MSG No. 228.135 $Fd\bar{3}c1'$ [Type II, cubic]

Table 1: Wyckoff site: 16a, site symmetry: 23.1'

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

Table 2: Wyckoff site: 32b, site symmetry: .321'

No.	position	mapping
1	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[1,12,14,16,17,18,193,204,206,208,209,210]
2	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{2}\right]$	[2,7,15,105,115,120,194,199,207,297,307,312]
3	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[3,4,11,154,164,165,195,196,203,346,356,357]
4	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}\right]$	[5,6,13,56,70,71,197,198,205,248,262,263]
5	$\left[\frac{1}{4}, 0, 0\right]$	[8,22,23,53,54,61,200,214,215,245,246,253]
6	$\left[0, \frac{1}{4}, 0\right]$	[9,19,24,98,103,111,201,211,216,290,295,303]
7	$\left[0, 0, \frac{1}{4}\right]$	[10,20,21,147,148,155,202,212,213,339,340,347]
8	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[25,36,38,40,41,42,217,228,230,232,233,234]
9	$\left[0, \frac{3}{4}, 0\right]$	[26,31,39,129,139,144,218,223,231,321,331,336]
10	$\left[0, 0, \frac{3}{4}\right]$	[27,28,35,178,188,189,219,220,227,370,380,381]
11	$\left[\frac{3}{4}, 0, 0\right]$	[29,30,37,80,94,95,221,222,229,272,286,287]
12	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}\right]$	[32,46,47,77,78,85,224,238,239,269,270,277]
13	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{2}\right]$	[33,43,48,122,127,135,225,235,240,314,319,327]
14	$\left[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	[34,44,45,171,172,179,226,236,237,363,364,371]
15	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[49,60,62,64,65,66,241,252,254,256,257,258]
16	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	[50,55,63,153,163,168,242,247,255,345,355,360]
17	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[51,52,59,106,116,117,243,244,251,298,308,309]
18	$\left[0, \frac{3}{4}, \frac{1}{2}\right]$	[57,67,72,146,151,159,249,259,264,338,343,351]
19	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[58,68,69,99,100,107,250,260,261,291,292,299]
20	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[73,84,86,88,89,90,265,276,278,280,281,282]
21	$\left[0, \frac{1}{4}, \frac{1}{2}\right]$	[74,79,87,177,187,192,266,271,279,369,379,384]

continued ...

Table 2

No.	position	mapping
22	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[75,76,83,130,140,141,267,268,275,322,332,333]
23	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[81,91,96,170,175,183,273,283,288,362,367,375]
24	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[82,92,93,123,124,131,274,284,285,315,316,323]
25	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[97,108,110,112,113,114,289,300,302,304,305,306]
26	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	[101,102,109,152,166,167,293,294,301,344,358,359]
27	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	[104,118,119,149,150,157,296,310,311,341,342,349]
28	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[121,132,134,136,137,138,313,324,326,328,329,330]
29	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[125,126,133,176,190,191,317,318,325,368,382,383]
30	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	[128,142,143,173,174,181,320,334,335,365,366,373]
31	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[145,156,158,160,161,162,337,348,350,352,353,354]
32	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[169,180,182,184,185,186,361,372,374,376,377,378]

Table 3: Wyckoff site: 32c, site symmetry: .-3'.1'

No.	position	mapping
1	[0, 0, 0]	[1,17,18,25,41,42,193,209,210,217,233,234]
2	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[2,7,15,26,31,39,194,199,207,218,223,231]
3	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[3,4,11,27,28,35,195,196,203,219,220,227]
4	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[5,6,13,29,30,37,197,198,205,221,222,229]
5	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	[8,22,23,32,46,47,200,214,215,224,238,239]
6	$\left[\frac{1}{4}, 0, \frac{1}{4}\right]$	[9,19,24,33,43,48,201,211,216,225,235,240]
7	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	[10,20,21,34,44,45,202,212,213,226,236,237]
8	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[12,14,16,36,38,40,204,206,208,228,230,232]
9	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[49,65,66,73,89,90,241,257,258,265,281,282]
10	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	[50,55,63,74,79,87,242,247,255,266,271,279]
11	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[51,52,59,75,76,83,243,244,251,267,268,275]
12	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[53,54,61,77,78,85,245,246,253,269,270,277]
13	$\left[0, \frac{3}{4}, \frac{3}{4}\right]$	[56,70,71,80,94,95,248,262,263,272,286,287]
14	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[57,67,72,81,91,96,249,259,264,273,283,288]
15	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[58,68,69,82,92,93,250,260,261,274,284,285]
16	$\left[\frac{1}{2}, 0, 0\right]$	[60,62,64,84,86,88,252,254,256,276,278,280]
17	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[97,113,114,121,137,138,289,305,306,313,329,330]
18	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[98,103,111,122,127,135,290,295,303,314,319,327]
19	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[99,100,107,123,124,131,291,292,299,315,316,323]
20	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	[101,102,109,125,126,133,293,294,301,317,318,325]
21	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[104,118,119,128,142,143,296,310,311,320,334,335]
22	$\left[\frac{3}{4}, 0, \frac{3}{4}\right]$	[105,115,120,129,139,144,297,307,312,321,331,336]
23	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[106,116,117,130,140,141,298,308,309,322,332,333]
24	$\left[0, \frac{1}{2}, 0\right]$	[108,110,112,132,134,136,300,302,304,324,326,328]
25	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[145,161,162,169,185,186,337,353,354,361,377,378]
26	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	[146,151,159,170,175,183,338,343,351,362,367,375]
27	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[147,148,155,171,172,179,339,340,347,363,364,371]
28	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	[149,150,157,173,174,181,341,342,349,365,366,373]
29	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[152,166,167,176,190,191,344,358,359,368,382,383]

continued ...

Table 3

No.	position	mapping
30	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[153,163,168,177,187,192,345,355,360,369,379,384]
31	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	[154,164,165,178,188,189,346,356,357,370,380,381]
32	$\left[0, 0, \frac{1}{2}\right]$	[156,158,160,180,182,184,348,350,352,372,374,376]

Table 4: Wyckoff site: 48d, site symmetry: -4..1'

No.	position	mapping
1	$\left[\frac{7}{8}, \frac{1}{8}, \frac{1}{8}\right]$	[1,8,123,170,193,200,315,362]
2	$\left[\frac{1}{8}, \frac{3}{8}, \frac{3}{8}\right]$	[2,3,32,73,194,195,224,265]
3	$\left[\frac{3}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[4,16,91,143,196,208,283,335]
4	$\left[\frac{3}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[5,15,45,186,197,207,237,378]
5	$\left[\frac{3}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[6,11,48,137,198,203,240,329]
6	$\left[\frac{3}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[7,12,92,190,199,204,284,382]
7	$\left[\frac{3}{8}, \frac{1}{8}, \frac{1}{8}\right]$	[9,10,37,86,201,202,229,278]
8	$\left[\frac{5}{8}, \frac{3}{8}, \frac{3}{8}\right]$	[13,14,130,177,205,206,322,369]
9	$\left[\frac{1}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[17,24,83,174,209,216,275,366]
10	$\left[\frac{1}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[18,21,87,125,210,213,279,317]
11	$\left[\frac{1}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[19,23,28,184,211,215,220,376]
12	$\left[\frac{1}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[20,22,31,132,212,214,223,324]
13	$\left[\frac{1}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[25,50,51,80,217,242,243,272]
14	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[26,75,145,152,218,267,337,344]
15	$\left[\frac{3}{8}, \frac{1}{8}, \frac{5}{8}\right]$	[27,74,97,104,219,266,289,296]
16	$\left[\frac{5}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[29,114,117,183,221,306,309,375]
17	$\left[\frac{5}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[30,131,161,168,222,323,353,360]
18	$\left[\frac{1}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[33,82,157,158,225,274,349,350]
19	$\left[\frac{1}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[34,81,109,110,226,273,301,302]
20	$\left[\frac{1}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[35,65,72,126,227,257,264,318]
21	$\left[\frac{5}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[36,116,118,127,228,308,310,319]
22	$\left[\frac{3}{8}, \frac{5}{8}, \frac{5}{8}\right]$	[38,57,58,85,230,249,250,277]
23	$\left[\frac{1}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[39,66,69,173,231,258,261,365]
24	$\left[\frac{5}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[40,163,167,172,232,355,359,364]
25	$\left[\frac{7}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[41,102,107,144,233,294,299,336]
26	$\left[\frac{7}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[42,149,159,189,234,341,351,381]
27	$\left[\frac{3}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[43,52,64,191,235,244,256,383]
28	$\left[\frac{3}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[44,55,60,142,236,247,252,334]
29	$\left[\frac{7}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[46,140,151,156,238,332,343,348]
30	$\left[\frac{7}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[47,100,112,187,239,292,304,379]
31	$\left[\frac{7}{8}, \frac{5}{8}, \frac{5}{8}\right]$	[49,56,122,171,241,248,314,363]
32	$\left[\frac{3}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[53,63,93,138,245,255,285,330]
33	$\left[\frac{3}{8}, \frac{5}{8}, \frac{7}{8}\right]$	[54,59,96,185,246,251,288,377]
34	$\left[\frac{5}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[61,62,129,178,253,254,321,370]
35	$\left[\frac{1}{8}, \frac{5}{8}, \frac{7}{8}\right]$	[67,71,76,136,259,263,268,328]
36	$\left[\frac{1}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[68,70,79,180,260,262,271,372]
37	$\left[\frac{5}{8}, \frac{5}{8}, \frac{7}{8}\right]$	[77,135,162,165,269,327,354,357]

