MSG No. 226.123 $Fm\bar{3}c1'$ [Type II, cubic]

Table 1: Wyckoff site: 8a, site symmetry: 4321'

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

Table 2: Wyckoff site: 8b, site symmetry: m-3.1'

No.	position	mapping
1	$[0, 0, 0]$	[1,8,9,10,17,18,19,20,21,22,23,24,25,32,33,34,41,42,43,44,45,46,47,48, 193,200,201,202,209,210,211,212,213,214,215,216,217,224,225,226,233,234,235,236,237,238,239,240]
2	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[2,3,4,5,6,7,11,12,13,14,15,16,26,27,28,29,30,31,35,36,37,38,39,40, 194,195,196,197,198,199,203,204,205,206,207,208,218,219,220,221,222,223,227,228,229,230,231,232]
3	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[49,56,57,58,65,66,67,68,69,70,71,72,73,80,81,82,89,90,91,92,93,94,95,96, 241,248,249,250,257,258,259,260,261,262,263,264,265,272,273,274,281,282,283,284,285,286,287,288]
4	$\left[\frac{1}{2}, 0, 0\right]$	[50,51,52,53,54,55,59,60,61,62,63,64,74,75,76,77,78,79,83,84,85,86,87,88, 242,243,244,245,246,247,251,252,253,254,255,256,266,267,268,269,270,271,275,276,277,278,279,280]
5	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[97,104,105,106,113,114,115,116,117,118,119,120,121,128,129,130,137,138,139,140,141,142,143,144, 289,296,297,298,305,306,307,308,309,310,311,312,313,320,321,322,329,330,331,332,333,334,335,336]
6	$\left[0, \frac{1}{2}, 0\right]$	[98,99,100,101,102,103,107,108,109,110,111,112,122,123,124,125,126,127,131,132,133,134,135,136, 290,291,292,293,294,295,299,300,301,302,303,304,314,315,316,317,318,319,323,324,325,326,327,328]
7	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[145,152,153,154,161,162,163,164,165,166,167,168,169,176,177,178,185,186,187,188,189,190,191,192, 337,344,345,346,353,354,355,356,357,358,359,360,361,368,369,370,377,378,379,380,381,382,383,384]
8	$\left[0, 0, \frac{1}{2}\right]$	[146,147,148,149,150,151,155,156,157,158,159,160,170,171,172,173,174,175,179,180,181,182,183,184, 338,339,340,341,342,343,347,348,349,350,351,352,362,363,364,365,366,367,371,372,373,374,375,376]

Table 3: Wyckoff site: 24c, site symmetry: -4m.21'

No.	position	mapping
1	$\left[\frac{1}{4}, 0, 0\right]$	[1,8,33,34,61,62,74,75,193,200,225,226,253,254,266,267]
2	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}\right]$	[2,3,37,38,57,58,73,80,194,195,229,230,249,250,265,272]
3	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[4,16,29,39,162,165,187,191,196,208,221,231,354,357,379,383]
4	$\left[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	[5,15,28,40,163,167,186,189,197,207,220,232,355,359,378,381]
5	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{2}\right]$	[6,11,31,36,116,118,137,144,198,203,223,228,308,310,329,336]
6	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{2}\right]$	[7,12,30,35,113,120,140,142,199,204,222,227,305,312,332,334]
7	$\left[\frac{3}{4}, 0, 0\right]$	[9,10,25,32,50,51,85,86,201,202,217,224,242,243,277,278]
8	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}\right]$	[13,14,26,27,49,56,81,82,205,206,218,219,241,248,273,274]
9	$\left[0, \frac{1}{4}, 0\right]$	[17,24,44,46,103,108,126,131,209,216,236,238,295,300,318,323]
10	$\left[0, 0, \frac{1}{4}\right]$	[18,21,43,47,148,160,173,183,210,213,235,239,340,352,365,375]
11	$\left[0, 0, \frac{3}{4}\right]$	[19,23,42,45,149,159,172,184,211,215,234,237,341,351,364,376]
12	$\left[0, \frac{3}{4}, 0\right]$	[20,22,41,48,102,107,127,132,212,214,233,240,294,299,319,324]
13	$\left[\frac{1}{2}, 0, \frac{3}{4}\right]$	[52,64,77,87,114,117,139,143,244,256,269,279,306,309,331,335]
14	$\left[\frac{1}{2}, 0, \frac{1}{4}\right]$	[53,63,76,88,115,119,138,141,245,255,268,280,307,311,330,333]
15	$\left[\frac{1}{2}, \frac{1}{4}, 0\right]$	[54,59,79,84,164,166,185,192,246,251,271,276,356,358,377,384]
16	$\left[\frac{1}{2}, \frac{3}{4}, 0\right]$	[55,60,78,83,161,168,188,190,247,252,270,275,353,360,380,382]
17	$\left[0, \frac{3}{4}, \frac{1}{2}\right]$	[65,72,92,94,151,156,174,179,257,264,284,286,343,348,366,371]
18	$\left[0, \frac{1}{2}, \frac{3}{4}\right]$	[66,69,91,95,100,112,125,135,258,261,283,287,292,304,317,327]
19	$\left[0, \frac{1}{2}, \frac{1}{4}\right]$	[67,71,90,93,101,111,124,136,259,263,282,285,293,303,316,328]
20	$\left[0, \frac{1}{4}, \frac{1}{2}\right]$	[68,70,89,96,150,155,175,180,260,262,281,288,342,347,367,372]
21	$\left[\frac{3}{4}, 0, \frac{1}{2}\right]$	[97,104,129,130,157,158,170,171,289,296,321,322,349,350,362,363]
22	$\left[\frac{1}{4}, \frac{1}{2}, 0\right]$	[98,99,133,134,153,154,169,176,290,291,325,326,345,346,361,368]
23	$\left[\frac{1}{4}, 0, \frac{1}{2}\right]$	[105,106,121,128,146,147,181,182,297,298,313,320,338,339,373,374]
24	$\left[\frac{3}{4}, \frac{1}{2}, 0\right]$	[109,110,122,123,145,152,177,178,301,302,314,315,337,344,369,370]

Table 4: Wyckoff site: 24d, site symmetry: 4/m..1'

No.	position	mapping
1	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	[1,32,56,73,98,123,147,170,193,224,248,265,290,315,339,362]
2	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[2,27,51,74,97,128,152,169,194,219,243,266,289,320,344,361]
3	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[3,26,50,75,104,121,145,176,195,218,242,267,296,313,337,368]
4	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[4,40,67,95,119,139,160,172,196,232,259,287,311,331,352,364]
5	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[5,39,66,93,117,138,159,173,197,231,258,285,309,330,351,365]
6	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[6,35,65,96,107,126,168,185,198,227,257,288,299,318,360,377]
7	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[7,36,68,94,108,127,166,188,199,228,260,286,300,319,358,380]
8	$\left[0, \frac{3}{4}, \frac{3}{4}\right]$	[8,25,49,80,99,122,146,171,200,217,241,272,291,314,338,363]
9	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	[9,34,58,81,110,133,157,182,201,226,250,273,302,325,349,374]
10	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	[10,33,57,82,109,134,158,181,202,225,249,274,301,326,350,373]
11	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[11,30,72,89,102,131,161,192,203,222,264,281,294,323,353,384]
12	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[12,31,70,92,103,132,164,190,204,223,262,284,295,324,356,382]
13	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[13,38,62,85,106,129,153,178,205,230,254,277,298,321,345,370]
14	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[14,37,61,86,105,130,154,177,206,229,253,278,297,322,346,369]
15	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[15,29,69,90,114,141,149,183,207,221,261,282,306,333,341,375]

continued ...

