac{1}{4}-z\right]$	[9,271]
10	$\left[\frac{1}{4}-x,\ \frac{1}{4}-x,\ z\right]$	[10,227]
11	$\left[x+\frac{1}{4},\ x+\frac{1}{4},\ \frac{1}{2}-z\right]$	[11,226]
12	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[12,361]
13	$\left[\frac{1}{2}-x,\ z+\frac{1}{4},\ x+\frac{1}{4}\right]$	[13,335]
14	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[14,378]
15	$\left[z+\frac{1}{4},\ \frac{1}{2}-x,\ x+\frac{1}{4}\right]$	[15,288]
16	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	[16,377]
17	$[z,\ x,\ x]$	[17,376]
18	$[x,\ z,\ x]$	[18,374]
19	$\left[\frac{1}{4}-x,\ z,\ \frac{1}{4}-x\right]$	[19,266]
20	$\left[\frac{1}{4}-z,\ \frac{1}{4}-x,\ x\right]$	[20,220]
21	$\left[\frac{1}{4}-x,\ \frac{1}{4}-z,\ x\right]$	[21,219]
22	$\left[z,\ \frac{1}{4}-x,\ \frac{1}{4}-x\right]$	[22,317]
23	$\left[x,\ \frac{1}{4}-z,\ \frac{1}{4}-x\right]$	[23,325]
24	$\left[\frac{1}{4}-z,\ x,\ \frac{1}{4}-x\right]$	[24,279]
25	$[-x,\ -x,\ -z]$	[25,348]
26	$\left[\frac{1}{4}-x,\ z+\frac{1}{2},\ \frac{1}{4}-x\right]$	[26,259]
27	$\left[\frac{1}{4}-x,\ \frac{1}{4}-z,\ x+\frac{1}{2}\right]$	[27,213]
28	$\left[\frac{1}{4}-z,\ \frac{1}{4}-x,\ x+\frac{1}{2}\right]$	[28,212]
29	$\left[z+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{1}{4}-x\right]$	[29,310]
30	$\left[x+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{1}{4}-z\right]$	[30,296]
31	$\left[\frac{1}{4}-x,\ x+\frac{1}{2},\ \frac{1}{4}-z\right]$	[31,249]
32	$\left[-x,\ x+\frac{1}{4},\ z+\frac{1}{4}\right]$	[32,294]
33	$\left[x+\frac{1}{4},\ -x,\ z+\frac{1}{4}\right]$	[33,247]
34	$\left[x+\frac{1}{4},\ x+\frac{1}{4},\ -z\right]$	[34,203]
35	$\left[\frac{1}{4}-x,\ \frac{1}{4}-x,\ z+\frac{1}{2}\right]$	[35,202]
36	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[36,337]
37	$\left[x+\frac{1}{2},\ \frac{1}{4}-z,\ \frac{1}{4}-x\right]$	[37,311]
38	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$	[38,354]
39	$\left[\frac{1}{4}-z,\ x+\frac{1}{2},\ \frac{1}{4}-x\right]$	[39,264]
40	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ x+\frac{1}{2}\right]$	[40,353]
41	$[-z,\ -x,\ -x]$	[41,352]
42	$[-x,\ -z,\ -x]$	[42,350]
43	$\left[x+\frac{1}{4},\ -z,\ x+\frac{1}{4}\right]$	[43,242]
44	$\left[z+\frac{1}{4},\ x+\frac{1}{4},\ -x\right]$	[44,196]
45	$\left[x+\frac{1}{4},\ z+\frac{1}{4},\ -x\right]$	[45,195]
46	$\left[-z,\ x+\frac{1}{4},\ x+\frac{1}{4}\right]$	[46,293]
47	$\left[-x,\ z+\frac{1}{4},\ x+\frac{1}{4}\right]$	[47,301]
48	$\left[z+\frac{1}{4},\ -x,\ x+\frac{1}{4}\right]$	[48,255]
49	$\left[x,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[49,324]
50	$\left[x+\frac{1}{4},\ -z,\ x+\frac{3}{4}\right]$	[50,235]
51	$\left[x+\frac{1}{4},\ z+\frac{3}{4},\ -x\right]$	[51,285]

continued ...