continued ...

Table 4

No.	position	mapping
38	$\left[\frac{5}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[78,113,120,179,270,305,312,371]
39	$\left[\frac{5}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[84,164,166,175,276,356,358,367]
40	$\left[\frac{5}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[88,115,119,124,280,307,311,316]
41	$\left[\frac{7}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[89,150,155,192,281,342,347,384]
42	$\left[\frac{7}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[90,101,111,141,282,293,303,333]
43	$\left[\frac{7}{8}, \frac{5}{8}, \frac{7}{8}\right]$	[94,103,108,188,286,295,300,380]
44	$\left[\frac{7}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[95,139,148,160,287,331,340,352]
45	$\left[\frac{5}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[98,99,128,169,290,291,320,361]
46	$\left[\frac{7}{8}, \frac{1}{8}, \frac{5}{8}\right]$	[105,106,133,182,297,298,325,374]
47	$\left[\frac{5}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[121,146,147,176,313,338,339,368]
48	$\left[\frac{7}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[134,153,154,181,326,345,346,373]

Table 5: Wyckoff site: 64e, site symmetry: .3.1'

No.	position	mapping
1	$[x, x, x]$	[1,17,18,193,209,210]
2	$\left[x+\frac{1}{4}, \frac{1}{2}-x, x+\frac{1}{4}\right]$	[2,7,15,194,199,207]
3	$\left[x+\frac{1}{4}, x+\frac{1}{4}, \frac{1}{2}-x\right]$	[3,4,11,195,196,203]
4	$\left[\frac{1}{2}-x, x+\frac{1}{4}, x+\frac{1}{4}\right]$	[5,6,13,197,198,205]
5	$\left[x, \frac{1}{4}-x, \frac{1}{4}-x\right]$	[8,22,23,200,214,215]
6	$\left[\frac{1}{4}-x, x, \frac{1}{4}-x\right]$	[9,19,24,201,211,216]
7	$\left[\frac{1}{4}-x, \frac{1}{4}-x, x\right]$	[10,20,21,202,212,213]
8	$\left[\frac{1}{2}-x, \frac{1}{2}-x, \frac{1}{2}-x\right]$	[12,14,16,204,206,208]
9	$[-x, -x, -x]$	[25,41,42,217,233,234]
10	$\left[\frac{1}{4}-x, x+\frac{1}{2}, \frac{1}{4}-x\right]$	[26,31,39,218,223,231]
11	$\left[\frac{1}{4}-x, \frac{1}{4}-x, x+\frac{1}{2}\right]$	[27,28,35,219,220,227]
12	$\left[x+\frac{1}{2}, \frac{1}{4}-x, \frac{1}{4}-x\right]$	[29,30,37,221,222,229]
13	$\left[-x, x+\frac{1}{4}, x+\frac{1}{4}\right]$	[32,46,47,224,238,239]
14	$\left[x+\frac{1}{4}, -x, x+\frac{1}{4}\right]$	[33,43,48,225,235,240]
15	$\left[x+\frac{1}{4}, x+\frac{1}{4}, -x\right]$	[34,44,45,226,236,237]
16	$\left[x+\frac{1}{2}, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[36,38,40,228,230,232]
17	$\left[x, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[49,65,66,241,257,258]
18	$\left[x+\frac{1}{4}, -x, x+\frac{3}{4}\right]$	[50,55,63,242,247,255]
19	$\left[x+\frac{1}{4}, x+\frac{3}{4}, -x\right]$	[51,52,59,243,244,251]
20	$\left[\frac{1}{2}-x, x+\frac{3}{4}, x+\frac{3}{4}\right]$	[53,54,61,245,246,253]
21	$\left[x, \frac{3}{4}-x, \frac{3}{4}-x\right]$	[56,70,71,248,262,263]
22	$\left[\frac{1}{4}-x, x+\frac{1}{2}, \frac{3}{4}-x\right]$	[57,67,72,249,259,264]
23	$\left[\frac{1}{4}-x, \frac{3}{4}-x, x+\frac{1}{2}\right]$	[58,68,69,250,260,261]
24	$\left[\frac{1}{2}-x, -x, -x\right]$	[60,62,64,252,254,256]
25	$\left[-x, \frac{1}{2}-x, \frac{1}{2}-x\right]$	[73,89,90,265,281,282]
26	$\left[\frac{1}{4}-x, x, \frac{3}{4}-x\right]$	[74,79,87,266,271,279]
27	$\left[\frac{1}{4}-x, \frac{3}{4}-x, x\right]$	[75,76,83,267,268,275]
28	$\left[x+\frac{1}{2}, \frac{3}{4}-x, \frac{3}{4}-x\right]$	[77,78,85,269,270,277]
29	$\left[-x, x+\frac{3}{4}, x+\frac{3}{4}\right]$	[80,94,95,272,286,287]

continued ...

