MSG No. 210.53 $F4_132'$ [Type II, cubic]

Table 1: Wyckoff site: 8a, site symmetry: 23.1'

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

Table 2: Wyckoff site: 8b, site symmetry: 23.1'

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

Table 3: Wyckoff site: 16c, site symmetry: .321'

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

continued ...

Table 3

No.	position	mapping
16	$\left[\frac{5}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[73,84,86,88,89,90,169,180,182,184,185,186]

Table 4: Wyckoff site: 16d, site symmetry: .321'

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

Table 5: Wyckoff site: 32e, site symmetry: .3.1'

No.	position	mapping
1	$[x, x, x]$	[1,17,18,97,113,114]
2	$\left[x+\frac{1}{4}, \frac{1}{4}-x, x+\frac{1}{4}\right]$	[2,7,15,98,103,111]
3	$\left[x+\frac{1}{4}, x+\frac{1}{4}, \frac{1}{4}-x\right]$	[3,4,11,99,100,107]
4	$\left[\frac{1}{4}-x, x+\frac{1}{4}, x+\frac{1}{4}\right]$	[5,6,13,101,102,109]
5	$[x, -x, -x]$	[8,22,23,104,118,119]
6	$[-x, x, -x]$	[9,19,24,105,115,120]
7	$[-x, -x, x]$	[10,20,21,106,116,117]
8	$\left[\frac{1}{4}-x, \frac{1}{4}-x, \frac{1}{4}-x\right]$	[12,14,16,108,110,112]
9	$\left[x, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[25,41,42,121,137,138]
10	$\left[x+\frac{1}{4}, \frac{3}{4}-x, x+\frac{3}{4}\right]$	[26,31,39,122,127,135]
11	$\left[x+\frac{1}{4}, x+\frac{3}{4}, \frac{3}{4}-x\right]$	[27,28,35,123,124,131]
12	$\left[\frac{1}{4}-x, x+\frac{3}{4}, x+\frac{3}{4}\right]$	[29,30,37,125,126,133]
13	$\left[x, \frac{1}{2}-x, \frac{1}{2}-x\right]$	[32,46,47,128,142,143]
14	$\left[-x, x+\frac{1}{2}, \frac{1}{2}-x\right]$	[33,43,48,129,139,144]
15	$\left[-x, \frac{1}{2}-x, x+\frac{1}{2}\right]$	[34,44,45,130,140,141]
16	$\left[\frac{1}{4}-x, \frac{3}{4}-x, \frac{3}{4}-x\right]$	[36,38,40,132,134,136]
17	$\left[x+\frac{1}{2}, x, x+\frac{1}{2}\right]$	[49,65,66,145,161,162]

continued ...

Table 5

No.	position	mapping
18	$\left[x+\frac{3}{4},\ \frac{1}{4}-x,\ x+\frac{3}{4}\right]$	[50,55,63,146,151,159]
19	$\left[x+\frac{3}{4},\ x+\frac{1}{4},\ \frac{3}{4}-x\right]$	[51,52,59,147,148,155]
20	$\left[\frac{3}{4}-x,\ x+\frac{1}{4},\ x+\frac{3}{4}\right]$	[53,54,61,149,150,157]
21	$\left[x+\frac{1}{2},\ -x,\ \frac{1}{2}-x\right]$	[56,70,71,152,166,167]
22	$\left[\frac{1}{2}-x,\ x,\ \frac{1}{2}-x\right]$	[57,67,72,153,163,168]
23	$\left[\frac{1}{2}-x,\ -x,\ x+\frac{1}{2}\right]$	[58,68,69,154,164,165]
24	$\left[\frac{3}{4}-x,\ \frac{1}{4}-x,\ \frac{3}{4}-x\right]$	[60,62,64,156,158,160]
25	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ x\right]$	[73,89,90,169,185,186]
26	$\left[x+\frac{3}{4},\ \frac{3}{4}-x,\ x+\frac{1}{4}\right]$	[74,79,87,170,175,183]
27	$\left[x+\frac{3}{4},\ x+\frac{3}{4},\ \frac{1}{4}-x\right]$	[75,76,83,171,172,179]
28	$\left[\frac{3}{4}-x,\ x+\frac{3}{4},\ x+\frac{1}{4}\right]$	[77,78,85,173,174,181]
29	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ -x\right]$	[80,94,95,176,190,191]
30	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ -x\right]$	[81,91,96,177,187,192]
31	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ x\right]$	[82,92,93,178,188,189]
32	$\left[\frac{3}{4}-x,\ \frac{3}{4}-x,\ \frac{1}{4}-x\right]$	[84,86,88,180,182,184]