Table 11

No.	position	mapping
52	$\left[z+\frac{1}{4},\, x+\frac{3}{4},\, -x\right]$	[52,284]
53	$\left[\frac{1}{2}-z,\, x+\frac{3}{4},\, x+\frac{3}{4}\right]$	[53,382]
54	$\left[\frac{1}{2}-x,\, x+\frac{3}{4},\, z+\frac{3}{4}\right]$	[54,368]
55	$\left[x+\frac{1}{4},\, -x,\, z+\frac{3}{4}\right]$	[55,225]
56	$\left[x,\, \frac{3}{4}-x,\, \frac{3}{4}-z\right]$	[56,366]
57	$\left[\frac{1}{4}-x,\, x+\frac{1}{2},\, \frac{3}{4}-z\right]$	[57,223]
58	$\left[\frac{1}{4}-x,\, \frac{3}{4}-x,\, z+\frac{1}{2}\right]$	[58,275]
59	$\left[x+\frac{1}{4},\, x+\frac{3}{4},\, -z\right]$	[59,274]
60	$\left[\frac{1}{2}-x,\, -x,\, -z\right]$	[60,313]
61	$\left[\frac{1}{2}-x,\, z+\frac{3}{4},\, x+\frac{3}{4}\right]$	[61,383]
62	$\left[\frac{1}{2}-x,\, -z,\, -x\right]$	[62,330]
63	$\left[z+\frac{1}{4},\, -x,\, x+\frac{3}{4}\right]$	[63,240]
64	$\left[\frac{1}{2}-z,\, -x,\, -x\right]$	[64,329]
65	$\left[z,\, x+\frac{1}{2},\, x+\frac{1}{2}\right]$	[65,328]
66	$\left[x,\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[66,326]
67	$\left[\frac{1}{4}-x,\, z+\frac{1}{2},\, \frac{3}{4}-x\right]$	[67,218]
68	$\left[\frac{1}{4}-z,\, \frac{3}{4}-x,\, x+\frac{1}{2}\right]$	[68,268]
69	$\left[\frac{1}{4}-x,\, \frac{3}{4}-z,\, x+\frac{1}{2}\right]$	[69,267]
70	$\left[z,\, \frac{3}{4}-x,\, \frac{3}{4}-x\right]$	[70,365]
71	$\left[x,\, \frac{3}{4}-z,\, \frac{3}{4}-x\right]$	[71,373]
72	$\left[\frac{1}{4}-z,\, x+\frac{1}{2},\, \frac{3}{4}-x\right]$	[72,231]
73	$\left[-x,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[73,300]
74	$\left[\frac{1}{4}-x,\, z,\, \frac{3}{4}-x\right]$	[74,211]
75	$\left[\frac{1}{4}-x,\, \frac{3}{4}-z,\, x\right]$	[75,261]
76	$\left[\frac{1}{4}-z,\, \frac{3}{4}-x,\, x\right]$	[76,260]
77	$\left[z+\frac{1}{2},\, \frac{3}{4}-x,\, \frac{3}{4}-x\right]$	[77,358]
78	$\left[x+\frac{1}{2},\, \frac{3}{4}-x,\, \frac{3}{4}-z\right]$	[78,344]
79	$\left[\frac{1}{4}-x,\, x,\, \frac{3}{4}-z\right]$	[79,201]
80	$\left[-x,\, x+\frac{3}{4},\, z+\frac{3}{4}\right]$	[80,342]
81	$\left[x+\frac{1}{4},\, \frac{1}{2}-x,\, z+\frac{3}{4}\right]$	[81,199]
82	$\left[x+\frac{1}{4},\, x+\frac{3}{4},\, \frac{1}{2}-z\right]$	[82,251]
83	$\left[\frac{1}{4}-x,\, \frac{3}{4}-x,\, z\right]$	[83,250]
84	$\left[x+\frac{1}{2},\, x,\, z\right]$	[84,289]
85	$\left[x+\frac{1}{2},\, \frac{3}{4}-z,\, \frac{3}{4}-x\right]$	[85,359]
86	$\left[x+\frac{1}{2},\, z,\, x\right]$	[86,306]
87	$\left[\frac{1}{4}-z,\, x,\, \frac{3}{4}-x\right]$	[87,216]
88	$\left[z+\frac{1}{2},\, x,\, x\right]$	[88,305]
89	$\left[-z,\, \frac{1}{2}-x,\, \frac{1}{2}-x\right]$	[89,304]
90	$\left[-x,\, \frac{1}{2}-z,\, \frac{1}{2}-x\right]$	[90,302]
91	$\left[x+\frac{1}{4},\, \frac{1}{2}-z,\, x+\frac{3}{4}\right]$	[91,194]
92	$\left[z+\frac{1}{4},\, x+\frac{3}{4},\, \frac{1}{2}-x\right]$	[92,244]
93	$\left[x+\frac{1}{4},\, z+\frac{3}{4},\, \frac{1}{2}-x\right]$	[93,243]
94	$\left[-z,\, x+\frac{3}{4},\, x+\frac{3}{4}\right]$	[94,341]
95	$\left[-x,\, z+\frac{3}{4},\, x+\frac{3}{4}\right]$	[95,349]
96	$\left[z+\frac{1}{4},\, \frac{1}{2}-x,\, x+\frac{3}{4}\right]$	[96,207]
97	$\left[x+\frac{1}{2},\, x,\, z+\frac{1}{2}\right]$	[97,276]
98	$\left[x+\frac{3}{4},\, \frac{1}{2}-z,\, x+\frac{3}{4}\right]$	[98,379]

continued ...