Table 5

No.	position	mapping
30	$\left[x+\frac{1}{4},\ \frac{1}{2}-x,\ x+\frac{3}{4}\right]$	[81,91,96,273,283,288]
31	$\left[x+\frac{1}{4},\ x+\frac{3}{4},\ \frac{1}{2}-x\right]$	[82,92,93,274,284,285]
32	$\left[x+\frac{1}{2},\ x,\ x\right]$	[84,86,88,276,278,280]
33	$\left[x+\frac{1}{2},\ x,\ x+\frac{1}{2}\right]$	[97,113,114,289,305,306]
34	$\left[x+\frac{3}{4},\ \frac{1}{2}-x,\ x+\frac{3}{4}\right]$	[98,103,111,290,295,303]
35	$\left[x+\frac{3}{4},\ x+\frac{1}{4},\ -x\right]$	[99,100,107,291,292,299]
36	$\left[-x,\ x+\frac{1}{4},\ x+\frac{3}{4}\right]$	[101,102,109,293,294,301]
37	$\left[x+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{3}{4}-x\right]$	[104,118,119,296,310,311]
38	$\left[\frac{3}{4}-x,\ x,\ \frac{3}{4}-x\right]$	[105,115,120,297,307,312]
39	$\left[\frac{3}{4}-x,\ \frac{1}{4}-x,\ x+\frac{1}{2}\right]$	[106,116,117,298,308,309]
40	$\left[-x,\ \frac{1}{2}-x,\ -x\right]$	[108,110,112,300,302,304]
41	$\left[\frac{1}{2}-x,\ -x,\ \frac{1}{2}-x\right]$	[121,137,138,313,329,330]
42	$\left[\frac{3}{4}-x,\ x+\frac{1}{2},\ \frac{3}{4}-x\right]$	[122,127,135,314,319,327]
43	$\left[\frac{3}{4}-x,\ \frac{1}{4}-x,\ x\right]$	[123,124,131,315,316,323]
44	$\left[x,\ \frac{1}{4}-x,\ \frac{3}{4}-x\right]$	[125,126,133,317,318,325]
45	$\left[\frac{1}{2}-x,\ x+\frac{1}{4},\ x+\frac{3}{4}\right]$	[128,142,143,320,334,335]
46	$\left[x+\frac{3}{4},\ -x,\ x+\frac{3}{4}\right]$	[129,139,144,321,331,336]
47	$\left[x+\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{2}-x\right]$	[130,140,141,322,332,333]
48	$\left[x,\ x+\frac{1}{2},\ x\right]$	[132,134,136,324,326,328]
49	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ x\right]$	[145,161,162,337,353,354]
50	$\left[x+\frac{3}{4},\ -x,\ x+\frac{1}{4}\right]$	[146,151,159,338,343,351]
51	$\left[x+\frac{3}{4},\ x+\frac{3}{4},\ \frac{1}{2}-x\right]$	[147,148,155,339,340,347]
52	$\left[-x,\ x+\frac{3}{4},\ x+\frac{1}{4}\right]$	[149,150,157,341,342,349]
53	$\left[x+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{1}{4}-x\right]$	[152,166,167,344,358,359]
54	$\left[\frac{3}{4}-x,\ x+\frac{1}{2},\ \frac{1}{4}-x\right]$	[153,163,168,345,355,360]
55	$\left[\frac{3}{4}-x,\ \frac{3}{4}-x,\ x\right]$	[154,164,165,346,356,357]
56	$\left[-x,\ -x,\ \frac{1}{2}-x\right]$	[156,158,160,348,350,352]
57	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ -x\right]$	[169,185,186,361,377,378]
58	$\left[\frac{3}{4}-x,\ x,\ \frac{1}{4}-x\right]$	[170,175,183,362,367,375]
59	$\left[\frac{3}{4}-x,\ \frac{3}{4}-x,\ x+\frac{1}{2}\right]$	[171,172,179,363,364,371]
60	$\left[x,\ \frac{3}{4}-x,\ \frac{1}{4}-x\right]$	[173,174,181,365,366,373]
61	$\left[\frac{1}{2}-x,\ x+\frac{3}{4},\ x+\frac{1}{4}\right]$	[176,190,191,368,382,383]
62	$\left[x+\frac{3}{4},\ \frac{1}{2}-x,\ x+\frac{1}{4}\right]$	[177,187,192,369,379,384]
63	$\left[x+\frac{3}{4},\ x+\frac{3}{4},\ -x\right]$	[178,188,189,370,380,381]
64	$\left[x,\ x,\ x+\frac{1}{2}\right]$	[180,182,184,372,374,376]

Table 6: Wyckoff site: `96f`, site symmetry: `2..1'`

No.	position	mapping
1	$\left[x,\ \frac{1}{8},\ \frac{1}{8}\right]$	[1,8,193,200]
2	$\left[x+\frac{1}{4},\ \frac{3}{8},\ \frac{3}{8}\right]$	[2,3,194,195]
3	$\left[\frac{3}{8},\ \frac{3}{8},\ \frac{1}{2}-x\right]$	[4,16,196,208]
4	$\left[\frac{3}{8},\ \frac{3}{8},\ x+\frac{1}{4}\right]$	[5,15,197,207]
5	$\left[\frac{3}{8},\ x+\frac{1}{4},\ \frac{3}{8}\right]$	[6,11,198,203]

continued ...

Table 6

No.	position	mapping
6	$\left[\frac{3}{8}, \frac{1}{2} - x, \frac{3}{8}\right]$	[7,12,199,204]
7	$\left[\frac{1}{4} - x, \frac{1}{8}, \frac{1}{8}\right]$	[9,10,201,202]
8	$\left[\frac{1}{2} - x, \frac{3}{8}, \frac{3}{8}\right]$	[13,14,205,206]
9	$\left[\frac{1}{8}, x, \frac{1}{8}\right]$	[17,24,209,216]
10	$\left[\frac{1}{8}, \frac{1}{8}, x\right]$	[18,21,210,213]
11	$\left[\frac{1}{8}, \frac{1}{8}, \frac{1}{4} - x\right]$	[19,23,211,215]
12	$\left[\frac{1}{8}, \frac{1}{4} - x, \frac{1}{8}\right]$	[20,22,212,214]
13	$\left[-x, \frac{7}{8}, \frac{7}{8}\right]$	[25,80,217,272]
14	$\left[\frac{1}{4} - x, \frac{5}{8}, \frac{1}{8}\right]$	[26,75,218,267]
15	$\left[\frac{1}{4} - x, \frac{1}{8}, \frac{5}{8}\right]$	[27,74,219,266]
16	$\left[\frac{1}{8}, \frac{1}{8}, x + \frac{1}{2}\right]$	[28,184,220,376]
17	$\left[\frac{5}{8}, \frac{1}{8}, \frac{1}{4} - x\right]$	[29,183,221,375]
18	$\left[\frac{5}{8}, \frac{1}{4} - x, \frac{1}{8}\right]$	[30,131,222,323]
19	$\left[\frac{1}{8}, x + \frac{1}{2}, \frac{1}{8}\right]$	[31,132,223,324]
20	$\left[-x, \frac{3}{8}, \frac{3}{8}\right]$	[32,73,224,265]
21	$\left[x + \frac{1}{4}, \frac{7}{8}, \frac{3}{8}\right]$	[33,82,225,274]
22	$\left[x + \frac{1}{4}, \frac{3}{8}, \frac{7}{8}\right]$	[34,81,226,273]
23	$\left[\frac{1}{8}, \frac{1}{4} - x, \frac{5}{8}\right]$	[35,126,227,318]
24	$\left[\frac{5}{8}, x + \frac{1}{2}, \frac{5}{8}\right]$	[36,127,228,319]
25	$\left[x + \frac{1}{2}, \frac{1}{8}, \frac{1}{8}\right]$	[37,86,229,278]
26	$\left[x + \frac{1}{2}, \frac{5}{8}, \frac{5}{8}\right]$	[38,85,230,277]
27	$\left[\frac{1}{8}, \frac{5}{8}, \frac{1}{4} - x\right]$	[39,173,231,365]
28	$\left[\frac{5}{8}, \frac{5}{8}, x + \frac{1}{2}\right]$	[40,172,232,364]
29	$\left[\frac{7}{8}, -x, \frac{7}{8}\right]$	[41,144,233,336]
30	$\left[\frac{7}{8}, \frac{7}{8}, -x\right]$	[42,189,234,381]
31	$\left[\frac{3}{8}, \frac{7}{8}, x + \frac{1}{4}\right]$	[43,191,235,383]
32	$\left[\frac{3}{8}, x + \frac{1}{4}, \frac{7}{8}\right]$	[44,142,236,334]
33	$\left[\frac{3}{8}, \frac{3}{8}, -x\right]$	[45,186,237,378]
34	$\left[\frac{7}{8}, x + \frac{1}{4}, \frac{3}{8}\right]$	[46,140,238,332]
35	$\left[\frac{7}{8}, \frac{3}{8}, x + \frac{1}{4}\right]$	[47,187,239,379]
36	$\left[\frac{3}{8}, -x, \frac{3}{8}\right]$	[48,137,240,329]
37	$\left[x, \frac{5}{8}, \frac{5}{8}\right]$	[49,56,241,248]
38	$\left[x + \frac{1}{4}, \frac{7}{8}, \frac{7}{8}\right]$	[50,51,242,243]
39	$\left[\frac{3}{8}, \frac{7}{8}, -x\right]$	[52,64,244,256]
40	$\left[\frac{3}{8}, \frac{7}{8}, x + \frac{3}{4}\right]$	[53,63,245,255]
41	$\left[\frac{3}{8}, x + \frac{3}{4}, \frac{7}{8}\right]$	[54,59,246,251]
42	$\left[\frac{3}{8}, -x, \frac{7}{8}\right]$	[55,60,247,252]
43	$\left[\frac{1}{4} - x, \frac{5}{8}, \frac{5}{8}\right]$	[57,58,249,250]
44	$\left[\frac{1}{2} - x, \frac{7}{8}, \frac{7}{8}\right]$	[61,62,253,254]
45	$\left[\frac{1}{8}, x + \frac{1}{2}, \frac{5}{8}\right]$	[65,72,257,264]
46	$\left[\frac{1}{8}, \frac{5}{8}, x + \frac{1}{2}\right]$	[66,69,258,261]
47	$\left[\frac{1}{8}, \frac{5}{8}, \frac{3}{4} - x\right]$	[67,71,259,263]
48	$\left[\frac{1}{8}, \frac{3}{4} - x, \frac{5}{8}\right]$	[68,70,260,262]
49	$\left[\frac{1}{8}, \frac{5}{8}, x\right]$	[76,136,268,328]
50	$\left[\frac{5}{8}, \frac{5}{8}, \frac{3}{4} - x\right]$	[77,135,269,327]
51	$\left[\frac{5}{8}, \frac{3}{4} - x, \frac{5}{8}\right]$	[78,179,270,371]
52	$\left[\frac{1}{8}, x, \frac{5}{8}\right]$	[79,180,271,372]