Table 4

No.	position	mapping
16	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[16,28,71,91,115,143,148,184,208,220,263,283,307,335,340,376]
17	$\left[\frac{1}{4}, 0, \frac{1}{4}\right]$	[17,48,54,83,120,137,155,174,209,240,246,275,312,329,347,366]
18	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	[18,45,53,87,111,125,165,186,210,237,245,279,303,317,357,378]
19	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[19,47,52,88,112,124,167,187,211,239,244,280,304,316,359,379]
20	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	[20,46,55,84,118,140,156,175,212,238,247,276,310,332,348,367]
21	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	[21,42,63,77,101,135,162,189,213,234,255,269,293,327,354,381]
22	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	[22,44,60,79,116,142,151,180,214,236,252,271,308,334,343,372]
23	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[23,43,64,76,100,136,163,191,215,235,256,268,292,328,355,383]
24	$\left[\frac{3}{4}, 0, \frac{3}{4}\right]$	[24,41,59,78,113,144,150,179,216,233,251,270,305,336,342,371]

Table 5: Wyckoff site: 48e, site symmetry: 2mm..1'

No.	position	mapping
1	$[x, 0, 0]$	[1,8,33,34,193,200,225,226]
2	$\left[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[2,3,37,38,194,195,229,230]
3	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x\right]$	[4,16,29,39,196,208,221,231]
4	$\left[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}\right]$	[5,15,28,40,197,207,220,232]
5	$\left[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}\right]$	[6,11,31,36,198,203,223,228]
6	$\left[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}\right]$	[7,12,30,35,199,204,222,227]
7	$[-x, 0, 0]$	[9,10,25,32,201,202,217,224]
8	$\left[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}\right]$	[13,14,26,27,205,206,218,219]
9	$[0, x, 0]$	[17,24,44,46,209,216,236,238]
10	$[0, 0, x]$	[18,21,43,47,210,213,235,239]
11	$[0, 0, -x]$	[19,23,42,45,211,215,234,237]
12	$[0, -x, 0]$	[20,22,41,48,212,214,233,240]
13	$\left[x, \frac{1}{2}, \frac{1}{2}\right]$	[49,56,81,82,241,248,273,274]
14	$\left[x + \frac{1}{2}, 0, 0\right]$	[50,51,85,86,242,243,277,278]
15	$\left[\frac{1}{2}, 0, -x\right]$	[52,64,77,87,244,256,269,279]
16	$\left[\frac{1}{2}, 0, x\right]$	[53,63,76,88,245,255,268,280]
17	$\left[\frac{1}{2}, x, 0\right]$	[54,59,79,84,246,251,271,276]
18	$\left[\frac{1}{2}, -x, 0\right]$	[55,60,78,83,247,252,270,275]
19	$\left[-x, \frac{1}{2}, \frac{1}{2}\right]$	[57,58,73,80,249,250,265,272]
20	$\left[\frac{1}{2} - x, 0, 0\right]$	[61,62,74,75,253,254,266,267]
21	$\left[0, x + \frac{1}{2}, \frac{1}{2}\right]$	[65,72,92,94,257,264,284,286]
22	$\left[0, \frac{1}{2}, x + \frac{1}{2}\right]$	[66,69,91,95,258,261,283,287]
23	$\left[0, \frac{1}{2}, \frac{1}{2} - x\right]$	[67,71,90,93,259,263,282,285]
24	$\left[0, \frac{1}{2} - x, \frac{1}{2}\right]$	[68,70,89,96,260,262,281,288]
25	$\left[x + \frac{1}{2}, 0, \frac{1}{2}\right]$	[97,104,129,130,289,296,321,322]
26	$\left[x, \frac{1}{2}, 0\right]$	[98,99,133,134,290,291,325,326]
27	$\left[0, \frac{1}{2}, -x\right]$	[100,112,125,135,292,304,317,327]
28	$\left[0, \frac{1}{2}, x\right]$	[101,111,124,136,293,303,316,328]
29	$\left[0, x + \frac{1}{2}, 0\right]$	[102,107,127,132,294,299,319,324]
30	$\left[0, \frac{1}{2} - x, 0\right]$	[103,108,126,131,295,300,318,323]
31	$\left[\frac{1}{2} - x, 0, \frac{1}{2}\right]$	[105,106,121,128,297,298,313,320]

continued ...

Table 5

No.	position	mapping
32	$\left[-x, \frac{1}{2}, 0\right]$	[109,110,122,123,301,302,314,315]
33	$\left[\frac{1}{2}, x, \frac{1}{2}\right]$	[113,120,140,142,305,312,332,334]
34	$\left[\frac{1}{2}, 0, x+\frac{1}{2}\right]$	[114,117,139,143,306,309,331,335]
35	$\left[\frac{1}{2}, 0, \frac{1}{2}-x\right]$	[115,119,138,141,307,311,330,333]
36	$\left[\frac{1}{2}, -x, \frac{1}{2}\right]$	[116,118,137,144,308,310,329,336]
37	$\left[x+\frac{1}{2}, \frac{1}{2}, 0\right]$	[145,152,177,178,337,344,369,370]
38	$\left[x, 0, \frac{1}{2}\right]$	[146,147,181,182,338,339,373,374]
39	$\left[0, 0, \frac{1}{2}-x\right]$	[148,160,173,183,340,352,365,375]
40	$\left[0, 0, x+\frac{1}{2}\right]$	[149,159,172,184,341,351,364,376]
41	$\left[0, x, \frac{1}{2}\right]$	[150,155,175,180,342,347,367,372]
42	$\left[0, -x, \frac{1}{2}\right]$	[151,156,174,179,343,348,366,371]
43	$\left[\frac{1}{2}-x, \frac{1}{2}, 0\right]$	[153,154,169,176,345,346,361,368]
44	$\left[-x, 0, \frac{1}{2}\right]$	[157,158,170,171,349,350,362,363]
45	$\left[\frac{1}{2}, x+\frac{1}{2}, 0\right]$	[161,168,188,190,353,360,380,382]
46	$\left[\frac{1}{2}, \frac{1}{2}, x\right]$	[162,165,187,191,354,357,379,383]
47	$\left[\frac{1}{2}, \frac{1}{2}, -x\right]$	[163,167,186,189,355,359,378,381]
48	$\left[\frac{1}{2}, \frac{1}{2}-x, 0\right]$	[164,166,185,192,356,358,377,384]