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Table 11

No.	position	mapping
99	$\left[x+\frac{3}{4}, z+\frac{1}{4}, -x\right]$	[99,333]
100	$\left[z+\frac{3}{4}, x+\frac{1}{4}, -x\right]$	[100,332]
101	$\left[-z, x+\frac{1}{4}, x+\frac{3}{4}\right]$	[101,238]
102	$\left[-x, x+\frac{1}{4}, z+\frac{3}{4}\right]$	[102,224]
103	$\left[x+\frac{3}{4}, \frac{1}{2}-x, z+\frac{3}{4}\right]$	[103,369]
104	$\left[x+\frac{1}{2}, \frac{1}{4}-x, \frac{3}{4}-z\right]$	[104,222]
105	$\left[\frac{3}{4}-x, x, \frac{3}{4}-z\right]$	[105,367]
106	$\left[\frac{3}{4}-x, \frac{1}{4}-x, z+\frac{1}{2}\right]$	[106,323]
107	$\left[x+\frac{3}{4}, x+\frac{1}{4}, -z\right]$	[107,322]
108	$\left[-x, \frac{1}{2}-x, -z\right]$	[108,265]
109	$\left[-x, z+\frac{1}{4}, x+\frac{3}{4}\right]$	[109,239]
110	$\left[-x, \frac{1}{2}-z, -x\right]$	[110,282]
111	$\left[z+\frac{3}{4}, \frac{1}{2}-x, x+\frac{3}{4}\right]$	[111,384]
112	$\left[-z, \frac{1}{2}-x, -x\right]$	[112,281]
113	$\left[z+\frac{1}{2}, x, x+\frac{1}{2}\right]$	[113,280]
114	$\left[x+\frac{1}{2}, z, x+\frac{1}{2}\right]$	[114,278]
115	$\left[\frac{3}{4}-x, z, \frac{3}{4}-x\right]$	[115,362]
116	$\left[\frac{3}{4}-z, \frac{1}{4}-x, x+\frac{1}{2}\right]$	[116,316]
117	$\left[\frac{3}{4}-x, \frac{1}{4}-z, x+\frac{1}{2}\right]$	[117,315]
118	$\left[z+\frac{1}{2}, \frac{1}{4}-x, \frac{3}{4}-x\right]$	[118,221]
119	$\left[x+\frac{1}{2}, \frac{1}{4}-z, \frac{3}{4}-x\right]$	[119,229]
120	$\left[\frac{3}{4}-z, x, \frac{3}{4}-x\right]$	[120,375]
121	$\left[\frac{1}{2}-x, -x, \frac{1}{2}-z\right]$	[121,252]
122	$\left[\frac{3}{4}-x, z+\frac{1}{2}, \frac{3}{4}-x\right]$	[122,355]
123	$\left[\frac{3}{4}-x, \frac{1}{4}-z, x\right]$	[123,309]
124	$\left[\frac{3}{4}-z, \frac{1}{4}-x, x\right]$	[124,308]
125	$\left[z, \frac{1}{4}-x, \frac{3}{4}-x\right]$	[125,214]
126	$\left[x, \frac{1}{4}-x, \frac{3}{4}-z\right]$	[126,200]
127	$\left[\frac{3}{4}-x, x+\frac{1}{2}, \frac{3}{4}-z\right]$	[127,345]
128	$\left[\frac{1}{2}-x, x+\frac{1}{4}, z+\frac{3}{4}\right]$	[128,198]
129	$\left[x+\frac{3}{4}, -x, z+\frac{3}{4}\right]$	[129,343]
130	$\left[x+\frac{3}{4}, x+\frac{1}{4}, \frac{1}{2}-z\right]$	[130,299]
131	$\left[\frac{3}{4}-x, \frac{1}{4}-x, z\right]$	[131,298]
132	$\left[x, x+\frac{1}{2}, z\right]$	[132,241]
133	$\left[x, \frac{1}{4}-z, \frac{3}{4}-x\right]$	[133,215]
134	$\left[x, z+\frac{1}{2}, x\right]$	[134,258]
135	$\left[\frac{3}{4}-z, x+\frac{1}{2}, \frac{3}{4}-x\right]$	[135,360]
136	$\left[z, x+\frac{1}{2}, x\right]$	[136,257]
137	$\left[\frac{1}{2}-z, -x, \frac{1}{2}-x\right]$	[137,256]
138	$\left[\frac{1}{2}-x, -z, \frac{1}{2}-x\right]$	[138,254]
139	$\left[x+\frac{3}{4}, -z, x+\frac{3}{4}\right]$	[139,338]
140	$\left[z+\frac{3}{4}, x+\frac{1}{4}, \frac{1}{2}-x\right]$	[140,292]
141	$\left[x+\frac{3}{4}, z+\frac{1}{4}, \frac{1}{2}-x\right]$	[141,291]
142	$\left[\frac{1}{2}-z, x+\frac{1}{4}, x+\frac{3}{4}\right]$	[142,197]
143	$\left[\frac{1}{2}-x, z+\frac{1}{4}, x+\frac{3}{4}\right]$	[143,205]
144	$\left[z+\frac{3}{4}, -x, x+\frac{3}{4}\right]$	[144,351]
145	$\left[x+\frac{1}{2}, x+\frac{1}{2}, z\right]$	[145,228]

continued ...