Table 6: Wyckoff site: 48f, site symmetry: 2..1'

No.	position	mapping
1	$[x,\ 0,\ 0]$	[1,8,97,104]
2	$\left[x+\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	[2,3,98,99]
3	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}-x\right]$	[4,16,100,112]
4	$\left[\frac{1}{4},\ \frac{1}{4},\ x+\frac{1}{4}\right]$	[5,15,101,111]
5	$\left[\frac{1}{4},\ x+\frac{1}{4},\ \frac{1}{4}\right]$	[6,11,102,107]
6	$\left[\frac{1}{4},\ \frac{1}{4}-x,\ \frac{1}{4}\right]$	[7,12,103,108]
7	$[-x,\ 0,\ 0]$	[9,10,105,106]
8	$\left[\frac{1}{4}-x,\ \frac{1}{4},\ \frac{1}{4}\right]$	[13,14,109,110]
9	$[0,\ x,\ 0]$	[17,24,113,120]
10	$[0,\ 0,\ x]$	[18,21,114,117]
11	$[0,\ 0,\ -x]$	[19,23,115,119]
12	$[0,\ -x,\ 0]$	[20,22,116,118]
13	$\left[x,\ \frac{1}{2},\ \frac{1}{2}\right]$	[25,32,121,128]
14	$\left[x+\frac{1}{4},\ \frac{3}{4},\ \frac{3}{4}\right]$	[26,27,122,123]
15	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{3}{4}-x\right]$	[28,40,124,136]
16	$\left[\frac{1}{4},\ \frac{3}{4},\ x+\frac{3}{4}\right]$	[29,39,125,135]
17	$\left[\frac{1}{4},\ x+\frac{3}{4},\ \frac{3}{4}\right]$	[30,35,126,131]
18	$\left[\frac{1}{4},\ \frac{3}{4}-x,\ \frac{3}{4}\right]$	[31,36,127,132]
19	$\left[-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	[33,34,129,130]
20	$\left[\frac{1}{4}-x,\ \frac{3}{4},\ \frac{3}{4}\right]$	[37,38,133,134]
21	$\left[0,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[41,48,137,144]
22	$\left[0,\ \frac{1}{2},\ x+\frac{1}{2}\right]$	[42,45,138,141]
23	$\left[0,\ \frac{1}{2},\ \frac{1}{2}-x\right]$	[43,47,139,143]
24	$\left[0,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[44,46,140,142]
25	$\left[x+\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	[49,56,145,152]

continued ...

Table 6

No.	position	mapping
26	$\left[x+\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[50,51,146,147]
27	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}-x\right]$	[52,64,148,160]
28	$\left[\frac{3}{4}, \frac{1}{4}, x+\frac{3}{4}\right]$	[53,63,149,159]
29	$\left[\frac{3}{4}, x+\frac{1}{4}, \frac{3}{4}\right]$	[54,59,150,155]
30	$\left[\frac{3}{4}, \frac{1}{4}-x, \frac{3}{4}\right]$	[55,60,151,156]
31	$\left[\frac{1}{2}-x, 0, \frac{1}{2}\right]$	[57,58,153,154]
32	$\left[\frac{3}{4}-x, \frac{1}{4}, \frac{3}{4}\right]$	[61,62,157,158]
33	$\left[\frac{1}{2}, x, \frac{1}{2}\right]$	[65,72,161,168]
34	$\left[\frac{1}{2}, 0, x+\frac{1}{2}\right]$	[66,69,162,165]
35	$\left[\frac{1}{2}, 0, \frac{1}{2}-x\right]$	[67,71,163,167]
36	$\left[\frac{1}{2}, -x, \frac{1}{2}\right]$	[68,70,164,166]
37	$\left[x+\frac{1}{2}, \frac{1}{2}, 0\right]$	[73,80,169,176]
38	$\left[x+\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[74,75,170,171]
39	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}-x\right]$	[76,88,172,184]
40	$\left[\frac{3}{4}, \frac{3}{4}, x+\frac{1}{4}\right]$	[77,87,173,183]
41	$\left[\frac{3}{4}, x+\frac{3}{4}, \frac{1}{4}\right]$	[78,83,174,179]
42	$\left[\frac{3}{4}, \frac{3}{4}-x, \frac{1}{4}\right]$	[79,84,175,180]
43	$\left[\frac{1}{2}-x, \frac{1}{2}, 0\right]$	[81,82,177,178]
44	$\left[\frac{3}{4}-x, \frac{3}{4}, \frac{1}{4}\right]$	[85,86,181,182]
45	$\left[\frac{1}{2}, x+\frac{1}{2}, 0\right]$	[89,96,185,192]
46	$\left[\frac{1}{2}, \frac{1}{2}, x\right]$	[90,93,186,189]
47	$\left[\frac{1}{2}, \frac{1}{2}, -x\right]$	[91,95,187,191]
48	$\left[\frac{1}{2}, \frac{1}{2}-x, 0\right]$	[92,94,188,190]