continued ...

Table 6

No.	position	mapping
53	$\left[\frac{1}{8}, \frac{3}{4}-x, \frac{1}{8}\right]$	[83,174,275,366]
54	$\left[\frac{5}{8}, x, \frac{1}{8}\right]$	[84,175,276,367]
55	$\left[\frac{1}{8}, \frac{1}{8}, \frac{3}{4}-x\right]$	[87,125,279,317]
56	$\left[\frac{5}{8}, \frac{1}{8}, x\right]$	[88,124,280,316]
57	$\left[\frac{7}{8}, \frac{1}{2}-x, \frac{3}{8}\right]$	[89,192,281,384]
58	$\left[\frac{7}{8}, \frac{3}{8}, \frac{1}{2}-x\right]$	[90,141,282,333]
59	$\left[\frac{3}{8}, \frac{3}{8}, x+\frac{3}{4}\right]$	[91,143,283,335]
60	$\left[\frac{3}{8}, x+\frac{3}{4}, \frac{3}{8}\right]$	[92,190,284,382]
61	$\left[\frac{3}{8}, \frac{7}{8}, \frac{1}{2}-x\right]$	[93,138,285,330]
62	$\left[\frac{7}{8}, x+\frac{3}{4}, \frac{7}{8}\right]$	[94,188,286,380]
63	$\left[\frac{7}{8}, \frac{7}{8}, x+\frac{3}{4}\right]$	[95,139,287,331]
64	$\left[\frac{3}{8}, \frac{1}{2}-x, \frac{7}{8}\right]$	[96,185,288,377]
65	$\left[x+\frac{1}{2}, \frac{1}{8}, \frac{5}{8}\right]$	[97,104,289,296]
66	$\left[x+\frac{3}{4}, \frac{3}{8}, \frac{7}{8}\right]$	[98,99,290,291]
67	$\left[\frac{7}{8}, \frac{3}{8}, -x\right]$	[100,112,292,304]
68	$\left[\frac{7}{8}, \frac{3}{8}, x+\frac{3}{4}\right]$	[101,111,293,303]
69	$\left[\frac{7}{8}, x+\frac{1}{4}, \frac{7}{8}\right]$	[102,107,294,299]
70	$\left[\frac{7}{8}, \frac{1}{2}-x, \frac{7}{8}\right]$	[103,108,295,300]
71	$\left[\frac{3}{4}-x, \frac{1}{8}, \frac{5}{8}\right]$	[105,106,297,298]
72	$\left[-x, \frac{3}{8}, \frac{7}{8}\right]$	[109,110,301,302]
73	$\left[\frac{5}{8}, x, \frac{5}{8}\right]$	[113,120,305,312]
74	$\left[\frac{5}{8}, \frac{1}{8}, x+\frac{1}{2}\right]$	[114,117,306,309]
75	$\left[\frac{5}{8}, \frac{1}{8}, \frac{3}{4}-x\right]$	[115,119,307,311]
76	$\left[\frac{5}{8}, \frac{1}{4}-x, \frac{5}{8}\right]$	[116,118,308,310]
77	$\left[\frac{1}{2}-x, \frac{7}{8}, \frac{3}{8}\right]$	[121,176,313,368]
78	$\left[\frac{3}{4}-x, \frac{5}{8}, \frac{5}{8}\right]$	[122,171,314,363]
79	$\left[\frac{3}{4}-x, \frac{1}{8}, \frac{1}{8}\right]$	[123,170,315,362]
80	$\left[\frac{1}{2}-x, \frac{3}{8}, \frac{7}{8}\right]$	[128,169,320,361]
81	$\left[x+\frac{3}{4}, \frac{7}{8}, \frac{7}{8}\right]$	[129,178,321,370]
82	$\left[x+\frac{3}{4}, \frac{3}{8}, \frac{3}{8}\right]$	[130,177,322,369]
83	$\left[x, \frac{1}{8}, \frac{5}{8}\right]$	[133,182,325,374]
84	$\left[x, \frac{5}{8}, \frac{1}{8}\right]$	[134,181,326,373]
85	$\left[x+\frac{1}{2}, \frac{5}{8}, \frac{1}{8}\right]$	[145,152,337,344]
86	$\left[x+\frac{3}{4}, \frac{7}{8}, \frac{3}{8}\right]$	[146,147,338,339]
87	$\left[\frac{7}{8}, \frac{7}{8}, \frac{1}{2}-x\right]$	[148,160,340,352]
88	$\left[\frac{7}{8}, \frac{7}{8}, x+\frac{1}{4}\right]$	[149,159,341,351]
89	$\left[\frac{7}{8}, x+\frac{3}{4}, \frac{3}{8}\right]$	[150,155,342,347]
90	$\left[\frac{7}{8}, -x, \frac{3}{8}\right]$	[151,156,343,348]
91	$\left[\frac{3}{4}-x, \frac{5}{8}, \frac{1}{8}\right]$	[153,154,345,346]
92	$\left[-x, \frac{7}{8}, \frac{3}{8}\right]$	[157,158,349,350]
93	$\left[\frac{5}{8}, x+\frac{1}{2}, \frac{1}{8}\right]$	[161,168,353,360]
94	$\left[\frac{5}{8}, \frac{5}{8}, x\right]$	[162,165,354,357]
95	$\left[\frac{5}{8}, \frac{5}{8}, \frac{1}{4}-x\right]$	[163,167,355,359]
96	$\left[\frac{5}{8}, \frac{3}{4}-x, \frac{1}{8}\right]$	[164,166,356,358]