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Table 11

No.	position	mapping
146	$\left[x+\frac{3}{4},\,-z,\,x+\frac{1}{4}\right]$	[146,331]
147	$\left[x+\frac{3}{4},\,z+\frac{3}{4},\,\frac{1}{2}-x\right]$	[147,381]
148	$\left[z+\frac{3}{4},\,x+\frac{3}{4},\,\frac{1}{2}-x\right]$	[148,380]
149	$\left[-z,\,x+\frac{3}{4},\,x+\frac{1}{4}\right]$	[149,286]
150	$\left[-x,\,x+\frac{3}{4},\,z+\frac{1}{4}\right]$	[150,272]
151	$\left[x+\frac{3}{4},\,-x,\,z+\frac{1}{4}\right]$	[151,321]
152	$\left[x+\frac{1}{2},\,\frac{3}{4}-x,\,\frac{1}{4}-z\right]$	[152,270]
153	$\left[\frac{3}{4}-x,\,x+\frac{1}{2},\,\frac{1}{4}-z\right]$	[153,319]
154	$\left[\frac{3}{4}-x,\,\frac{3}{4}-x,\,z\right]$	[154,371]
155	$\left[x+\frac{3}{4},\,x+\frac{3}{4},\,\frac{1}{2}-z\right]$	[155,370]
156	$\left[-x,\,-x,\,\frac{1}{2}-z\right]$	[156,217]
157	$\left[-x,\,z+\frac{3}{4},\,x+\frac{1}{4}\right]$	[157,287]
158	$\left[-x,\,-z,\,\frac{1}{2}-x\right]$	[158,234]
159	$\left[z+\frac{3}{4},\,-x,\,x+\frac{1}{4}\right]$	[159,336]
160	$\left[-z,\,-x,\,\frac{1}{2}-x\right]$	[160,233]
161	$\left[z+\frac{1}{2},\,x+\frac{1}{2},\,x\right]$	[161,232]
162	$\left[x+\frac{1}{2},\,z+\frac{1}{2},\,x\right]$	[162,230]
163	$\left[\frac{3}{4}-x,\,z+\frac{1}{2},\,\frac{1}{4}-x\right]$	[163,314]
164	$\left[\frac{3}{4}-z,\,\frac{3}{4}-x,\,x\right]$	[164,364]
165	$\left[\frac{3}{4}-x,\,\frac{3}{4}-z,\,x\right]$	[165,363]
166	$\left[z+\frac{1}{2},\,\frac{3}{4}-x,\,\frac{1}{4}-x\right]$	[166,269]
167	$\left[x+\frac{1}{2},\,\frac{3}{4}-z,\,\frac{1}{4}-x\right]$	[167,277]
168	$\left[\frac{3}{4}-z,\,x+\frac{1}{2},\,\frac{1}{4}-x\right]$	[168,327]
169	$\left[\frac{1}{2}-x,\,\frac{1}{2}-x,\,-z\right]$	[169,204]
170	$\left[\frac{3}{4}-x,\,z,\,\frac{1}{4}-x\right]$	[170,307]
171	$\left[\frac{3}{4}-x,\,\frac{3}{4}-z,\,x+\frac{1}{2}\right]$	[171,357]
172	$\left[\frac{3}{4}-z,\,\frac{3}{4}-x,\,x+\frac{1}{2}\right]$	[172,356]
173	$\left[z,\,\frac{3}{4}-x,\,\frac{1}{4}-x\right]$	[173,262]
174	$\left[x,\,\frac{3}{4}-x,\,\frac{1}{4}-z\right]$	[174,248]
175	$\left[\frac{3}{4}-x,\,x,\,\frac{1}{4}-z\right]$	[175,297]
176	$\left[\frac{1}{2}-x,\,x+\frac{3}{4},\,z+\frac{1}{4}\right]$	[176,246]
177	$\left[x+\frac{3}{4},\,\frac{1}{2}-x,\,z+\frac{1}{4}\right]$	[177,295]
178	$\left[x+\frac{3}{4},\,x+\frac{3}{4},\,-z\right]$	[178,347]
179	$\left[\frac{3}{4}-x,\,\frac{3}{4}-x,\,z+\frac{1}{2}\right]$	[179,346]
180	$\left[x,\,x,\,z+\frac{1}{2}\right]$	[180,193]
181	$\left[x,\,\frac{3}{4}-z,\,\frac{1}{4}-x\right]$	[181,263]
182	$\left[x,\,z,\,x+\frac{1}{2}\right]$	[182,210]
183	$\left[\frac{3}{4}-z,\,x,\,\frac{1}{4}-x\right]$	[183,312]
184	$\left[z,\,x,\,x+\frac{1}{2}\right]$	[184,209]
185	$\left[\frac{1}{2}-z,\,\frac{1}{2}-x,\,-x\right]$	[185,208]
186	$\left[\frac{1}{2}-x,\,\frac{1}{2}-z,\,-x\right]$	[186,206]
187	$\left[x+\frac{3}{4},\,\frac{1}{2}-z,\,x+\frac{1}{4}\right]$	[187,290]
188	$\left[z+\frac{3}{4},\,x+\frac{3}{4},\,-x\right]$	[188,340]
189	$\left[x+\frac{3}{4},\,z+\frac{3}{4},\,-x\right]$	[189,339]
190	$\left[\frac{1}{2}-z,\,x+\frac{3}{4},\,x+\frac{1}{4}\right]$	[190,245]
191	$\left[\frac{1}{2}-x,\,z+\frac{3}{4},\,x+\frac{1}{4}\right]$	[191,253]
192	$\left[z+\frac{3}{4},\,\frac{1}{2}-x,\,x+\frac{1}{4}\right]$	[192,303]