Table 6: Wyckoff site: `48f`, site symmetry: `4..1'`

No.	position	mapping
1	$\left[x, \frac{1}{4}, \frac{1}{4}\right]$	[1,56,98,147,193,248,290,339]
2	$\left[x+\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[2,51,97,152,194,243,289,344]
3	$\left[x+\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[3,50,104,145,195,242,296,337]
4	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}-x\right]$	[4,67,119,160,196,259,311,352]
5	$\left[\frac{1}{4}, \frac{3}{4}, x+\frac{1}{2}\right]$	[5,66,117,159,197,258,309,351]
6	$\left[\frac{1}{4}, x+\frac{1}{2}, \frac{3}{4}\right]$	[6,65,107,168,198,257,299,360]
7	$\left[\frac{3}{4}, \frac{1}{2}-x, \frac{3}{4}\right]$	[7,68,108,166,199,260,300,358]
8	$\left[x, \frac{3}{4}, \frac{3}{4}\right]$	[8,49,99,146,200,241,291,338]
9	$\left[-x, \frac{1}{4}, \frac{3}{4}\right]$	[9,58,110,157,201,250,302,349]
10	$\left[-x, \frac{3}{4}, \frac{1}{4}\right]$	[10,57,109,158,202,249,301,350]
11	$\left[\frac{3}{4}, x+\frac{1}{2}, \frac{1}{4}\right]$	[11,72,102,161,203,264,294,353]
12	$\left[\frac{1}{4}, \frac{1}{2}-x, \frac{1}{4}\right]$	[12,70,103,164,204,262,295,356]
13	$\left[\frac{1}{2}-x, \frac{3}{4}, \frac{3}{4}\right]$	[13,62,106,153,205,254,298,345]
14	$\left[\frac{1}{2}-x, \frac{1}{4}, \frac{1}{4}\right]$	[14,61,105,154,206,253,297,346]
15	$\left[\frac{3}{4}, \frac{1}{4}, x+\frac{1}{2}\right]$	[15,69,114,149,207,261,306,341]
16	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}-x\right]$	[16,71,115,148,208,263,307,340]
17	$\left[\frac{1}{4}, x, \frac{1}{4}\right]$	[17,54,120,155,209,246,312,347]
18	$\left[\frac{1}{4}, \frac{1}{4}, x\right]$	[18,53,111,165,210,245,303,357]
19	$\left[\frac{3}{4}, \frac{1}{4}, -x\right]$	[19,52,112,167,211,244,304,359]
20	$\left[\frac{3}{4}, -x, \frac{1}{4}\right]$	[20,55,118,156,212,247,310,348]
21	$\left[\frac{3}{4}, \frac{3}{4}, x\right]$	[21,63,101,162,213,255,293,354]
22	$\left[\frac{1}{4}, -x, \frac{3}{4}\right]$	[22,60,116,151,214,252,308,343]
23	$\left[\frac{1}{4}, \frac{3}{4}, -x\right]$	[23,64,100,163,215,256,292,355]

continued ...

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Table 6

No.	position	mapping
24	$\left[\frac{3}{4}, x, \frac{3}{4}\right]$	[24,59,113,150,216,251,305,342]
25	$\left[-x, \frac{3}{4}, \frac{3}{4}\right]$	[25,80,122,171,217,272,314,363]
26	$\left[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}\right]$	[26,75,121,176,218,267,313,368]
27	$\left[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}\right]$	[27,74,128,169,219,266,320,361]
28	$\left[\frac{1}{4}, \frac{1}{4}, x + \frac{1}{2}\right]$	[28,91,143,184,220,283,335,376]
29	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - x\right]$	[29,90,141,183,221,282,333,375]
30	$\left[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{4}\right]$	[30,89,131,192,222,281,323,384]
31	$\left[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{4}\right]$	[31,92,132,190,223,284,324,382]
32	$\left[-x, \frac{1}{4}, \frac{1}{4}\right]$	[32,73,123,170,224,265,315,362]
33	$\left[x, \frac{3}{4}, \frac{1}{4}\right]$	[33,82,134,181,225,274,326,373]
34	$\left[x, \frac{1}{4}, \frac{3}{4}\right]$	[34,81,133,182,226,273,325,374]
35	$\left[\frac{1}{4}, \frac{1}{2} - x, \frac{3}{4}\right]$	[35,96,126,185,227,288,318,377]
36	$\left[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}\right]$	[36,94,127,188,228,286,319,380]
37	$\left[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[37,86,130,177,229,278,322,369]
38	$\left[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[38,85,129,178,230,277,321,370]
39	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - x\right]$	[39,93,138,173,231,285,330,365]
40	$\left[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}\right]$	[40,95,139,172,232,287,331,364]
41	$\left[\frac{3}{4}, -x, \frac{3}{4}\right]$	[41,78,144,179,233,270,336,371]
42	$\left[\frac{3}{4}, \frac{3}{4}, -x\right]$	[42,77,135,189,234,269,327,381]
43	$\left[\frac{1}{4}, \frac{3}{4}, x\right]$	[43,76,136,191,235,268,328,383]
44	$\left[\frac{1}{4}, x, \frac{3}{4}\right]$	[44,79,142,180,236,271,334,372]
45	$\left[\frac{1}{4}, \frac{1}{4}, -x\right]$	[45,87,125,186,237,279,317,378]
46	$\left[\frac{3}{4}, x, \frac{1}{4}\right]$	[46,84,140,175,238,276,332,367]
47	$\left[\frac{3}{4}, \frac{1}{4}, x\right]$	[47,88,124,187,239,280,316,379]
48	$\left[\frac{1}{4}, -x, \frac{1}{4}\right]$	[48,83,137,174,240,275,329,366]

Table 7: Wyckoff site: 64g, site symmetry: .3.1'

No.	position	mapping
1	$[x, x, x]$	[1,17,18,193,209,210]
2	$\left[x + \frac{1}{2}, \frac{1}{2} - x, x + \frac{1}{2}\right]$	[2,7,15,194,199,207]
3	$\left[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - x\right]$	[3,4,11,195,196,203]
4	$\left[\frac{1}{2} - x, x + \frac{1}{2}, x + \frac{1}{2}\right]$	[5,6,13,197,198,205]
5	$[x, -x, -x]$	[8,22,23,200,214,215]
6	$[-x, x, -x]$	[9,19,24,201,211,216]
7	$[-x, -x, x]$	[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	$\left[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - x\right]$	[26,31,39,218,223,231]
11	$\left[\frac{1}{2} - x, \frac{1}{2} - x, x + \frac{1}{2}\right]$	[27,28,35,219,220,227]
12	$\left[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x\right]$	[29,30,37,221,222,229]
13	$[-x, x, x]$	[32,46,47,224,238,239]
14	$[x, -x, x]$	[33,43,48,225,235,240]
15	$[x, x, -x]$	[34,44,45,226,236,237]

continued ...