Table 7: Wyckoff site: `96g`, site symmetry: `..21'`

No.	position	mapping
1	$\left[\frac{1}{4}, y, -y\right]$	[1,62,193,254]
2	$\left[\frac{1}{2}, y+\frac{1}{2}, y+\frac{1}{4}\right]$	[2,153,194,345]
3	$\left[\frac{1}{2}, \frac{1}{4}-y, \frac{1}{2}-y\right]$	[3,106,195,298]
4	$\left[\frac{1}{4}-y, y+\frac{1}{4}, \frac{1}{4}\right]$	[4,21,196,213]
5	$\left[y+\frac{1}{2}, y+\frac{1}{4}, \frac{1}{2}\right]$	[5,119,197,311]
6	$\left[\frac{1}{2}-y, \frac{1}{2}, \frac{1}{4}-y\right]$	[6,166,198,358]
7	$\left[y+\frac{1}{4}, \frac{1}{4}, \frac{1}{4}-y\right]$	[7,24,199,216]
8	$\left[\frac{1}{4}, \frac{1}{4}-y, y+\frac{1}{4}\right]$	[8,13,200,205]
9	$\left[0, y, y+\frac{1}{4}\right]$	[9,146,201,338]
10	$\left[0, \frac{1}{4}-y, -y\right]$	[10,99,202,291]
11	$\left[y+\frac{1}{4}, \frac{1}{2}, y+\frac{1}{2}\right]$	[11,68,203,260]
12	$\left[\frac{1}{2}-y, \frac{1}{4}, y+\frac{1}{2}\right]$	[12,113,204,305]
13	$\left[\frac{1}{4}, y+\frac{1}{2}, \frac{1}{2}-y\right]$	[14,49,206,241]
14	$\left[\frac{1}{4}-y, \frac{1}{2}-y, \frac{1}{2}\right]$	[15,67,207,259]
15	$\left[y+\frac{1}{2}, \frac{1}{2}-y, \frac{1}{4}\right]$	[16,162,208,354]
16	$\left[-y, \frac{1}{4}, y\right]$	[17,108,209,300]
17	$\left[y, -y, \frac{1}{4}\right]$	[18,160,210,352]
18	$\left[\frac{1}{4}-y, -y, 0\right]$	[19,63,211,255]
19	$\left[y+\frac{1}{4}, 0, y\right]$	[20,59,212,251]
20	$\left[-y, 0, \frac{1}{4}-y\right]$	[22,150,214,342]
21	$\left[y, y+\frac{1}{4}, 0\right]$	[23,101,215,293]
22	$\left[\frac{3}{4}, -y, y\right]$	[25,86,217,278]
23	$\left[0, \frac{1}{2}-y, \frac{1}{4}-y\right]$	[26,177,218,369]
24	$\left[0, y+\frac{1}{4}, y+\frac{1}{2}\right]$	[27,130,219,322]
25	$\left[y+\frac{1}{4}, \frac{1}{4}-y, \frac{3}{4}\right]$	[28,45,220,237]
26	$\left[\frac{1}{2}-y, \frac{1}{4}-y, 0\right]$	[29,143,221,335]
27	$\left[y+\frac{1}{2}, 0, y+\frac{1}{4}\right]$	[30,190,222,382]
28	$\left[\frac{1}{4}-y, \frac{3}{4}, y+\frac{1}{4}\right]$	[31,48,223,240]
29	$\left[\frac{3}{4}, y+\frac{1}{4}, \frac{1}{4}-y\right]$	[32,37,224,229]
30	$\left[\frac{1}{2}, -y, \frac{1}{4}-y\right]$	[33,170,225,362]
31	$\left[\frac{1}{2}, y+\frac{1}{4}, y\right]$	[34,123,226,315]
32	$\left[\frac{1}{4}-y, 0, \frac{1}{2}-y\right]$	[35,92,227,284]
33	$\left[y+\frac{1}{2}, \frac{3}{4}, \frac{1}{2}-y\right]$	[36,137,228,329]
34	$\left[\frac{3}{4}, \frac{1}{2}-y, y+\frac{1}{2}\right]$	[38,73,230,265]
35	$\left[y+\frac{1}{4}, y+\frac{1}{2}, 0\right]$	[39,91,231,283]
36	$\left[\frac{1}{2}-y, y+\frac{1}{2}, \frac{3}{4}\right]$	[40,186,232,378]
37	$\left[y, \frac{3}{4}, -y\right]$	[41,132,233,324]
38	$\left[-y, y, \frac{3}{4}\right]$	[42,184,234,376]
39	$\left[y+\frac{1}{4}, y, \frac{1}{2}\right]$	[43,87,235,279]
40	$\left[\frac{1}{4}-y, \frac{1}{2}, -y\right]$	[44,83,236,275]
41	$\left[y, \frac{1}{2}, y+\frac{1}{4}\right]$	[46,174,238,366]
42	$\left[-y, \frac{1}{4}-y, \frac{1}{2}\right]$	[47,125,239,317]
43	$\left[\frac{1}{2}, y, y+\frac{3}{4}\right]$	[50,105,242,297]
44	$\left[\frac{1}{2}, \frac{3}{4}-y, -y\right]$	[51,154,243,346]
45	$\left[\frac{1}{4}-y, y+\frac{3}{4}, \frac{3}{4}\right]$	[52,69,244,261]
46	$\left[y+\frac{1}{2}, y+\frac{3}{4}, 0\right]$	[53,167,245,359]

continued ...

Table 7

No.	position	mapping
47	$\left[\frac{1}{2}-y,\ 0,\ \frac{3}{4}-y\right]$	[54,118,246,310]
48	$\left[y+\frac{1}{4},\ \frac{3}{4},\ \frac{3}{4}-y\right]$	[55,72,247,264]
49	$\left[\frac{1}{4},\ \frac{3}{4}-y,\ y+\frac{3}{4}\right]$	[56,61,248,253]
50	$\left[0,\ y+\frac{1}{2},\ y+\frac{3}{4}\right]$	[57,98,249,290]
51	$\left[0,\ \frac{3}{4}-y,\ \frac{1}{2}-y\right]$	[58,147,250,339]
52	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ y\right]$	[60,161,252,353]
53	$\left[y+\frac{1}{2},\ -y,\ \frac{3}{4}\right]$	[64,114,256,306]
54	$\left[-y,\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[65,156,257,348]
55	$\left[y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[66,112,258,304]
56	$\left[-y,\ \frac{1}{2},\ \frac{3}{4}-y\right]$	[70,102,262,294]
57	$\left[y,\ y+\frac{3}{4},\ \frac{1}{2}\right]$	[71,149,263,341]
58	$\left[0,\ -y,\ \frac{3}{4}-y\right]$	[74,129,266,321]
59	$\left[0,\ y+\frac{3}{4},\ y\right]$	[75,178,267,370]
60	$\left[y+\frac{1}{4},\ \frac{3}{4}-y,\ \frac{1}{4}\right]$	[76,93,268,285]
61	$\left[\frac{1}{2}-y,\ \frac{3}{4}-y,\ \frac{1}{2}\right]$	[77,191,269,383]
62	$\left[y+\frac{1}{2},\ \frac{1}{2},\ y+\frac{3}{4}\right]$	[78,142,270,334]
63	$\left[\frac{1}{4}-y,\ \frac{1}{4},\ y+\frac{3}{4}\right]$	[79,96,271,288]
64	$\left[\frac{3}{4},\ y+\frac{3}{4},\ \frac{3}{4}-y\right]$	[80,85,272,277]
65	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ \frac{3}{4}-y\right]$	[81,122,273,314]
66	$\left[\frac{1}{2},\ y+\frac{3}{4},\ y+\frac{1}{2}\right]$	[82,171,274,363]
67	$\left[y+\frac{1}{2},\ \frac{1}{4},\ -y\right]$	[84,185,276,377]
68	$\left[\frac{1}{2}-y,\ y,\ \frac{1}{4}\right]$	[88,138,280,330]
69	$\left[y,\ \frac{1}{4},\ \frac{1}{2}-y\right]$	[89,180,281,372]
70	$\left[-y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[90,136,282,328]
71	$\left[y,\ 0,\ y+\frac{3}{4}\right]$	[94,126,286,318]
72	$\left[-y,\ \frac{3}{4}-y,\ 0\right]$	[95,173,287,365]
73	$\left[\frac{3}{4},\ y,\ \frac{1}{2}-y\right]$	[97,158,289,350]
74	$\left[\frac{3}{4}-y,\ y+\frac{1}{4},\ \frac{3}{4}\right]$	[100,117,292,309]
75	$\left[y+\frac{3}{4},\ \frac{1}{4},\ \frac{3}{4}-y\right]$	[103,120,295,312]
76	$\left[\frac{3}{4},\ \frac{1}{4}-y,\ y+\frac{3}{4}\right]$	[104,109,296,301]
77	$\left[y+\frac{3}{4},\ \frac{1}{2},\ y\right]$	[107,164,299,356]
78	$\left[\frac{3}{4},\ y+\frac{1}{2},\ -y\right]$	[110,145,302,337]
79	$\left[\frac{3}{4}-y,\ \frac{1}{2}-y,\ 0\right]$	[111,163,303,355]
80	$\left[\frac{3}{4}-y,\ -y,\ \frac{1}{2}\right]$	[115,159,307,351]
81	$\left[y+\frac{3}{4},\ 0,\ y+\frac{1}{2}\right]$	[116,155,308,347]
82	$\left[\frac{1}{4},\ -y,\ y+\frac{1}{2}\right]$	[121,182,313,374]
83	$\left[y+\frac{3}{4},\ \frac{1}{4}-y,\ \frac{1}{4}\right]$	[124,141,316,333]
84	$\left[\frac{3}{4}-y,\ \frac{3}{4},\ y+\frac{3}{4}\right]$	[127,144,319,336]
85	$\left[\frac{1}{4},\ y+\frac{1}{4},\ \frac{3}{4}-y\right]$	[128,133,320,325]
86	$\left[\frac{3}{4}-y,\ 0,\ -y\right]$	[131,188,323,380]
87	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ y\right]$	[134,169,326,361]
88	$\left[y+\frac{3}{4},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[135,187,327,379]
89	$\left[y+\frac{3}{4},\ y,\ 0\right]$	[139,183,331,375]
90	$\left[\frac{3}{4}-y,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[140,179,332,371]
91	$\left[\frac{3}{4}-y,\ y+\frac{3}{4},\ \frac{1}{4}\right]$	[148,165,340,357]
92	$\left[y+\frac{3}{4},\ \frac{3}{4},\ \frac{1}{4}-y\right]$	[151,168,343,360]
93	$\left[\frac{3}{4},\ \frac{3}{4}-y,\ y+\frac{1}{4}\right]$	[152,157,344,349]