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

No.	position	mapping
1	$[x, y, z]$	[1]
2	$\left[x + \frac{1}{4}, \frac{1}{2} - z, y + \frac{1}{4}\right]$	[2]
3	$\left[x + \frac{1}{4}, z + \frac{1}{4}, \frac{1}{2} - y\right]$	[3]
4	$\left[z + \frac{1}{4}, y + \frac{1}{4}, \frac{1}{2} - x\right]$	[4]
5	$\left[\frac{1}{2} - z, y + \frac{1}{4}, x + \frac{1}{4}\right]$	[5]
6	$\left[\frac{1}{2} - y, x + \frac{1}{4}, z + \frac{1}{4}\right]$	[6]
7	$\left[y + \frac{1}{4}, \frac{1}{2} - x, z + \frac{1}{4}\right]$	[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	$\left[y + \frac{1}{4}, x + \frac{1}{4}, \frac{1}{2} - z\right]$	[11]
12	$\left[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z\right]$	[12]
13	$\left[\frac{1}{2} - x, z + \frac{1}{4}, y + \frac{1}{4}\right]$	[13]
14	$\left[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y\right]$	[14]
15	$\left[z + \frac{1}{4}, \frac{1}{2} - y, x + \frac{1}{4}\right]$	[15]
16	$\left[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2} - x\right]$	[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	$\left[\frac{1}{4} - x, z + \frac{1}{2}, \frac{1}{4} - y\right]$	[26]
27	$\left[\frac{1}{4} - x, \frac{1}{4} - z, y + \frac{1}{2}\right]$	[27]
28	$\left[\frac{1}{4} - z, \frac{1}{4} - y, x + \frac{1}{2}\right]$	[28]
29	$\left[z + \frac{1}{2}, \frac{1}{4} - y, \frac{1}{4} - x\right]$	[29]
30	$\left[y + \frac{1}{2}, \frac{1}{4} - x, \frac{1}{4} - z\right]$	[30]
31	$\left[\frac{1}{4} - y, x + \frac{1}{2}, \frac{1}{4} - z\right]$	[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	$\left[\frac{1}{4} - y, \frac{1}{4} - x, z + \frac{1}{2}\right]$	[35]
36	$\left[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}\right]$	[36]
37	$\left[x + \frac{1}{2}, \frac{1}{4} - z, \frac{1}{4} - y\right]$	[37]
38	$\left[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}\right]$	[38]
39	$\left[\frac{1}{4} - z, y + \frac{1}{2}, \frac{1}{4} - x\right]$	[39]
40	$\left[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}\right]$	[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 ...

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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	$\left[x + \frac{1}{4}, -z, y + \frac{3}{4}\right]$	[50]
51	$\left[x + \frac{1}{4}, z + \frac{3}{4}, -y\right]$	[51]
52	$\left[z + \frac{1}{4}, y + \frac{3}{4}, -x\right]$	[52]
53	$\left[\frac{1}{2} - z, y + \frac{3}{4}, x + \frac{3}{4}\right]$	[53]
54	$\left[\frac{1}{2} - y, x + \frac{3}{4}, z + \frac{3}{4}\right]$	[54]
55	$\left[y + \frac{1}{4}, -x, z + \frac{3}{4}\right]$	[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	$\left[y + \frac{1}{4}, x + \frac{3}{4}, -z\right]$	[59]
60	$\left[\frac{1}{2} - y, -x, -z\right]$	[60]
61	$\left[\frac{1}{2} - x, z + \frac{3}{4}, y + \frac{3}{4}\right]$	[61]
62	$\left[\frac{1}{2} - x, -z, -y\right]$	[62]
63	$\left[z + \frac{1}{4}, -y, x + \frac{3}{4}\right]$	[63]
64	$\left[\frac{1}{2} - z, -y, -x\right]$	[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	$\left[\frac{1}{4} - x, z, \frac{3}{4} - y\right]$	[74]
75	$\left[\frac{1}{4} - x, \frac{3}{4} - z, y\right]$	[75]
76	$\left[\frac{1}{4} - z, \frac{3}{4} - y, x\right]$	[76]
77	$\left[z + \frac{1}{2}, \frac{3}{4} - y, \frac{3}{4} - x\right]$	[77]
78	$\left[y + \frac{1}{2}, \frac{3}{4} - x, \frac{3}{4} - z\right]$	[78]
79	$\left[\frac{1}{4} - y, x, \frac{3}{4} - z\right]$	[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	$\left[\frac{1}{4} - y, \frac{3}{4} - x, z\right]$	[83]
84	$\left[y + \frac{1}{2}, x, z\right]$	[84]
85	$\left[x + \frac{1}{2}, \frac{3}{4} - z, \frac{3}{4} - y\right]$	[85]
86	$\left[x + \frac{1}{2}, z, y\right]$	[86]
87	$\left[\frac{1}{4} - z, y, \frac{3}{4} - x\right]$	[87]
88	$\left[z + \frac{1}{2}, y, x\right]$	[88]
89	$\left[-z, \frac{1}{2} - x, \frac{1}{2} - y\right]$	[89]
90	$\left[-y, \frac{1}{2} - z, \frac{1}{2} - x\right]$	[90]
91	$\left[y + \frac{1}{4}, \frac{1}{2} - z, x + \frac{3}{4}\right]$	[91]

continued ...