Table 7

No.	position	mapping
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	$\left[x+\frac{1}{2}, -x, x\right]$	[50,55,63,242,247,255]
19	$\left[x+\frac{1}{2}, x, -x\right]$	[51,52,59,243,244,251]
20	$\left[\frac{1}{2}-x, x, x\right]$	[53,54,61,245,246,253]
21	$\left[x, \frac{1}{2}-x, \frac{1}{2}-x\right]$	[56,70,71,248,262,263]
22	$\left[-x, x+\frac{1}{2}, \frac{1}{2}-x\right]$	[57,67,72,249,259,264]
23	$\left[-x, \frac{1}{2}-x, x+\frac{1}{2}\right]$	[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	$\left[\frac{1}{2}-x, x, -x\right]$	[74,79,87,266,271,279]
27	$\left[\frac{1}{2}-x, -x, x\right]$	[75,76,83,267,268,275]
28	$\left[x+\frac{1}{2}, -x, -x\right]$	[77,78,85,269,270,277]
29	$\left[-x, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[80,94,95,272,286,287]
30	$\left[x, \frac{1}{2}-x, x+\frac{1}{2}\right]$	[81,91,96,273,283,288]
31	$\left[x, x+\frac{1}{2}, \frac{1}{2}-x\right]$	[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	$\left[x, \frac{1}{2}-x, x\right]$	[98,103,111,290,295,303]
35	$\left[x, x+\frac{1}{2}, -x\right]$	[99,100,107,291,292,299]
36	$\left[-x, x+\frac{1}{2}, x\right]$	[101,102,109,293,294,301]
37	$\left[x+\frac{1}{2}, -x, \frac{1}{2}-x\right]$	[104,118,119,296,310,311]
38	$\left[\frac{1}{2}-x, x, \frac{1}{2}-x\right]$	[105,115,120,297,307,312]
39	$\left[\frac{1}{2}-x, -x, x+\frac{1}{2}\right]$	[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	$\left[-x, x+\frac{1}{2}, -x\right]$	[122,127,135,314,319,327]
43	$\left[-x, \frac{1}{2}-x, x\right]$	[123,124,131,315,316,323]
44	$\left[x, \frac{1}{2}-x, -x\right]$	[125,126,133,317,318,325]
45	$\left[\frac{1}{2}-x, x, x+\frac{1}{2}\right]$	[128,142,143,320,334,335]
46	$\left[x+\frac{1}{2}, -x, x+\frac{1}{2}\right]$	[129,139,144,321,331,336]
47	$\left[x+\frac{1}{2}, x, \frac{1}{2}-x\right]$	[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	$\left[x, -x, x+\frac{1}{2}\right]$	[146,151,159,338,343,351]
51	$\left[x, x, \frac{1}{2}-x\right]$	[147,148,155,339,340,347]
52	$\left[-x, x, x+\frac{1}{2}\right]$	[149,150,157,341,342,349]
53	$\left[x+\frac{1}{2}, \frac{1}{2}-x, -x\right]$	[152,166,167,344,358,359]
54	$\left[\frac{1}{2}-x, x+\frac{1}{2}, -x\right]$	[153,163,168,345,355,360]
55	$\left[\frac{1}{2}-x, \frac{1}{2}-x, x\right]$	[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	$\left[-x, x, \frac{1}{2}-x\right]$	[170,175,183,362,367,375]
59	$\left[-x, -x, x+\frac{1}{2}\right]$	[171,172,179,363,364,371]
60	$\left[x, -x, \frac{1}{2}-x\right]$	[173,174,181,365,366,373]
61	$\left[\frac{1}{2}-x, x+\frac{1}{2}, x\right]$	[176,190,191,368,382,383]
62	$\left[x+\frac{1}{2}, \frac{1}{2}-x, x\right]$	[177,187,192,369,379,384]

Table 7

No.	position	mapping
63	$\left[x+\frac{1}{2},\, x+\frac{1}{2},\, -x\right]$	[178,188,189,370,380,381]
64	$\left[x,\, x,\, x+\frac{1}{2}\right]$	[180,182,184,372,374,376]

Table 8: Wyckoff site: `96h`, site symmetry: `..21'`

No.	position	mapping
1	$\left[\frac{1}{4},\, y,\, y\right]$	[1,61,193,253]
2	$\left[\frac{3}{4},\, \frac{1}{2}-y,\, y+\frac{1}{2}\right]$	[2,58,194,250]
3	$\left[\frac{3}{4},\, y+\frac{1}{2},\, \frac{1}{2}-y\right]$	[3,57,195,249]
4	$\left[y+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{4}\right]$	[4,162,196,354]
5	$\left[\frac{1}{2}-y,\, y+\frac{1}{2},\, \frac{3}{4}\right]$	[5,163,197,355]
6	$\left[\frac{1}{2}-y,\, \frac{3}{4},\, y+\frac{1}{2}\right]$	[6,116,198,308]
7	$\left[y+\frac{1}{2},\, \frac{1}{4},\, y+\frac{1}{2}\right]$	[7,113,199,305]
8	$\left[\frac{1}{4},\, -y,\, -y\right]$	[8,62,200,254]
9	$\left[\frac{3}{4},\, y,\, -y\right]$	[9,51,201,243]
10	$\left[\frac{3}{4},\, -y,\, y\right]$	[10,50,202,242]
11	$\left[y+\frac{1}{2},\, \frac{3}{4},\, \frac{1}{2}-y\right]$	[11,118,203,310]
12	$\left[\frac{1}{2}-y,\, \frac{1}{4},\, \frac{1}{2}-y\right]$	[12,120,204,312]
13	$\left[\frac{1}{4},\, y+\frac{1}{2},\, y+\frac{1}{2}\right]$	[13,49,205,241]
14	$\left[\frac{1}{4},\, \frac{1}{2}-y,\, \frac{1}{2}-y\right]$	[14,56,206,248]
15	$\left[y+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{3}{4}\right]$	[15,167,207,359]
16	$\left[\frac{1}{2}-y,\, \frac{1}{2}-y,\, \frac{1}{4}\right]$	[16,165,208,357]
17	$\left[y,\, \frac{1}{4},\, y\right]$	[17,103,209,295]
18	$\left[y,\, y,\, \frac{1}{4}\right]$	[18,148,210,340]
19	$\left[-y,\, y,\, \frac{3}{4}\right]$	[19,149,211,341]
20	$\left[-y,\, \frac{3}{4},\, y\right]$	[20,102,212,294]
21	$\left[-y,\, -y,\, \frac{1}{4}\right]$	[21,160,213,352]
22	$\left[y,\, \frac{3}{4},\, -y\right]$	[22,107,214,299]
23	$\left[y,\, -y,\, \frac{3}{4}\right]$	[23,159,215,351]
24	$\left[-y,\, \frac{1}{4},\, -y\right]$	[24,108,216,300]
25	$\left[\frac{3}{4},\, -y,\, -y\right]$	[25,85,217,277]
26	$\left[\frac{1}{4},\, y+\frac{1}{2},\, \frac{1}{2}-y\right]$	[26,82,218,274]
27	$\left[\frac{1}{4},\, \frac{1}{2}-y,\, y+\frac{1}{2}\right]$	[27,81,219,273]
28	$\left[\frac{1}{2}-y,\, \frac{1}{2}-y,\, \frac{3}{4}\right]$	[28,186,220,378]
29	$\left[y+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{4}\right]$	[29,187,221,379]
30	$\left[y+\frac{1}{2},\, \frac{1}{4},\, \frac{1}{2}-y\right]$	[30,140,222,332]
31	$\left[\frac{1}{2}-y,\, \frac{3}{4},\, \frac{1}{2}-y\right]$	[31,137,223,329]
32	$\left[\frac{3}{4},\, y,\, y\right]$	[32,86,224,278]
33	$\left[\frac{1}{4},\, -y,\, y\right]$	[33,75,225,267]
34	$\left[\frac{1}{4},\, y,\, -y\right]$	[34,74,226,266]
35	$\left[\frac{1}{2}-y,\, \frac{1}{4},\, y+\frac{1}{2}\right]$	[35,142,227,334]
36	$\left[y+\frac{1}{2},\, \frac{3}{4},\, y+\frac{1}{2}\right]$	[36,144,228,336]
37	$\left[\frac{3}{4},\, \frac{1}{2}-y,\, \frac{1}{2}-y\right]$	[37,73,229,265]
38	$\left[\frac{3}{4},\, y+\frac{1}{2},\, y+\frac{1}{2}\right]$	[38,80,230,272]