Table 7: Wyckoff site: 48g, site symmetry: ..21'

No.	position	mapping
1	$\left[\frac{1}{8}, y, \frac{1}{4}-y\right]$	[1,14,97,110]
2	$\left[\frac{3}{8}, y, y+\frac{1}{4}\right]$	[2,57,98,153]
3	$\left[\frac{3}{8}, \frac{1}{2}-y, \frac{1}{4}-y\right]$	[3,82,99,178]
4	$\left[\frac{1}{2}-y, y+\frac{1}{4}, \frac{1}{8}\right]$	[4,93,100,189]
5	$\left[y, y+\frac{1}{4}, \frac{3}{8}\right]$	[5,47,101,143]
6	$\left[\frac{1}{4}-y, \frac{3}{8}, \frac{1}{2}-y\right]$	[6,46,102,142]
7	$\left[y+\frac{1}{4}, \frac{1}{8}, \frac{1}{2}-y\right]$	[7,72,103,168]
8	$\left[\frac{1}{8}, -y, y+\frac{3}{4}\right]$	[8,37,104,133]
9	$\left[\frac{7}{8}, y, y+\frac{3}{4}\right]$	[9,50,105,146]
10	$\left[\frac{7}{8}, -y, \frac{1}{4}-y\right]$	[10,75,106,171]
11	$\left[y+\frac{1}{4}, \frac{3}{8}, y\right]$	[11,92,107,188]
12	$\left[\frac{1}{4}-y, \frac{1}{8}, y\right]$	[12,17,108,113]
13	$\left[\frac{1}{8}, \frac{1}{2}-y, y+\frac{1}{4}\right]$	[13,32,109,128]
14	$\left[\frac{1}{2}-y, \frac{1}{4}-y, \frac{3}{8}\right]$	[15,67,111,163]
15	$\left[y, \frac{1}{4}-y, \frac{1}{8}\right]$	[16,18,112,114]
16	$\left[-y, \frac{1}{4}-y, \frac{7}{8}\right]$	[19,63,115,159]
17	$\left[y+\frac{3}{4}, \frac{7}{8}, y\right]$	[20,83,116,179]

continued ...