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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	$\left[x + \frac{3}{4},\, \frac{1}{2} - z,\, y + \frac{3}{4}\right]$	[98]
99	$\left[x + \frac{3}{4},\, z + \frac{1}{4},\, -y\right]$	[99]
100	$\left[z + \frac{3}{4},\, y + \frac{1}{4},\, -x\right]$	[100]
101	$\left[-z,\, y + \frac{1}{4},\, x + \frac{3}{4}\right]$	[101]
102	$\left[-y,\, x + \frac{1}{4},\, z + \frac{3}{4}\right]$	[102]
103	$\left[y + \frac{3}{4},\, \frac{1}{2} - x,\, z + \frac{3}{4}\right]$	[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	$\left[y + \frac{3}{4},\, x + \frac{1}{4},\, -z\right]$	[107]
108	$\left[-y,\, \frac{1}{2} - x,\, -z\right]$	[108]
109	$\left[-x,\, z + \frac{1}{4},\, y + \frac{3}{4}\right]$	[109]
110	$\left[-x,\, \frac{1}{2} - z,\, -y\right]$	[110]
111	$\left[z + \frac{3}{4},\, \frac{1}{2} - y,\, x + \frac{3}{4}\right]$	[111]
112	$\left[-z,\, \frac{1}{2} - y,\, -x\right]$	[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	$\left[\frac{3}{4} - x,\, z + \frac{1}{2},\, \frac{3}{4} - y\right]$	[122]
123	$\left[\frac{3}{4} - x,\, \frac{1}{4} - z,\, y\right]$	[123]
124	$\left[\frac{3}{4} - z,\, \frac{1}{4} - y,\, x\right]$	[124]
125	$\left[z,\, \frac{1}{4} - y,\, \frac{3}{4} - x\right]$	[125]
126	$\left[y,\, \frac{1}{4} - x,\, \frac{3}{4} - z\right]$	[126]
127	$\left[\frac{3}{4} - y,\, x + \frac{1}{2},\, \frac{3}{4} - z\right]$	[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	$\left[\frac{3}{4} - y,\, \frac{1}{4} - x,\, z\right]$	[131]
132	$\left[y,\, x + \frac{1}{2},\, z\right]$	[132]
133	$\left[x,\, \frac{1}{4} - z,\, \frac{3}{4} - y\right]$	[133]
134	$\left[x,\, z + \frac{1}{2},\, y\right]$	[134]
135	$\left[\frac{3}{4} - z,\, y + \frac{1}{2},\, \frac{3}{4} - x\right]$	[135]
136	$\left[z,\, y + \frac{1}{2},\, x\right]$	[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	$\left[x + \frac{3}{4}, -z, y + \frac{1}{4}\right]$	[146]
147	$\left[x + \frac{3}{4}, z + \frac{3}{4}, \frac{1}{2} - y\right]$	[147]
148	$\left[z + \frac{3}{4}, y + \frac{3}{4}, \frac{1}{2} - x\right]$	[148]
149	$\left[-z, y + \frac{3}{4}, x + \frac{1}{4}\right]$	[149]
150	$\left[-y, x + \frac{3}{4}, z + \frac{1}{4}\right]$	[150]
151	$\left[y + \frac{3}{4}, -x, z + \frac{1}{4}\right]$	[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	$\left[y + \frac{3}{4}, x + \frac{3}{4}, \frac{1}{2} - z\right]$	[155]
156	$\left[-y, -x, \frac{1}{2} - z\right]$	[156]
157	$\left[-x, z + \frac{3}{4}, y + \frac{1}{4}\right]$	[157]
158	$\left[-x, -z, \frac{1}{2} - y\right]$	[158]
159	$\left[z + \frac{3}{4}, -y, x + \frac{1}{4}\right]$	[159]
160	$\left[-z, -y, \frac{1}{2} - x\right]$	[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	$\left[\frac{3}{4} - x, z, \frac{1}{4} - y\right]$	[170]
171	$\left[\frac{3}{4} - x, \frac{3}{4} - z, y + \frac{1}{2}\right]$	[171]
172	$\left[\frac{3}{4} - z, \frac{3}{4} - y, x + \frac{1}{2}\right]$	[172]
173	$\left[z, \frac{3}{4} - y, \frac{1}{4} - x\right]$	[173]
174	$\left[y, \frac{3}{4} - x, \frac{1}{4} - z\right]$	[174]
175	$\left[\frac{3}{4} - y, x, \frac{1}{4} - z\right]$	[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	$\left[\frac{3}{4} - y, \frac{3}{4} - x, z + \frac{1}{2}\right]$	[179]
180	$\left[y, x, z + \frac{1}{2}\right]$	[180]
181	$\left[x, \frac{3}{4} - z, \frac{1}{4} - y\right]$	[181]
182	$\left[x, z, y + \frac{1}{2}\right]$	[182]
183	$\left[\frac{3}{4} - z, y, \frac{1}{4} - x\right]$	[183]
184	$\left[z, y, x + \frac{1}{2}\right]$	[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	$\left[x + \frac{1}{4},\ \frac{1}{2} - z,\ y + \frac{3}{4}\right]$	[194]
195	$\left[x + \frac{1}{4},\ z + \frac{1}{4},\ -y\right]$	[195]
196	$\left[z + \frac{1}{4},\ y + \frac{1}{4},\ -x\right]$	[196]
197	$\left[\frac{1}{2} - z,\ y + \frac{1}{4},\ x + \frac{3}{4}\right]$	[197]
198	$\left[\frac{1}{2} - y,\ x + \frac{1}{4},\ z + \frac{3}{4}\right]$	[198]
199	$\left[y + \frac{1}{4},\ \frac{1}{2} - x,\ z + \frac{3}{4}\right]$	[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	$\left[y + \frac{1}{4},\ x + \frac{1}{4},\ -z\right]$	[203]
204	$\left[\frac{1}{2} - y,\ \frac{1}{2} - x,\ -z\right]$	[204]
205	$\left[\frac{1}{2} - x,\ z + \frac{1}{4},\ y + \frac{3}{4}\right]$	[205]
206	$\left[\frac{1}{2} - x,\ \frac{1}{2} - z,\ -y\right]$	[206]
207	$\left[z + \frac{1}{4},\ \frac{1}{2} - y,\ x + \frac{3}{4}\right]$	[207]
208	$\left[\frac{1}{2} - z,\ \frac{1}{2} - y,\ -x\right]$	[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	$\left[\frac{1}{4} - x,\ z + \frac{1}{2},\ \frac{3}{4} - y\right]$	[218]
219	$\left[\frac{1}{4} - x,\ \frac{1}{4} - z,\ y\right]$	[219]
220	$\left[\frac{1}{4} - z,\ \frac{1}{4} - y,\ x\right]$	[220]
221	$\left[z + \frac{1}{2},\ \frac{1}{4} - y,\ \frac{3}{4} - x\right]$	[221]
222	$\left[y + \frac{1}{2},\ \frac{1}{4} - x,\ \frac{3}{4} - z\right]$	[222]
223	$\left[\frac{1}{4} - y,\ x + \frac{1}{2},\ \frac{3}{4} - z\right]$	[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	$\left[\frac{1}{4} - y,\ \frac{1}{4} - x,\ z\right]$	[227]
228	$\left[y + \frac{1}{2},\ x + \frac{1}{2},\ z\right]$	[228]
229	$\left[x + \frac{1}{2},\ \frac{1}{4} - z,\ \frac{3}{4} - y\right]$	[229]
230	$\left[x + \frac{1}{2},\ z + \frac{1}{2},\ y\right]$	[230]
231	$\left[\frac{1}{4} - z,\ y + \frac{1}{2},\ \frac{3}{4} - x\right]$	[231]
232	$\left[z + \frac{1}{2},\ y + \frac{1}{2},\ x\right]$	[232]