continued …

Table 8

No.	position	mapping
39	$\left[\frac{1}{2}-y, y+\frac{1}{2}, \frac{1}{4}\right]$	[39,191,231,383]
40	$\left[y+\frac{1}{2}, y+\frac{1}{2}, \frac{3}{4}\right]$	[40,189,232,381]
41	$\left[-y, \frac{3}{4}, -y\right]$	[41,127,233,319]
42	$\left[-y, -y, \frac{3}{4}\right]$	[42,172,234,364]
43	$\left[y, -y, \frac{1}{4}\right]$	[43,173,235,365]
44	$\left[y, \frac{1}{4}, -y\right]$	[44,126,236,318]
45	$\left[y, y, \frac{3}{4}\right]$	[45,184,237,376]
46	$\left[-y, \frac{1}{4}, y\right]$	[46,131,238,323]
47	$\left[-y, y, \frac{1}{4}\right]$	[47,183,239,375]
48	$\left[y, \frac{3}{4}, y\right]$	[48,132,240,324]
49	$\left[y+\frac{1}{2}, y, \frac{3}{4}\right]$	[52,114,244,306]
50	$\left[\frac{1}{2}-y, y, \frac{1}{4}\right]$	[53,115,245,307]
51	$\left[\frac{1}{2}-y, \frac{1}{4}, y\right]$	[54,164,246,356]
52	$\left[y+\frac{1}{2}, \frac{3}{4}, y\right]$	[55,161,247,353]
53	$\left[y+\frac{1}{2}, \frac{1}{4}, -y\right]$	[59,166,251,358]
54	$\left[\frac{1}{2}-y, \frac{3}{4}, -y\right]$	[60,168,252,360]
55	$\left[y+\frac{1}{2}, -y, \frac{1}{4}\right]$	[63,119,255,311]
56	$\left[\frac{1}{2}-y, -y, \frac{3}{4}\right]$	[64,117,256,309]
57	$\left[y, \frac{3}{4}, y+\frac{1}{2}\right]$	[65,151,257,343]
58	$\left[y, y+\frac{1}{2}, \frac{3}{4}\right]$	[66,100,258,292]
59	$\left[-y, y+\frac{1}{2}, \frac{1}{4}\right]$	[67,101,259,293]
60	$\left[-y, \frac{1}{4}, y+\frac{1}{2}\right]$	[68,150,260,342]
61	$\left[-y, \frac{1}{2}-y, \frac{3}{4}\right]$	[69,112,261,304]
62	$\left[y, \frac{1}{4}, \frac{1}{2}-y\right]$	[70,155,262,347]
63	$\left[y, \frac{1}{2}-y, \frac{1}{4}\right]$	[71,111,263,303]
64	$\left[-y, \frac{3}{4}, \frac{1}{2}-y\right]$	[72,156,264,348]
65	$\left[\frac{1}{2}-y, -y, \frac{1}{4}\right]$	[76,138,268,330]
66	$\left[y+\frac{1}{2}, -y, \frac{3}{4}\right]$	[77,139,269,331]
67	$\left[y+\frac{1}{2}, \frac{3}{4}, -y\right]$	[78,188,270,380]
68	$\left[\frac{1}{2}-y, \frac{1}{4}, -y\right]$	[79,185,271,377]
69	$\left[\frac{1}{2}-y, \frac{3}{4}, y\right]$	[83,190,275,382]
70	$\left[y+\frac{1}{2}, \frac{1}{4}, y\right]$	[84,192,276,384]
71	$\left[\frac{1}{2}-y, y, \frac{3}{4}\right]$	[87,143,279,335]
72	$\left[y+\frac{1}{2}, y, \frac{1}{4}\right]$	[88,141,280,333]
73	$\left[-y, \frac{1}{4}, \frac{1}{2}-y\right]$	[89,175,281,367]
74	$\left[-y, \frac{1}{2}-y, \frac{1}{4}\right]$	[90,124,282,316]
75	$\left[y, \frac{1}{2}-y, \frac{3}{4}\right]$	[91,125,283,317]
76	$\left[y, \frac{3}{4}, \frac{1}{2}-y\right]$	[92,174,284,366]
77	$\left[y, y+\frac{1}{2}, \frac{1}{4}\right]$	[93,136,285,328]
78	$\left[-y, \frac{3}{4}, y+\frac{1}{2}\right]$	[94,179,286,371]
79	$\left[-y, y+\frac{1}{2}, \frac{3}{4}\right]$	[95,135,287,327]
80	$\left[y, \frac{1}{4}, y+\frac{1}{2}\right]$	[96,180,288,372]
81	$\left[\frac{3}{4}, y, y+\frac{1}{2}\right]$	[97,157,289,349]
82	$\left[\frac{1}{4}, \frac{1}{2}-y, y\right]$	[98,154,290,346]
83	$\left[\frac{1}{4}, y+\frac{1}{2}, -y\right]$	[99,153,291,345]
84	$\left[\frac{3}{4}, -y, \frac{1}{2}-y\right]$	[104,158,296,350]
85	$\left[\frac{1}{4}, y, \frac{1}{2}-y\right]$	[105,147,297,339]

continued ...

8

Table 8

No.	position	mapping
86	$\left[\frac{1}{4}, -y, y+\frac{1}{2}\right]$	[106,146,298,338]
87	$\left[\frac{3}{4}, y+\frac{1}{2}, y\right]$	[109,145,301,337]
88	$\left[\frac{3}{4}, \frac{1}{2}-y, -y\right]$	[110,152,302,344]
89	$\left[\frac{1}{4}, -y, \frac{1}{2}-y\right]$	[121,181,313,373]
90	$\left[\frac{3}{4}, y+\frac{1}{2}, -y\right]$	[122,178,314,370]
91	$\left[\frac{3}{4}, \frac{1}{2}-y, y\right]$	[123,177,315,369]
92	$\left[\frac{1}{4}, y, y+\frac{1}{2}\right]$	[128,182,320,374]
93	$\left[\frac{3}{4}, -y, y+\frac{1}{2}\right]$	[129,171,321,363]
94	$\left[\frac{3}{4}, y, \frac{1}{2}-y\right]$	[130,170,322,362]
95	$\left[\frac{1}{4}, \frac{1}{2}-y, -y\right]$	[133,169,325,361]
96	$\left[\frac{1}{4}, y+\frac{1}{2}, y\right]$	[134,176,326,368]

Table 9: Wyckoff site: 96i, site symmetry: m..1'