Table 7

No.	position	mapping
18	$\left[-y,\, y+\frac{3}{4},\, \frac{1}{8}\right]$	[21,76,117,172]
19	$\left[\frac{1}{4}-y,\, \frac{7}{8},\, -y\right]$	[22,30,118,126]
20	$\left[y,\, y+\frac{3}{4},\, \frac{7}{8}\right]$	[23,29,119,125]
21	$\left[y+\frac{3}{4},\, \frac{1}{8},\, -y\right]$	[24,55,120,151]
22	$\left[\frac{1}{8},\, y+\frac{1}{2},\, \frac{3}{4}-y\right]$	[25,38,121,134]
23	$\left[\frac{3}{8},\, y+\frac{1}{2},\, y+\frac{3}{4}\right]$	[26,81,122,177]
24	$\left[\frac{3}{8},\, -y,\, \frac{3}{4}-y\right]$	[27,58,123,154]
25	$\left[\frac{1}{2}-y,\, y+\frac{3}{4},\, \frac{5}{8}\right]$	[28,69,124,165]
26	$\left[y+\frac{1}{4},\, \frac{5}{8},\, -y\right]$	[31,96,127,192]
27	$\left[\frac{7}{8},\, y+\frac{1}{2},\, y+\frac{1}{4}\right]$	[33,74,129,170]
28	$\left[\frac{7}{8},\, \frac{1}{2}-y,\, \frac{3}{4}-y\right]$	[34,51,130,147]
29	$\left[y+\frac{1}{4},\, \frac{7}{8},\, y+\frac{1}{2}\right]$	[35,68,131,164]
30	$\left[\frac{1}{4}-y,\, \frac{5}{8},\, y+\frac{1}{2}\right]$	[36,41,132,137]
31	$\left[\frac{1}{2}-y,\, \frac{3}{4}-y,\, \frac{7}{8}\right]$	[39,91,135,187]
32	$\left[y,\, \frac{3}{4}-y,\, \frac{5}{8}\right]$	[40,42,136,138]
33	$\left[-y,\, \frac{3}{4}-y,\, \frac{3}{8}\right]$	[43,87,139,183]
34	$\left[y+\frac{3}{4},\, \frac{3}{8},\, y+\frac{1}{2}\right]$	[44,59,140,155]
35	$\left[-y,\, y+\frac{1}{4},\, \frac{5}{8}\right]$	[45,52,141,148]
36	$\left[y+\frac{3}{4},\, \frac{5}{8},\, \frac{1}{2}-y\right]$	[48,79,144,175]
37	$\left[\frac{5}{8},\, y,\, \frac{3}{4}-y\right]$	[49,62,145,158]
38	$\left[y+\frac{1}{2},\, y+\frac{1}{4},\, \frac{7}{8}\right]$	[53,95,149,191]
39	$\left[\frac{3}{4}-y,\, \frac{3}{8},\, -y\right]$	[54,94,150,190]
40	$\left[\frac{5}{8},\, -y,\, y+\frac{1}{4}\right]$	[56,85,152,181]
41	$\left[\frac{3}{4}-y,\, \frac{1}{8},\, y+\frac{1}{2}\right]$	[60,65,156,161]
42	$\left[\frac{5}{8},\, \frac{1}{2}-y,\, y+\frac{3}{4}\right]$	[61,80,157,176]
43	$\left[y+\frac{1}{2},\, \frac{1}{4}-y,\, \frac{5}{8}\right]$	[64,66,160,162]
44	$\left[\frac{3}{4}-y,\, \frac{7}{8},\, \frac{1}{2}-y\right]$	[70,78,166,174]
45	$\left[y+\frac{1}{2},\, y+\frac{3}{4},\, \frac{3}{8}\right]$	[71,77,167,173]
46	$\left[\frac{5}{8},\, y+\frac{1}{2},\, \frac{1}{4}-y\right]$	[73,86,169,182]
47	$\left[\frac{3}{4}-y,\, \frac{5}{8},\, y\right]$	[84,89,180,185]
48	$\left[y+\frac{1}{2},\, \frac{3}{4}-y,\, \frac{1}{8}\right]$	[88,90,184,186]

Table 8: Wyckoff site: 96h, site symmetry: 11'

No.	position	mapping
1	$[x,\, y,\, z]$	[1,97]
2	$\left[x+\frac{1}{4},\, \frac{1}{4}-z,\, y+\frac{1}{4}\right]$	[2,98]
3	$\left[x+\frac{1}{4},\, z+\frac{1}{4},\, \frac{1}{4}-y\right]$	[3,99]
4	$\left[z+\frac{1}{4},\, y+\frac{1}{4},\, \frac{1}{4}-x\right]$	[4,100]
5	$\left[\frac{1}{4}-z,\, y+\frac{1}{4},\, x+\frac{1}{4}\right]$	[5,101]
6	$\left[\frac{1}{4}-y,\, x+\frac{1}{4},\, z+\frac{1}{4}\right]$	[6,102]
7	$\left[y+\frac{1}{4},\, \frac{1}{4}-x,\, z+\frac{1}{4}\right]$	[7,103]
8	$[x,\, -y,\, -z]$	[8,104]
9	$[-x,\, y,\, -z]$	[9,105]

continued ...