continued ...

Table 7

No.	position	mapping
94	$\left[y+\frac{3}{4},\ \frac{3}{4}-y,\ \frac{3}{4}\right]$	[172,189,364,381]
95	$\left[\frac{3}{4}-y,\ \frac{1}{4},\ y+\frac{1}{4}\right]$	[175,192,367,384]
96	$\left[\frac{1}{4},\ y+\frac{3}{4},\ \frac{1}{4}-y\right]$	[176,181,368,373]

Table 8: Wyckoff site: 192h, site symmetry: 11'

No.	position	mapping
1	$[x,\ y,\ z]$	[1,193]
2	$\left[x+\frac{1}{4},\ \frac{1}{2}-z,\ y+\frac{1}{4}\right]$	[2,194]
3	$\left[x+\frac{1}{4},\ z+\frac{1}{4},\ \frac{1}{2}-y\right]$	[3,195]
4	$\left[z+\frac{1}{4},\ y+\frac{1}{4},\ \frac{1}{2}-x\right]$	[4,196]
5	$\left[\frac{1}{2}-z,\ y+\frac{1}{4},\ x+\frac{1}{4}\right]$	[5,197]
6	$\left[\frac{1}{2}-y,\ x+\frac{1}{4},\ z+\frac{1}{4}\right]$	[6,198]
7	$\left[y+\frac{1}{4},\ \frac{1}{2}-x,\ z+\frac{1}{4}\right]$	[7,199]
8	$\left[x,\ \frac{1}{4}-y,\ \frac{1}{4}-z\right]$	[8,200]
9	$\left[\frac{1}{4}-x,\ y,\ \frac{1}{4}-z\right]$	[9,201]
10	$\left[\frac{1}{4}-x,\ \frac{1}{4}-y,\ z\right]$	[10,202]
11	$\left[y+\frac{1}{4},\ x+\frac{1}{4},\ \frac{1}{2}-z\right]$	[11,203]
12	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[12,204]
13	$\left[\frac{1}{2}-x,\ z+\frac{1}{4},\ y+\frac{1}{4}\right]$	[13,205]
14	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[14,206]
15	$\left[z+\frac{1}{4},\ \frac{1}{2}-y,\ x+\frac{1}{4}\right]$	[15,207]
16	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ \frac{1}{2}-x\right]$	[16,208]
17	$[z,\ x,\ y]$	[17,209]
18	$[y,\ z,\ x]$	[18,210]
19	$\left[\frac{1}{4}-y,\ z,\ \frac{1}{4}-x\right]$	[19,211]
20	$\left[\frac{1}{4}-z,\ \frac{1}{4}-x,\ y\right]$	[20,212]
21	$\left[\frac{1}{4}-y,\ \frac{1}{4}-z,\ x\right]$	[21,213]
22	$\left[z,\ \frac{1}{4}-x,\ \frac{1}{4}-y\right]$	[22,214]
23	$\left[y,\ \frac{1}{4}-z,\ \frac{1}{4}-x\right]$	[23,215]
24	$\left[\frac{1}{4}-z,\ x,\ \frac{1}{4}-y\right]$	[24,216]
25	$[-x,\ -y,\ -z]$	[25,217]
26	$\left[\frac{1}{4}-x,\ z+\frac{1}{2},\ \frac{1}{4}-y\right]$	[26,218]
27	$\left[\frac{1}{4}-x,\ \frac{1}{4}-z,\ y+\frac{1}{2}\right]$	[27,219]
28	$\left[\frac{1}{4}-z,\ \frac{1}{4}-y,\ x+\frac{1}{2}\right]$	[28,220]
29	$\left[z+\frac{1}{2},\ \frac{1}{4}-y,\ \frac{1}{4}-x\right]$	[29,221]
30	$\left[y+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{1}{4}-z\right]$	[30,222]
31	$\left[\frac{1}{4}-y,\ x+\frac{1}{2},\ \frac{1}{4}-z\right]$	[31,223]
32	$\left[-x,\ y+\frac{1}{4},\ z+\frac{1}{4}\right]$	[32,224]
33	$\left[x+\frac{1}{4},\ -y,\ z+\frac{1}{4}\right]$	[33,225]
34	$\left[x+\frac{1}{4},\ y+\frac{1}{4},\ -z\right]$	[34,226]
35	$\left[\frac{1}{4}-y,\ \frac{1}{4}-x,\ z+\frac{1}{2}\right]$	[35,227]
36	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[36,228]
37	$\left[x+\frac{1}{2},\ \frac{1}{4}-z,\ \frac{1}{4}-y\right]$	[37,229]

continued ...