No.	position	mapping
1	$[0, y, z]$	[1,32,193,224]
2	$\left[\frac{1}{2}, \frac{1}{2}-z, y+\frac{1}{2}\right]$	[2,27,194,219]
3	$\left[\frac{1}{2}, z+\frac{1}{2}, \frac{1}{2}-y\right]$	[3,26,195,218]
4	$\left[z+\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}\right]$	[4,40,196,232]
5	$\left[\frac{1}{2}-z, y+\frac{1}{2}, \frac{1}{2}\right]$	[5,39,197,231]
6	$\left[\frac{1}{2}-y, \frac{1}{2}, z+\frac{1}{2}\right]$	[6,35,198,227]
7	$\left[y+\frac{1}{2}, \frac{1}{2}, z+\frac{1}{2}\right]$	[7,36,199,228]
8	$[0, -y, -z]$	[8,25,200,217]
9	$[0, y, -z]$	[9,34,201,226]
10	$[0, -y, z]$	[10,33,202,225]
11	$\left[y+\frac{1}{2}, \frac{1}{2}, \frac{1}{2}-z\right]$	[11,30,203,222]
12	$\left[\frac{1}{2}-y, \frac{1}{2}, \frac{1}{2}-z\right]$	[12,31,204,223]
13	$\left[\frac{1}{2}, z+\frac{1}{2}, y+\frac{1}{2}\right]$	[13,38,205,230]
14	$\left[\frac{1}{2}, \frac{1}{2}-z, \frac{1}{2}-y\right]$	[14,37,206,229]
15	$\left[z+\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}\right]$	[15,29,207,221]
16	$\left[\frac{1}{2}-z, \frac{1}{2}-y, \frac{1}{2}\right]$	[16,28,208,220]
17	$[z, 0, y]$	[17,48,209,240]
18	$[y, z, 0]$	[18,45,210,237]
19	$[-y, z, 0]$	[19,47,211,239]
20	$[-z, 0, y]$	[20,46,212,238]
21	$[-y, -z, 0]$	[21,42,213,234]
22	$[z, 0, -y]$	[22,44,214,236]
23	$[y, -z, 0]$	[23,43,215,235]
24	$[-z, 0, -y]$	[24,41,216,233]
25	$\left[0, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[49,80,241,272]
26	$\left[\frac{1}{2}, -z, y\right]$	[50,75,242,267]
27	$\left[\frac{1}{2}, z, -y\right]$	[51,74,243,266]
28	$\left[z+\frac{1}{2}, y, 0\right]$	[52,88,244,280]
29	$\left[\frac{1}{2}-z, y, 0\right]$	[53,87,245,279]

continued ...

Table 9

No.	position	mapping
30	$\left[\frac{1}{2}-y,\,0,\,z\right]$	[54,83,246,275]
31	$\left[y+\frac{1}{2},\,0,\,z\right]$	[55,84,247,276]
32	$\left[0,\,\frac{1}{2}-y,\,\frac{1}{2}-z\right]$	[56,73,248,265]
33	$\left[0,\,y+\frac{1}{2},\,\frac{1}{2}-z\right]$	[57,82,249,274]
34	$\left[0,\,\frac{1}{2}-y,\,z+\frac{1}{2}\right]$	[58,81,250,273]
35	$\left[y+\frac{1}{2},\,0,\,-z\right]$	[59,78,251,270]
36	$\left[\frac{1}{2}-y,\,0,\,-z\right]$	[60,79,252,271]
37	$\left[\frac{1}{2},\,z,\,y\right]$	[61,86,253,278]
38	$\left[\frac{1}{2},\,-z,\,-y\right]$	[62,85,254,277]
39	$\left[z+\frac{1}{2},\,-y,\,0\right]$	[63,77,255,269]
40	$\left[\frac{1}{2}-z,\,-y,\,0\right]$	[64,76,256,268]
41	$\left[z,\,\frac{1}{2},\,y+\frac{1}{2}\right]$	[65,96,257,288]
42	$\left[y,\,z+\frac{1}{2},\,\frac{1}{2}\right]$	[66,93,258,285]
43	$\left[-y,\,z+\frac{1}{2},\,\frac{1}{2}\right]$	[67,95,259,287]
44	$\left[-z,\,\frac{1}{2},\,y+\frac{1}{2}\right]$	[68,94,260,286]
45	$\left[-y,\,\frac{1}{2}-z,\,\frac{1}{2}\right]$	[69,90,261,282]
46	$\left[z,\,\frac{1}{2},\,\frac{1}{2}-y\right]$	[70,92,262,284]
47	$\left[y,\,\frac{1}{2}-z,\,\frac{1}{2}\right]$	[71,91,263,283]
48	$\left[-z,\,\frac{1}{2},\,\frac{1}{2}-y\right]$	[72,89,264,281]
49	$\left[\frac{1}{2},\,y,\,z+\frac{1}{2}\right]$	[97,128,289,320]
50	$\left[0,\,\frac{1}{2}-z,\,y\right]$	[98,123,290,315]
51	$\left[0,\,z+\frac{1}{2},\,-y\right]$	[99,122,291,314]
52	$\left[z,\,y+\frac{1}{2},\,0\right]$	[100,136,292,328]
53	$\left[-z,\,y+\frac{1}{2},\,0\right]$	[101,135,293,327]
54	$\left[-y,\,\frac{1}{2},\,z\right]$	[102,131,294,323]
55	$\left[y,\,\frac{1}{2},\,z\right]$	[103,132,295,324]
56	$\left[\frac{1}{2},\,-y,\,\frac{1}{2}-z\right]$	[104,121,296,313]
57	$\left[\frac{1}{2},\,y,\,\frac{1}{2}-z\right]$	[105,130,297,322]
58	$\left[\frac{1}{2},\,-y,\,z+\frac{1}{2}\right]$	[106,129,298,321]
59	$\left[y,\,\frac{1}{2},\,-z\right]$	[107,126,299,318]
60	$\left[-y,\,\frac{1}{2},\,-z\right]$	[108,127,300,319]
61	$\left[0,\,z+\frac{1}{2},\,y\right]$	[109,134,301,326]
62	$\left[0,\,\frac{1}{2}-z,\,-y\right]$	[110,133,302,325]
63	$\left[z,\,\frac{1}{2}-y,\,0\right]$	[111,125,303,317]
64	$\left[-z,\,\frac{1}{2}-y,\,0\right]$	[112,124,304,316]
65	$\left[z+\frac{1}{2},\,0,\,y+\frac{1}{2}\right]$	[113,144,305,336]
66	$\left[y+\frac{1}{2},\,z,\,\frac{1}{2}\right]$	[114,141,306,333]
67	$\left[\frac{1}{2}-y,\,z,\,\frac{1}{2}\right]$	[115,143,307,335]
68	$\left[\frac{1}{2}-z,\,0,\,y+\frac{1}{2}\right]$	[116,142,308,334]
69	$\left[\frac{1}{2}-y,\,-z,\,\frac{1}{2}\right]$	[117,138,309,330]
70	$\left[z+\frac{1}{2},\,0,\,\frac{1}{2}-y\right]$	[118,140,310,332]
71	$\left[y+\frac{1}{2},\,-z,\,\frac{1}{2}\right]$	[119,139,311,331]
72	$\left[\frac{1}{2}-z,\,0,\,\frac{1}{2}-y\right]$	[120,137,312,329]
73	$\left[\frac{1}{2},\,y+\frac{1}{2},\,z\right]$	[145,176,337,368]
74	$\left[0,\,-z,\,y+\frac{1}{2}\right]$	[146,171,338,363]
75	$\left[0,\,z,\,\frac{1}{2}-y\right]$	[147,170,339,362]
76	$\left[z,\,y,\,\frac{1}{2}\right]$	[148,184,340,376]