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	$\left[x + \frac{1}{4},\, -z,\, y + \frac{1}{4}\right]$	[242]
243	$\left[x + \frac{1}{4},\, z + \frac{3}{4},\, \frac{1}{2} - y\right]$	[243]
244	$\left[z + \frac{1}{4},\, y + \frac{3}{4},\, \frac{1}{2} - x\right]$	[244]
245	$\left[\frac{1}{2} - z,\, y + \frac{3}{4},\, x + \frac{1}{4}\right]$	[245]
246	$\left[\frac{1}{2} - y,\, x + \frac{3}{4},\, z + \frac{1}{4}\right]$	[246]
247	$\left[y + \frac{1}{4},\, -x,\, z + \frac{1}{4}\right]$	[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	$\left[y + \frac{1}{4},\, x + \frac{3}{4},\, \frac{1}{2} - z\right]$	[251]
252	$\left[\frac{1}{2} - y,\, -x,\, \frac{1}{2} - z\right]$	[252]
253	$\left[\frac{1}{2} - x,\, z + \frac{3}{4},\, y + \frac{1}{4}\right]$	[253]
254	$\left[\frac{1}{2} - x,\, -z,\, \frac{1}{2} - y\right]$	[254]
255	$\left[z + \frac{1}{4},\, -y,\, x + \frac{1}{4}\right]$	[255]
256	$\left[\frac{1}{2} - z,\, -y,\, \frac{1}{2} - x\right]$	[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	$\left[\frac{1}{4} - x,\, z,\, \frac{1}{4} - y\right]$	[266]
267	$\left[\frac{1}{4} - x,\, \frac{3}{4} - z,\, y + \frac{1}{2}\right]$	[267]
268	$\left[\frac{1}{4} - z,\, \frac{3}{4} - y,\, x + \frac{1}{2}\right]$	[268]
269	$\left[z + \frac{1}{2},\, \frac{3}{4} - y,\, \frac{1}{4} - x\right]$	[269]
270	$\left[y + \frac{1}{2},\, \frac{3}{4} - x,\, \frac{1}{4} - z\right]$	[270]
271	$\left[\frac{1}{4} - y,\, x,\, \frac{1}{4} - z\right]$	[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	$\left[\frac{1}{4} - y,\, \frac{3}{4} - x,\, z + \frac{1}{2}\right]$	[275]
276	$\left[y + \frac{1}{2},\, x,\, z + \frac{1}{2}\right]$	[276]
277	$\left[x + \frac{1}{2},\, \frac{3}{4} - z,\, \frac{1}{4} - y\right]$	[277]
278	$\left[x + \frac{1}{2},\, z,\, y + \frac{1}{2}\right]$	[278]
279	$\left[\frac{1}{4} - z,\, y,\, \frac{1}{4} - x\right]$	[279]

continued ...