Table 8

No.	position	mapping
38	$\left[x+\frac{1}{2}, z+\frac{1}{2}, y+\frac{1}{2}\right]$	[38,230]
39	$\left[\frac{1}{4}-z, y+\frac{1}{2}, \frac{1}{4}-x\right]$	[39,231]
40	$\left[z+\frac{1}{2}, y+\frac{1}{2}, x+\frac{1}{2}\right]$	[40,232]
41	$[-z, -x, -y]$	[41,233]
42	$[-y, -z, -x]$	[42,234]
43	$\left[y+\frac{1}{4}, -z, x+\frac{1}{4}\right]$	[43,235]
44	$\left[z+\frac{1}{4}, x+\frac{1}{4}, -y\right]$	[44,236]
45	$\left[y+\frac{1}{4}, z+\frac{1}{4}, -x\right]$	[45,237]
46	$\left[-z, x+\frac{1}{4}, y+\frac{1}{4}\right]$	[46,238]
47	$\left[-y, z+\frac{1}{4}, x+\frac{1}{4}\right]$	[47,239]
48	$\left[z+\frac{1}{4}, -x, y+\frac{1}{4}\right]$	[48,240]
49	$\left[x, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[49,241]
50	$\left[x+\frac{1}{4}, -z, y+\frac{3}{4}\right]$	[50,242]
51	$\left[x+\frac{1}{4}, z+\frac{3}{4}, -y\right]$	[51,243]
52	$\left[z+\frac{1}{4}, y+\frac{3}{4}, -x\right]$	[52,244]
53	$\left[\frac{1}{2}-z, y+\frac{3}{4}, x+\frac{3}{4}\right]$	[53,245]
54	$\left[\frac{1}{2}-y, x+\frac{3}{4}, z+\frac{3}{4}\right]$	[54,246]
55	$\left[y+\frac{1}{4}, -x, z+\frac{3}{4}\right]$	[55,247]
56	$\left[x, \frac{3}{4}-y, \frac{3}{4}-z\right]$	[56,248]
57	$\left[\frac{1}{4}-x, y+\frac{1}{2}, \frac{3}{4}-z\right]$	[57,249]
58	$\left[\frac{1}{4}-x, \frac{3}{4}-y, z+\frac{1}{2}\right]$	[58,250]
59	$\left[y+\frac{1}{4}, x+\frac{3}{4}, -z\right]$	[59,251]
60	$\left[\frac{1}{2}-y, -x, -z\right]$	[60,252]
61	$\left[\frac{1}{2}-x, z+\frac{3}{4}, y+\frac{3}{4}\right]$	[61,253]
62	$\left[\frac{1}{2}-x, -z, -y\right]$	[62,254]
63	$\left[z+\frac{1}{4}, -y, x+\frac{3}{4}\right]$	[63,255]
64	$\left[\frac{1}{2}-z, -y, -x\right]$	[64,256]
65	$\left[z, x+\frac{1}{2}, y+\frac{1}{2}\right]$	[65,257]
66	$\left[y, z+\frac{1}{2}, x+\frac{1}{2}\right]$	[66,258]
67	$\left[\frac{1}{4}-y, z+\frac{1}{2}, \frac{3}{4}-x\right]$	[67,259]
68	$\left[\frac{1}{4}-z, \frac{3}{4}-x, y+\frac{1}{2}\right]$	[68,260]
69	$\left[\frac{1}{4}-y, \frac{3}{4}-z, x+\frac{1}{2}\right]$	[69,261]
70	$\left[z, \frac{3}{4}-x, \frac{3}{4}-y\right]$	[70,262]
71	$\left[y, \frac{3}{4}-z, \frac{3}{4}-x\right]$	[71,263]
72	$\left[\frac{1}{4}-z, x+\frac{1}{2}, \frac{3}{4}-y\right]$	[72,264]
73	$\left[-x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[73,265]
74	$\left[\frac{1}{4}-x, z, \frac{3}{4}-y\right]$	[74,266]
75	$\left[\frac{1}{4}-x, \frac{3}{4}-z, y\right]$	[75,267]
76	$\left[\frac{1}{4}-z, \frac{3}{4}-y, x\right]$	[76,268]
77	$\left[z+\frac{1}{2}, \frac{3}{4}-y, \frac{3}{4}-x\right]$	[77,269]
78	$\left[y+\frac{1}{2}, \frac{3}{4}-x, \frac{3}{4}-z\right]$	[78,270]
79	$\left[\frac{1}{4}-y, x, \frac{3}{4}-z\right]$	[79,271]
80	$\left[-x, y+\frac{3}{4}, z+\frac{3}{4}\right]$	[80,272]
81	$\left[x+\frac{1}{4}, \frac{1}{2}-y, z+\frac{3}{4}\right]$	[81,273]
82	$\left[x+\frac{1}{4}, y+\frac{3}{4}, \frac{1}{2}-z\right]$	[82,274]
83	$\left[\frac{1}{4}-y, \frac{3}{4}-x, z\right]$	[83,275]
84	$\left[y+\frac{1}{2}, x, z\right]$	[84,276]

continued ...

Table 8

No.	position	mapping
85	$\left[x+\frac{1}{2},\ \frac{3}{4}-z,\ \frac{3}{4}-y\right]$	[85,277]
86	$\left[x+\frac{1}{2},\ z,\ y\right]$	[86,278]
87	$\left[\frac{1}{4}-z,\ y,\ \frac{3}{4}-x\right]$	[87,279]
88	$\left[z+\frac{1}{2},\ y,\ x\right]$	[88,280]
89	$\left[-z,\ \frac{1}{2}-x,\ \frac{1}{2}-y\right]$	[89,281]
90	$\left[-y,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[90,282]
91	$\left[y+\frac{1}{4},\ \frac{1}{2}-z,\ x+\frac{3}{4}\right]$	[91,283]
92	$\left[z+\frac{1}{4},\ x+\frac{3}{4},\ \frac{1}{2}-y\right]$	[92,284]
93	$\left[y+\frac{1}{4},\ z+\frac{3}{4},\ \frac{1}{2}-x\right]$	[93,285]
94	$\left[-z,\ x+\frac{3}{4},\ y+\frac{3}{4}\right]$	[94,286]
95	$\left[-y,\ z+\frac{3}{4},\ x+\frac{3}{4}\right]$	[95,287]
96	$\left[z+\frac{1}{4},\ \frac{1}{2}-x,\ y+\frac{3}{4}\right]$	[96,288]
97	$\left[x+\frac{1}{2},\ y,\ z+\frac{1}{2}\right]$	[97,289]
98	$\left[x+\frac{3}{4},\ \frac{1}{2}-z,\ y+\frac{3}{4}\right]$	[98,290]
99	$\left[x+\frac{3}{4},\ z+\frac{1}{4},\ -y\right]$	[99,291]
100	$\left[z+\frac{3}{4},\ y+\frac{1}{4},\ -x\right]$	[100,292]
101	$\left[-z,\ y+\frac{1}{4},\ x+\frac{3}{4}\right]$	[101,293]
102	$\left[-y,\ x+\frac{1}{4},\ z+\frac{3}{4}\right]$	[102,294]
103	$\left[y+\frac{3}{4},\ \frac{1}{2}-x,\ z+\frac{3}{4}\right]$	[103,295]
104	$\left[x+\frac{1}{2},\ \frac{1}{4}-y,\ \frac{3}{4}-z\right]$	[104,296]
105	$\left[\frac{3}{4}-x,\ y,\ \frac{3}{4}-z\right]$	[105,297]
106	$\left[\frac{3}{4}-x,\ \frac{1}{4}-y,\ z+\frac{1}{2}\right]$	[106,298]
107	$\left[y+\frac{3}{4},\ x+\frac{1}{4},\ -z\right]$	[107,299]
108	$\left[-y,\ \frac{1}{2}-x,\ -z\right]$	[108,300]
109	$\left[-x,\ z+\frac{1}{4},\ y+\frac{3}{4}\right]$	[109,301]
110	$\left[-x,\ \frac{1}{2}-z,\ -y\right]$	[110,302]
111	$\left[z+\frac{3}{4},\ \frac{1}{2}-y,\ x+\frac{3}{4}\right]$	[111,303]
112	$\left[-z,\ \frac{1}{2}-y,\ -x\right]$	[112,304]
113	$\left[z+\frac{1}{2},\ x,\ y+\frac{1}{2}\right]$	[113,305]
114	$\left[y+\frac{1}{2},\ z,\ x+\frac{1}{2}\right]$	[114,306]
115	$\left[\frac{3}{4}-y,\ z,\ \frac{3}{4}-x\right]$	[115,307]
116	$\left[\frac{3}{4}-z,\ \frac{1}{4}-x,\ y+\frac{1}{2}\right]$	[116,308]
117	$\left[\frac{3}{4}-y,\ \frac{1}{4}-z,\ x+\frac{1}{2}\right]$	[117,309]
118	$\left[z+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{3}{4}-y\right]$	[118,310]
119	$\left[y+\frac{1}{2},\ \frac{1}{4}-z,\ \frac{3}{4}-x\right]$	[119,311]
120	$\left[\frac{3}{4}-z,\ x,\ \frac{3}{4}-y\right]$	[120,312]
121	$\left[\frac{1}{2}-x,\ -y,\ \frac{1}{2}-z\right]$	[121,313]
122	$\left[\frac{3}{4}-x,\ z+\frac{1}{2},\ \frac{3}{4}-y\right]$	[122,314]
123	$\left[\frac{3}{4}-x,\ \frac{1}{4}-z,\ y\right]$	[123,315]
124	$\left[\frac{3}{4}-z,\ \frac{1}{4}-y,\ x\right]$	[124,316]
125	$\left[z,\ \frac{1}{4}-y,\ \frac{3}{4}-x\right]$	[125,317]
126	$\left[y,\ \frac{1}{4}-x,\ \frac{3}{4}-z\right]$	[126,318]
127	$\left[\frac{3}{4}-y,\ x+\frac{1}{2},\ \frac{3}{4}-z\right]$	[127,319]
128	$\left[\frac{1}{2}-x,\ y+\frac{1}{4},\ z+\frac{3}{4}\right]$	[128,320]
129	$\left[x+\frac{3}{4},\ -y,\ z+\frac{3}{4}\right]$	[129,321]
130	$\left[x+\frac{3}{4},\ y+\frac{1}{4},\ \frac{1}{2}-z\right]$	[130,322]
131	$\left[\frac{3}{4}-y,\ \frac{1}{4}-x,\ z\right]$	[131,323]

continued ...