Table 9

No.	position	mapping
77	$\left[-z,\, y,\, \frac{1}{2}\right]$	[149,183,341,375]
78	$\left[-y,\, 0,\, z+\frac{1}{2}\right]$	[150,179,342,371]
79	$\left[y,\, 0,\, z+\frac{1}{2}\right]$	[151,180,343,372]
80	$\left[\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	[152,169,344,361]
81	$\left[\frac{1}{2},\, y+\frac{1}{2},\, -z\right]$	[153,178,345,370]
82	$\left[\frac{1}{2},\, \frac{1}{2}-y,\, z\right]$	[154,177,346,369]
83	$\left[y,\, 0,\, \frac{1}{2}-z\right]$	[155,174,347,366]
84	$\left[-y,\, 0,\, \frac{1}{2}-z\right]$	[156,175,348,367]
85	$\left[0,\, z,\, y+\frac{1}{2}\right]$	[157,182,349,374]
86	$\left[0,\, -z,\, \frac{1}{2}-y\right]$	[158,181,350,373]
87	$\left[z,\, -y,\, \frac{1}{2}\right]$	[159,173,351,365]
88	$\left[-z,\, -y,\, \frac{1}{2}\right]$	[160,172,352,364]
89	$\left[z+\frac{1}{2},\, \frac{1}{2},\, y\right]$	[161,192,353,384]
90	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, 0\right]$	[162,189,354,381]
91	$\left[\frac{1}{2}-y,\, z+\frac{1}{2},\, 0\right]$	[163,191,355,383]
92	$\left[\frac{1}{2}-z,\, \frac{1}{2},\, y\right]$	[164,190,356,382]
93	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, 0\right]$	[165,186,357,378]
94	$\left[z+\frac{1}{2},\, \frac{1}{2},\, -y\right]$	[166,188,358,380]
95	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, 0\right]$	[167,187,359,379]
96	$\left[\frac{1}{2}-z,\, \frac{1}{2},\, -y\right]$	[168,185,360,377]

Table 10: Wyckoff site: `192j`, site symmetry: `11'`

No.	position	mapping
1	$[x,\, y,\, z]$	[1,193]
2	$\left[x+\frac{1}{2},\, \frac{1}{2}-z,\, y+\frac{1}{2}\right]$	[2,194]
3	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, \frac{1}{2}-y\right]$	[3,195]
4	$\left[z+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}-x\right]$	[4,196]
5	$\left[\frac{1}{2}-z,\, y+\frac{1}{2},\, x+\frac{1}{2}\right]$	[5,197]
6	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[6,198]
7	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$	[7,199]
8	$[x,\, -y,\, -z]$	[8,200]
9	$[-x,\, y,\, -z]$	[9,201]
10	$[-x,\, -y,\, z]$	[10,202]
11	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[11,203]
12	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[12,204]
13	$\left[\frac{1}{2}-x,\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[13,205]
14	$\left[\frac{1}{2}-x,\, \frac{1}{2}-z,\, \frac{1}{2}-y\right]$	[14,206]
15	$\left[z+\frac{1}{2},\, \frac{1}{2}-y,\, x+\frac{1}{2}\right]$	[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	$[-y,\, z,\, -x]$	[19,211]
20	$[-z,\, -x,\, y]$	[20,212]

continued ...

Table 10

No.	position	mapping
21	$[-y, -z, x]$	[21,213]
22	$[z, -x, -y]$	[22,214]
23	$[y, -z, -x]$	[23,215]
24	$[-z, x, -y]$	[24,216]
25	$[-x, -y, -z]$	[25,217]
26	$\left[\frac{1}{2} - x, z + \frac{1}{2}, \frac{1}{2} - y\right]$	[26,218]
27	$\left[\frac{1}{2} - x, \frac{1}{2} - z, y + \frac{1}{2}\right]$	[27,219]
28	$\left[\frac{1}{2} - z, \frac{1}{2} - y, x + \frac{1}{2}\right]$	[28,220]
29	$\left[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - x\right]$	[29,221]
30	$\left[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z\right]$	[30,222]
31	$\left[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z\right]$	[31,223]
32	$[-x, y, z]$	[32,224]
33	$[x, -y, z]$	[33,225]
34	$[x, y, -z]$	[34,226]
35	$\left[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}\right]$	[35,227]
36	$\left[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}\right]$	[36,228]
37	$\left[x + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y\right]$	[37,229]
38	$\left[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}\right]$	[38,230]
39	$\left[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2} - x\right]$	[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	$[y, -z, x]$	[43,235]
44	$[z, x, -y]$	[44,236]
45	$[y, z, -x]$	[45,237]
46	$[-z, x, y]$	[46,238]
47	$[-y, z, x]$	[47,239]
48	$[z, -x, y]$	[48,240]
49	$\left[x, y + \frac{1}{2}, z + \frac{1}{2}\right]$	[49,241]
50	$\left[x + \frac{1}{2}, -z, y\right]$	[50,242]
51	$\left[x + \frac{1}{2}, z, -y\right]$	[51,243]
52	$\left[z + \frac{1}{2}, y, -x\right]$	[52,244]
53	$\left[\frac{1}{2} - z, y, x\right]$	[53,245]
54	$\left[\frac{1}{2} - y, x, z\right]$	[54,246]
55	$\left[y + \frac{1}{2}, -x, z\right]$	[55,247]
56	$\left[x, \frac{1}{2} - y, \frac{1}{2} - z\right]$	[56,248]
57	$\left[-x, y + \frac{1}{2}, \frac{1}{2} - z\right]$	[57,249]
58	$\left[-x, \frac{1}{2} - y, z + \frac{1}{2}\right]$	[58,250]
59	$\left[y + \frac{1}{2}, x, -z\right]$	[59,251]
60	$\left[\frac{1}{2} - y, -x, -z\right]$	[60,252]
61	$\left[\frac{1}{2} - x, z, y\right]$	[61,253]
62	$\left[\frac{1}{2} - x, -z, -y\right]$	[62,254]
63	$\left[z + \frac{1}{2}, -y, x\right]$	[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	$\left[-y, z + \frac{1}{2}, \frac{1}{2} - x\right]$	[67,259]

continued ...

Table 10

No.	position	mapping
68	$\left[-z, \frac{1}{2} - x, y + \frac{1}{2}\right]$	[68,260]
69	$\left[-y, \frac{1}{2} - z, x + \frac{1}{2}\right]$	[69,261]
70	$\left[z, \frac{1}{2} - x, \frac{1}{2} - y\right]$	[70,262]
71	$\left[y, \frac{1}{2} - z, \frac{1}{2} - x\right]$	[71,263]
72	$\left[-z, x + \frac{1}{2}, \frac{1}{2} - y\right]$	[72,264]
73	$\left[-x, \frac{1}{2} - y, \frac{1}{2} - z\right]$	[73,265]
74	$\left[\frac{1}{2} - x, z, -y\right]$	[74,266]
75	$\left[\frac{1}{2} - x, -z, y\right]$	[75,267]
76	$\left[\frac{1}{2} - z, -y, x\right]$	[76,268]
77	$\left[z + \frac{1}{2}, -y, -x\right]$	[77,269]
78	$\left[y + \frac{1}{2}, -x, -z\right]$	[78,270]
79	$\left[\frac{1}{2} - y, x, -z\right]$	[79,271]
80	$\left[-x, y + \frac{1}{2}, z + \frac{1}{2}\right]$	[80,272]
81	$\left[x, \frac{1}{2} - y, z + \frac{1}{2}\right]$	[81,273]
82	$\left[x, y + \frac{1}{2}, \frac{1}{2} - z\right]$	[82,274]
83	$\left[\frac{1}{2} - y, -x, z\right]$	[83,275]
84	$\left[y + \frac{1}{2}, x, z\right]$	[84,276]
85	$\left[x + \frac{1}{2}, -z, -y\right]$	[85,277]
86	$\left[x + \frac{1}{2}, z, y\right]$	[86,278]
87	$\left[\frac{1}{2} - z, y, -x\right]$	[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	$\left[y, \frac{1}{2} - z, x + \frac{1}{2}\right]$	[91,283]
92	$\left[z, x + \frac{1}{2}, \frac{1}{2} - y\right]$	[92,284]
93	$\left[y, z + \frac{1}{2}, \frac{1}{2} - x\right]$	[93,285]
94	$\left[-z, x + \frac{1}{2}, y + \frac{1}{2}\right]$	[94,286]
95	$\left[-y, z + \frac{1}{2}, x + \frac{1}{2}\right]$	[95,287]
96	$\left[z, \frac{1}{2} - x, y + \frac{1}{2}\right]$	[96,288]
97	$\left[x + \frac{1}{2}, y, z + \frac{1}{2}\right]$	[97,289]
98	$\left[x, \frac{1}{2} - z, y\right]$	[98,290]
99	$\left[x, z + \frac{1}{2}, -y\right]$	[99,291]
100	$\left[z, y + \frac{1}{2}, -x\right]$	[100,292]
101	$\left[-z, y + \frac{1}{2}, x\right]$	[101,293]
102	$\left[-y, x + \frac{1}{2}, z\right]$	[102,294]
103	$\left[y, \frac{1}{2} - x, z\right]$	[103,295]
104	$\left[x + \frac{1}{2}, -y, \frac{1}{2} - z\right]$	[104,296]
105	$\left[\frac{1}{2} - x, y, \frac{1}{2} - z\right]$	[105,297]
106	$\left[\frac{1}{2} - x, -y, z + \frac{1}{2}\right]$	[106,298]
107	$\left[y, x + \frac{1}{2}, -z\right]$	[107,299]
108	$\left[-y, \frac{1}{2} - x, -z\right]$	[108,300]
109	$\left[-x, z + \frac{1}{2}, y\right]$	[109,301]
110	$\left[-x, \frac{1}{2} - z, -y\right]$	[110,302]
111	$\left[z, \frac{1}{2} - y, x\right]$	[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]