Table 12

No.	position	mapping
280	$\left[z + \frac{1}{2}, y, x + \frac{1}{2}\right]$	[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	$\left[x + \frac{3}{4}, \frac{1}{2} - z, y + \frac{1}{4}\right]$	[290]
291	$\left[x + \frac{3}{4}, z + \frac{1}{4}, \frac{1}{2} - y\right]$	[291]
292	$\left[z + \frac{3}{4}, y + \frac{1}{4}, \frac{1}{2} - x\right]$	[292]
293	$\left[-z, y + \frac{1}{4}, x + \frac{1}{4}\right]$	[293]
294	$\left[-y, x + \frac{1}{4}, z + \frac{1}{4}\right]$	[294]
295	$\left[y + \frac{3}{4}, \frac{1}{2} - x, z + \frac{1}{4}\right]$	[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	$\left[y + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{2} - z\right]$	[299]
300	$\left[-y, \frac{1}{2} - x, \frac{1}{2} - z\right]$	[300]
301	$\left[-x, z + \frac{1}{4}, y + \frac{1}{4}\right]$	[301]
302	$\left[-x, \frac{1}{2} - z, \frac{1}{2} - y\right]$	[302]
303	$\left[z + \frac{3}{4}, \frac{1}{2} - y, x + \frac{1}{4}\right]$	[303]
304	$\left[-z, \frac{1}{2} - y, \frac{1}{2} - x\right]$	[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	$\left[\frac{3}{4} - x, z + \frac{1}{2}, \frac{1}{4} - y\right]$	[314]
315	$\left[\frac{3}{4} - x, \frac{1}{4} - z, y + \frac{1}{2}\right]$	[315]
316	$\left[\frac{3}{4} - z, \frac{1}{4} - y, x + \frac{1}{2}\right]$	[316]
317	$\left[z, \frac{1}{4} - y, \frac{1}{4} - x\right]$	[317]
318	$\left[y, \frac{1}{4} - x, \frac{1}{4} - z\right]$	[318]
319	$\left[\frac{3}{4} - y, x + \frac{1}{2}, \frac{1}{4} - z\right]$	[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	$\left[\frac{3}{4} - y, \frac{1}{4} - x, z + \frac{1}{2}\right]$	[323]
324	$\left[y, x + \frac{1}{2}, z + \frac{1}{2}\right]$	[324]
325	$\left[x, \frac{1}{4} - z, \frac{1}{4} - y\right]$	[325]
326	$\left[x, z + \frac{1}{2}, y + \frac{1}{2}\right]$	[326]

continued …

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Table 12

No.	position	mapping
327	$\left[\frac{3}{4} - z, y + \frac{1}{2}, \frac{1}{4} - x\right]$	[327]
328	$\left[z, y + \frac{1}{2}, x + \frac{1}{2}\right]$	[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	$\left[x + \frac{3}{4}, -z, y + \frac{3}{4}\right]$	[338]
339	$\left[x + \frac{3}{4}, z + \frac{3}{4}, -y\right]$	[339]
340	$\left[z + \frac{3}{4}, y + \frac{3}{4}, -x\right]$	[340]
341	$\left[-z, y + \frac{3}{4}, x + \frac{3}{4}\right]$	[341]
342	$\left[-y, x + \frac{3}{4}, z + \frac{3}{4}\right]$	[342]
343	$\left[y + \frac{3}{4}, -x, z + \frac{3}{4}\right]$	[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	$\left[y + \frac{3}{4}, x + \frac{3}{4}, -z\right]$	[347]
348	$\left[-y, -x, -z\right]$	[348]
349	$\left[-x, z + \frac{3}{4}, y + \frac{3}{4}\right]$	[349]
350	$\left[-x, -z, -y\right]$	[350]
351	$\left[z + \frac{3}{4}, -y, x + \frac{3}{4}\right]$	[351]
352	$\left[-z, -y, -x\right]$	[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	$\left[\frac{3}{4} - x, z, \frac{3}{4} - y\right]$	[362]
363	$\left[\frac{3}{4} - x, \frac{3}{4} - z, y\right]$	[363]
364	$\left[\frac{3}{4} - z, \frac{3}{4} - y, x\right]$	[364]
365	$\left[z, \frac{3}{4} - y, \frac{3}{4} - x\right]$	[365]
366	$\left[y, \frac{3}{4} - x, \frac{3}{4} - z\right]$	[366]
367	$\left[\frac{3}{4} - y, x, \frac{3}{4} - z\right]$	[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	$\left[\frac{3}{4} - y, \frac{3}{4} - x, z\right]$	[371]
372	$\left[y, x, z\right]$	[372]
373	$\left[x, \frac{3}{4} - z, \frac{3}{4} - y\right]$	[373]

continued ...

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Table 12

No.	position	mapping
374	$[x,\, z,\, y]$	[374]
375	$\left[\frac{3}{4} - z,\, y,\, \frac{3}{4} - x\right]$	[375]
376	$[z,\, y,\, x]$	[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]