Table 8

No.	position	mapping
132	$\left[y,\, x+\frac{1}{2},\, z\right]$	[132,324]
133	$\left[x,\, \frac{1}{4}-z,\, \frac{3}{4}-y\right]$	[133,325]
134	$\left[x,\, z+\frac{1}{2},\, y\right]$	[134,326]
135	$\left[\frac{3}{4}-z,\, y+\frac{1}{2},\, \frac{3}{4}-x\right]$	[135,327]
136	$\left[z,\, y+\frac{1}{2},\, x\right]$	[136,328]
137	$\left[\frac{1}{2}-z,\, -x,\, \frac{1}{2}-y\right]$	[137,329]
138	$\left[\frac{1}{2}-y,\, -z,\, \frac{1}{2}-x\right]$	[138,330]
139	$\left[y+\frac{3}{4},\, -z,\, x+\frac{3}{4}\right]$	[139,331]
140	$\left[z+\frac{3}{4},\, x+\frac{1}{4},\, \frac{1}{2}-y\right]$	[140,332]
141	$\left[y+\frac{3}{4},\, z+\frac{1}{4},\, \frac{1}{2}-x\right]$	[141,333]
142	$\left[\frac{1}{2}-z,\, x+\frac{1}{4},\, y+\frac{3}{4}\right]$	[142,334]
143	$\left[\frac{1}{2}-y,\, z+\frac{1}{4},\, x+\frac{3}{4}\right]$	[143,335]
144	$\left[z+\frac{3}{4},\, -x,\, y+\frac{3}{4}\right]$	[144,336]
145	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z\right]$	[145,337]
146	$\left[x+\frac{3}{4},\, -z,\, y+\frac{1}{4}\right]$	[146,338]
147	$\left[x+\frac{3}{4},\, z+\frac{3}{4},\, \frac{1}{2}-y\right]$	[147,339]
148	$\left[z+\frac{3}{4},\, y+\frac{3}{4},\, \frac{1}{2}-x\right]$	[148,340]
149	$\left[-z,\, y+\frac{3}{4},\, x+\frac{1}{4}\right]$	[149,341]
150	$\left[-y,\, x+\frac{3}{4},\, z+\frac{1}{4}\right]$	[150,342]
151	$\left[y+\frac{3}{4},\, -x,\, z+\frac{1}{4}\right]$	[151,343]
152	$\left[x+\frac{1}{2},\, \frac{3}{4}-y,\, \frac{1}{4}-z\right]$	[152,344]
153	$\left[\frac{3}{4}-x,\, y+\frac{1}{2},\, \frac{1}{4}-z\right]$	[153,345]
154	$\left[\frac{3}{4}-x,\, \frac{3}{4}-y,\, z\right]$	[154,346]
155	$\left[y+\frac{3}{4},\, x+\frac{3}{4},\, \frac{1}{2}-z\right]$	[155,347]
156	$\left[-y,\, -x,\, \frac{1}{2}-z\right]$	[156,348]
157	$\left[-x,\, z+\frac{3}{4},\, y+\frac{1}{4}\right]$	[157,349]
158	$\left[-x,\, -z,\, \frac{1}{2}-y\right]$	[158,350]
159	$\left[z+\frac{3}{4},\, -y,\, x+\frac{1}{4}\right]$	[159,351]
160	$\left[-z,\, -y,\, \frac{1}{2}-x\right]$	[160,352]
161	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, y\right]$	[161,353]
162	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, x\right]$	[162,354]
163	$\left[\frac{3}{4}-y,\, z+\frac{1}{2},\, \frac{1}{4}-x\right]$	[163,355]
164	$\left[\frac{3}{4}-z,\, \frac{3}{4}-x,\, y\right]$	[164,356]
165	$\left[\frac{3}{4}-y,\, \frac{3}{4}-z,\, x\right]$	[165,357]
166	$\left[z+\frac{1}{2},\, \frac{3}{4}-x,\, \frac{1}{4}-y\right]$	[166,358]
167	$\left[y+\frac{1}{2},\, \frac{3}{4}-z,\, \frac{1}{4}-x\right]$	[167,359]
168	$\left[\frac{3}{4}-z,\, x+\frac{1}{2},\, \frac{1}{4}-y\right]$	[168,360]
169	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, -z\right]$	[169,361]
170	$\left[\frac{3}{4}-x,\, z,\, \frac{1}{4}-y\right]$	[170,362]
171	$\left[\frac{3}{4}-x,\, \frac{3}{4}-z,\, y+\frac{1}{2}\right]$	[171,363]
172	$\left[\frac{3}{4}-z,\, \frac{3}{4}-y,\, x+\frac{1}{2}\right]$	[172,364]
173	$\left[z,\, \frac{3}{4}-y,\, \frac{1}{4}-x\right]$	[173,365]
174	$\left[y,\, \frac{3}{4}-x,\, \frac{1}{4}-z\right]$	[174,366]
175	$\left[\frac{3}{4}-y,\, x,\, \frac{1}{4}-z\right]$	[175,367]
176	$\left[\frac{1}{2}-x,\, y+\frac{3}{4},\, z+\frac{1}{4}\right]$	[176,368]
177	$\left[x+\frac{3}{4},\, \frac{1}{2}-y,\, z+\frac{1}{4}\right]$	[177,369]
178	$\left[x+\frac{3}{4},\, y+\frac{3}{4},\, -z\right]$	[178,370]

continued ...

Table 8

No.	position	mapping
179	$\left[\frac{3}{4}-y,\ \frac{3}{4}-x,\ z+\frac{1}{2}\right]$	[179,371]
180	$\left[y,\ x,\ z+\frac{1}{2}\right]$	[180,372]
181	$\left[x,\ \frac{3}{4}-z,\ \frac{1}{4}-y\right]$	[181,373]
182	$\left[x,\ z,\ y+\frac{1}{2}\right]$	[182,374]
183	$\left[\frac{3}{4}-z,\ y,\ \frac{1}{4}-x\right]$	[183,375]
184	$\left[z,\ y,\ x+\frac{1}{2}\right]$	[184,376]
185	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ -y\right]$	[185,377]
186	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ -x\right]$	[186,378]
187	$\left[y+\frac{3}{4},\ \frac{1}{2}-z,\ x+\frac{1}{4}\right]$	[187,379]
188	$\left[z+\frac{3}{4},\ x+\frac{3}{4},\ -y\right]$	[188,380]
189	$\left[y+\frac{3}{4},\ z+\frac{3}{4},\ -x\right]$	[189,381]
190	$\left[\frac{1}{2}-z,\ x+\frac{3}{4},\ y+\frac{1}{4}\right]$	[190,382]
191	$\left[\frac{1}{2}-y,\ z+\frac{3}{4},\ x+\frac{1}{4}\right]$	[191,383]
192	$\left[z+\frac{3}{4},\ \frac{1}{2}-x,\ y+\frac{1}{4}\right]$	[192,384]