continued ...

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Table 10

No.	position	mapping
115	$\left[\frac{1}{2} - y, z, \frac{1}{2} - x\right]$	[115,307]
116	$\left[\frac{1}{2} - z, -x, y + \frac{1}{2}\right]$	[116,308]
117	$\left[\frac{1}{2} - y, -z, x + \frac{1}{2}\right]$	[117,309]
118	$\left[z + \frac{1}{2}, -x, \frac{1}{2} - y\right]$	[118,310]
119	$\left[y + \frac{1}{2}, -z, \frac{1}{2} - x\right]$	[119,311]
120	$\left[\frac{1}{2} - z, x, \frac{1}{2} - y\right]$	[120,312]
121	$\left[\frac{1}{2} - x, -y, \frac{1}{2} - z\right]$	[121,313]
122	$\left[-x, z + \frac{1}{2}, -y\right]$	[122,314]
123	$\left[-x, \frac{1}{2} - z, y\right]$	[123,315]
124	$\left[-z, \frac{1}{2} - y, x\right]$	[124,316]
125	$\left[z, \frac{1}{2} - y, -x\right]$	[125,317]
126	$\left[y, \frac{1}{2} - x, -z\right]$	[126,318]
127	$\left[-y, x + \frac{1}{2}, -z\right]$	[127,319]
128	$\left[\frac{1}{2} - x, y, z + \frac{1}{2}\right]$	[128,320]
129	$\left[x + \frac{1}{2}, -y, z + \frac{1}{2}\right]$	[129,321]
130	$\left[x + \frac{1}{2}, y, \frac{1}{2} - z\right]$	[130,322]
131	$\left[-y, \frac{1}{2} - x, z\right]$	[131,323]
132	$\left[y, x + \frac{1}{2}, z\right]$	[132,324]
133	$\left[x, \frac{1}{2} - z, -y\right]$	[133,325]
134	$\left[x, z + \frac{1}{2}, y\right]$	[134,326]
135	$\left[-z, y + \frac{1}{2}, -x\right]$	[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	$\left[y + \frac{1}{2}, -z, x + \frac{1}{2}\right]$	[139,331]
140	$\left[z + \frac{1}{2}, x, \frac{1}{2} - y\right]$	[140,332]
141	$\left[y + \frac{1}{2}, z, \frac{1}{2} - x\right]$	[141,333]
142	$\left[\frac{1}{2} - z, x, y + \frac{1}{2}\right]$	[142,334]
143	$\left[\frac{1}{2} - y, z, x + \frac{1}{2}\right]$	[143,335]
144	$\left[z + \frac{1}{2}, -x, y + \frac{1}{2}\right]$	[144,336]
145	$\left[x + \frac{1}{2}, y + \frac{1}{2}, z\right]$	[145,337]
146	$\left[x, -z, y + \frac{1}{2}\right]$	[146,338]
147	$\left[x, z, \frac{1}{2} - y\right]$	[147,339]
148	$\left[z, y, \frac{1}{2} - x\right]$	[148,340]
149	$\left[-z, y, x + \frac{1}{2}\right]$	[149,341]
150	$\left[-y, x, z + \frac{1}{2}\right]$	[150,342]
151	$\left[y, -x, z + \frac{1}{2}\right]$	[151,343]
152	$\left[x + \frac{1}{2}, \frac{1}{2} - y, -z\right]$	[152,344]
153	$\left[\frac{1}{2} - x, y + \frac{1}{2}, -z\right]$	[153,345]
154	$\left[\frac{1}{2} - x, \frac{1}{2} - y, z\right]$	[154,346]
155	$\left[y, x, \frac{1}{2} - z\right]$	[155,347]
156	$\left[-y, -x, \frac{1}{2} - z\right]$	[156,348]
157	$\left[-x, z, y + \frac{1}{2}\right]$	[157,349]
158	$\left[-x, -z, \frac{1}{2} - y\right]$	[158,350]
159	$\left[z, -y, x + \frac{1}{2}\right]$	[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]

continued ...

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Table 10

No.	position	mapping
162	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, x\right]$	[162,354]
163	$\left[\frac{1}{2}-y,\, z+\frac{1}{2},\, -x\right]$	[163,355]
164	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, y\right]$	[164,356]
165	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, x\right]$	[165,357]
166	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, -y\right]$	[166,358]
167	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, -x\right]$	[167,359]
168	$\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, -y\right]$	[168,360]
169	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, -z\right]$	[169,361]
170	$\left[-x,\, z,\, \frac{1}{2}-y\right]$	[170,362]
171	$\left[-x,\, -z,\, y+\frac{1}{2}\right]$	[171,363]
172	$\left[-z,\, -y,\, x+\frac{1}{2}\right]$	[172,364]
173	$\left[z,\, -y,\, \frac{1}{2}-x\right]$	[173,365]
174	$\left[y,\, -x,\, \frac{1}{2}-z\right]$	[174,366]
175	$\left[-y,\, x,\, \frac{1}{2}-z\right]$	[175,367]
176	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z\right]$	[176,368]
177	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z\right]$	[177,369]
178	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, -z\right]$	[178,370]
179	$\left[-y,\, -x,\, z+\frac{1}{2}\right]$	[179,371]
180	$\left[y,\, x,\, z+\frac{1}{2}\right]$	[180,372]
181	$\left[x,\, -z,\, \frac{1}{2}-y\right]$	[181,373]
182	$\left[x,\, z,\, y+\frac{1}{2}\right]$	[182,374]
183	$\left[-z,\, y,\, \frac{1}{2}-x\right]$	[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	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, x\right]$	[187,379]
188	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, -y\right]$	[188,380]
189	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, -x\right]$	[189,381]
190	$\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, y\right]$	[190,382]
191	$\left[\frac{1}{2}-y,\, z+\frac{1}{2},\, x\right]$	[191,383]
192	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, y\right]$	[192,384]