Table 8

No.	position	mapping
10	$[-x, -y, z]$	[10,106]
11	$\left[y+\frac{1}{4}, x+\frac{1}{4}, \frac{1}{4}-z\right]$	[11,107]
12	$\left[\frac{1}{4}-y, \frac{1}{4}-x, \frac{1}{4}-z\right]$	[12,108]
13	$\left[\frac{1}{4}-x, z+\frac{1}{4}, y+\frac{1}{4}\right]$	[13,109]
14	$\left[\frac{1}{4}-x, \frac{1}{4}-z, \frac{1}{4}-y\right]$	[14,110]
15	$\left[z+\frac{1}{4}, \frac{1}{4}-y, x+\frac{1}{4}\right]$	[15,111]
16	$\left[\frac{1}{4}-z, \frac{1}{4}-y, \frac{1}{4}-x\right]$	[16,112]
17	$[z, x, y]$	[17,113]
18	$[y, z, x]$	[18,114]
19	$[-y, z, -x]$	[19,115]
20	$[-z, -x, y]$	[20,116]
21	$[-y, -z, x]$	[21,117]
22	$[z, -x, -y]$	[22,118]
23	$[y, -z, -x]$	[23,119]
24	$[-z, x, -y]$	[24,120]
25	$\left[x, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[25,121]
26	$\left[x+\frac{1}{4}, \frac{3}{4}-z, y+\frac{3}{4}\right]$	[26,122]
27	$\left[x+\frac{1}{4}, z+\frac{3}{4}, \frac{3}{4}-y\right]$	[27,123]
28	$\left[z+\frac{1}{4}, y+\frac{3}{4}, \frac{3}{4}-x\right]$	[28,124]
29	$\left[\frac{1}{4}-z, y+\frac{3}{4}, x+\frac{3}{4}\right]$	[29,125]
30	$\left[\frac{1}{4}-y, x+\frac{3}{4}, z+\frac{3}{4}\right]$	[30,126]
31	$\left[y+\frac{1}{4}, \frac{3}{4}-x, z+\frac{3}{4}\right]$	[31,127]
32	$\left[x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[32,128]
33	$\left[-x, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[33,129]
34	$\left[-x, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[34,130]
35	$\left[y+\frac{1}{4}, x+\frac{3}{4}, \frac{3}{4}-z\right]$	[35,131]
36	$\left[\frac{1}{4}-y, \frac{3}{4}-x, \frac{3}{4}-z\right]$	[36,132]
37	$\left[\frac{1}{4}-x, z+\frac{3}{4}, y+\frac{3}{4}\right]$	[37,133]
38	$\left[\frac{1}{4}-x, \frac{3}{4}-z, \frac{3}{4}-y\right]$	[38,134]
39	$\left[z+\frac{1}{4}, \frac{3}{4}-y, x+\frac{3}{4}\right]$	[39,135]
40	$\left[\frac{1}{4}-z, \frac{3}{4}-y, \frac{3}{4}-x\right]$	[40,136]
41	$\left[z, x+\frac{1}{2}, y+\frac{1}{2}\right]$	[41,137]
42	$\left[y, z+\frac{1}{2}, x+\frac{1}{2}\right]$	[42,138]
43	$\left[-y, z+\frac{1}{2}, \frac{1}{2}-x\right]$	[43,139]
44	$\left[-z, \frac{1}{2}-x, y+\frac{1}{2}\right]$	[44,140]
45	$\left[-y, \frac{1}{2}-z, x+\frac{1}{2}\right]$	[45,141]
46	$\left[z, \frac{1}{2}-x, \frac{1}{2}-y\right]$	[46,142]
47	$\left[y, \frac{1}{2}-z, \frac{1}{2}-x\right]$	[47,143]
48	$\left[-z, x+\frac{1}{2}, \frac{1}{2}-y\right]$	[48,144]
49	$\left[x+\frac{1}{2}, y, z+\frac{1}{2}\right]$	[49,145]
50	$\left[x+\frac{3}{4}, \frac{1}{4}-z, y+\frac{3}{4}\right]$	[50,146]
51	$\left[x+\frac{3}{4}, z+\frac{1}{4}, \frac{3}{4}-y\right]$	[51,147]
52	$\left[z+\frac{3}{4}, y+\frac{1}{4}, \frac{3}{4}-x\right]$	[52,148]
53	$\left[\frac{3}{4}-z, y+\frac{1}{4}, x+\frac{3}{4}\right]$	[53,149]
54	$\left[\frac{3}{4}-y, x+\frac{1}{4}, z+\frac{3}{4}\right]$	[54,150]
55	$\left[y+\frac{3}{4}, \frac{1}{4}-x, z+\frac{3}{4}\right]$	[55,151]
56	$\left[x+\frac{1}{2}, -y, \frac{1}{2}-z\right]$	[56,152]

continued ...

Table 8

No.	position	mapping
57	$\left[\frac{1}{2}-x,\, y,\, \frac{1}{2}-z\right]$	[57,153]
58	$\left[\frac{1}{2}-x,\, -y,\, z+\frac{1}{2}\right]$	[58,154]
59	$\left[y+\frac{3}{4},\, x+\frac{1}{4},\, \frac{3}{4}-z\right]$	[59,155]
60	$\left[\frac{3}{4}-y,\, \frac{1}{4}-x,\, \frac{3}{4}-z\right]$	[60,156]
61	$\left[\frac{3}{4}-x,\, z+\frac{1}{4},\, y+\frac{3}{4}\right]$	[61,157]
62	$\left[\frac{3}{4}-x,\, \frac{1}{4}-z,\, \frac{3}{4}-y\right]$	[62,158]
63	$\left[z+\frac{3}{4},\, \frac{1}{4}-y,\, x+\frac{3}{4}\right]$	[63,159]
64	$\left[\frac{3}{4}-z,\, \frac{1}{4}-y,\, \frac{3}{4}-x\right]$	[64,160]
65	$\left[z+\frac{1}{2},\, x,\, y+\frac{1}{2}\right]$	[65,161]
66	$\left[y+\frac{1}{2},\, z,\, x+\frac{1}{2}\right]$	[66,162]
67	$\left[\frac{1}{2}-y,\, z,\, \frac{1}{2}-x\right]$	[67,163]
68	$\left[\frac{1}{2}-z,\, -x,\, y+\frac{1}{2}\right]$	[68,164]
69	$\left[\frac{1}{2}-y,\, -z,\, x+\frac{1}{2}\right]$	[69,165]
70	$\left[z+\frac{1}{2},\, -x,\, \frac{1}{2}-y\right]$	[70,166]
71	$\left[y+\frac{1}{2},\, -z,\, \frac{1}{2}-x\right]$	[71,167]
72	$\left[\frac{1}{2}-z,\, x,\, \frac{1}{2}-y\right]$	[72,168]
73	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z\right]$	[73,169]
74	$\left[x+\frac{3}{4},\, \frac{3}{4}-z,\, y+\frac{1}{4}\right]$	[74,170]
75	$\left[x+\frac{3}{4},\, z+\frac{3}{4},\, \frac{1}{4}-y\right]$	[75,171]
76	$\left[z+\frac{3}{4},\, y+\frac{3}{4},\, \frac{1}{4}-x\right]$	[76,172]
77	$\left[\frac{3}{4}-z,\, y+\frac{3}{4},\, x+\frac{1}{4}\right]$	[77,173]
78	$\left[\frac{3}{4}-y,\, x+\frac{3}{4},\, z+\frac{1}{4}\right]$	[78,174]
79	$\left[y+\frac{3}{4},\, \frac{3}{4}-x,\, z+\frac{1}{4}\right]$	[79,175]
80	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	[80,176]
81	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, -z\right]$	[81,177]
82	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z\right]$	[82,178]
83	$\left[y+\frac{3}{4},\, x+\frac{3}{4},\, \frac{1}{4}-z\right]$	[83,179]
84	$\left[\frac{3}{4}-y,\, \frac{3}{4}-x,\, \frac{1}{4}-z\right]$	[84,180]
85	$\left[\frac{3}{4}-x,\, z+\frac{3}{4},\, y+\frac{1}{4}\right]$	[85,181]
86	$\left[\frac{3}{4}-x,\, \frac{3}{4}-z,\, \frac{1}{4}-y\right]$	[86,182]
87	$\left[z+\frac{3}{4},\, \frac{3}{4}-y,\, x+\frac{1}{4}\right]$	[87,183]
88	$\left[\frac{3}{4}-z,\, \frac{3}{4}-y,\, \frac{1}{4}-x\right]$	[88,184]
89	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, y\right]$	[89,185]
90	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, x\right]$	[90,186]
91	$\left[\frac{1}{2}-y,\, z+\frac{1}{2},\, -x\right]$	[91,187]
92	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, y\right]$	[92,188]
93	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, x\right]$	[93,189]
94	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, -y\right]$	[94,190]
95	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, -x\right]$	[95,191]
96	$\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, -y\right]$	[96,192]