MSG No. 230.146 $Ia\bar{3}d1'$ [Type II, cubic]

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

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

Table 2: Wyckoff site: `16b`, 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	$\left[\frac{3}{8}, \frac{1}{8}, \frac{7}{8}\right]$	[2,7,9,15,19,24,98,103,105,111,115,120]
3	$\left[\frac{7}{8}, \frac{3}{8}, \frac{1}{8}\right]$	[3,4,10,11,20,21,99,100,106,107,116,117]
4	$\left[\frac{1}{8}, \frac{7}{8}, \frac{3}{8}\right]$	[5,6,8,13,22,23,101,102,104,109,118,119]
5	$\left[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}\right]$	[25,41,42,84,86,88,121,137,138,180,182,184]
6	$\left[\frac{1}{8}, \frac{3}{8}, \frac{5}{8}\right]$	[26,31,39,81,91,96,122,127,135,177,187,192]
7	$\left[\frac{5}{8}, \frac{1}{8}, \frac{3}{8}\right]$	[27,28,35,82,92,93,123,124,131,178,188,189]
8	$\left[\frac{3}{8}, \frac{5}{8}, \frac{1}{8}\right]$	[29,30,37,80,94,95,125,126,133,176,190,191]
9	$\left[\frac{7}{8}, \frac{1}{8}, \frac{5}{8}\right]$	[32,46,47,77,78,85,128,142,143,173,174,181]
10	$\left[\frac{5}{8}, \frac{7}{8}, \frac{1}{8}\right]$	[33,43,48,74,79,87,129,139,144,170,175,183]
11	$\left[\frac{1}{8}, \frac{5}{8}, \frac{7}{8}\right]$	[34,44,45,75,76,83,130,140,141,171,172,179]
12	$\left[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}\right]$	[36,38,40,73,89,90,132,134,136,169,185,186]
13	$\left[\frac{5}{8}, \frac{5}{8}, \frac{5}{8}\right]$	[49,60,62,64,65,66,145,156,158,160,161,162]
14	$\left[\frac{7}{8}, \frac{5}{8}, \frac{3}{8}\right]$	[50,55,57,63,67,72,146,151,153,159,163,168]
15	$\left[\frac{3}{8}, \frac{7}{8}, \frac{5}{8}\right]$	[51,52,58,59,68,69,147,148,154,155,164,165]
16	$\left[\frac{5}{8}, \frac{3}{8}, \frac{7}{8}\right]$	[53,54,56,61,70,71,149,150,152,157,166,167]

Table 3: Wyckoff site: `24c`, site symmetry: `2.221'`

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

Table 4: Wyckoff site: `24d`, site symmetry: `-4..1'`

No.	position	mapping
1	$\left[\frac{3}{8}, 0, \frac{1}{4}\right]$	`[1,8,27,74,97,104,123,170]`
2	$\left[\frac{5}{8}, 0, \frac{3}{4}\right]$	`[2,25,32,51,98,121,128,147]`
3	$\left[\frac{1}{8}, \frac{1}{2}, \frac{1}{4}\right]$	`[3,50,73,80,99,146,169,176]`
4	$\left[0, \frac{1}{4}, \frac{7}{8}\right]$	`[4,16,47,91,100,112,143,187]`
5	$\left[0, \frac{3}{4}, \frac{5}{8}\right]$	`[5,42,45,63,101,138,141,159]`
6	$\left[\frac{1}{4}, \frac{1}{8}, \frac{1}{2}\right]$	`[6,59,89,96,102,155,185,192]`
7	$\left[\frac{1}{4}, \frac{7}{8}, 0\right]$	`[7,12,44,94,103,108,140,190]`
8	$\left[\frac{1}{8}, 0, \frac{3}{4}\right]$	`[9,58,85,86,105,154,181,182]`
9	$\left[\frac{5}{8}, \frac{1}{2}, \frac{1}{4}\right]$	`[10,37,38,57,106,133,134,153]`
10	$\left[\frac{3}{4}, \frac{5}{8}, 0\right]$	`[11,41,48,54,107,137,144,150]`
11	$\left[\frac{7}{8}, 0, \frac{1}{4}\right]$	`[13,14,33,82,109,110,129,178]`
12	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{8}\right]$	`[15,53,90,93,111,149,186,189]`
13	$\left[\frac{1}{4}, \frac{3}{8}, 0\right]$	`[17,24,30,83,113,120,126,179]`
14	$\left[0, \frac{1}{4}, \frac{3}{8}\right]$	`[18,21,39,77,114,117,135,173]`
15	$\left[\frac{1}{2}, \frac{1}{4}, \frac{5}{8}\right]$	`[19,28,40,71,115,124,136,167]`

continued ...

Table 4

No.	position	mapping
16	$\left[\frac{3}{4}, \frac{1}{8}, 0\right]$	[20,70,79,84,116,166,175,180]
17	$\left[\frac{1}{4}, \frac{5}{8}, \frac{1}{2}\right]$	[22,31,36,68,118,127,132,164]
18	$\left[0, \frac{3}{4}, \frac{1}{8}\right]$	[23,67,76,88,119,163,172,184]
19	$\left[\frac{7}{8}, \frac{1}{2}, \frac{3}{4}\right]$	[26,49,56,75,122,145,152,171]
20	$\left[\frac{1}{2}, \frac{3}{4}, \frac{7}{8}\right]$	[29,66,69,87,125,162,165,183]
21	$\left[\frac{3}{8}, \frac{1}{2}, \frac{3}{4}\right]$	[34,61,62,81,130,157,158,177]
22	$\left[\frac{3}{4}, \frac{7}{8}, \frac{1}{2}\right]$	[35,65,72,78,131,161,168,174]
23	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{8}\right]$	[43,52,64,95,139,148,160,191]
24	$\left[\frac{3}{4}, \frac{3}{8}, \frac{1}{2}\right]$	[46,55,60,92,142,151,156,188]

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

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

continued ...

Table 5

No.	position	mapping
32	$\left[x+\frac{3}{4}, x+\frac{3}{4}, x+\frac{3}{4}\right]$	[84,86,88,180,182,184]

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

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

continued ...

Table 6

No.	position	mapping
40	$\left[\frac{3}{4}-x,\ \frac{1}{2},\ \frac{3}{4}\right]$	[61,62,157,158]
41	$\left[\frac{3}{4},\ x+\frac{1}{2},\ \frac{1}{2}\right]$	[65,72,161,168]
42	$\left[\frac{1}{2},\ \frac{3}{4},\ x+\frac{1}{2}\right]$	[66,69,162,165]
43	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{4}\right]$	[73,80,169,176]
44	$\left[0,\ \frac{3}{4},\ x+\frac{3}{4}\right]$	[76,88,172,184]
45	$\left[\frac{3}{4},\ x+\frac{3}{4},\ 0\right]$	[79,84,175,180]
46	$\left[x+\frac{3}{4},\ 0,\ \frac{3}{4}\right]$	[85,86,181,182]
47	$\left[\frac{1}{4},\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	[89,96,185,192]
48	$\left[\frac{1}{2},\ \frac{1}{4},\ \frac{1}{2}-x\right]$	[90,93,186,189]

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	$\left[\frac{3}{8},\ y,\ y+\frac{3}{4}\right]$	[2,9,98,105]
3	$\left[\frac{7}{8},\ \frac{1}{2}-y,\ \frac{1}{4}-y\right]$	[3,10,99,106]
4	$\left[-y,\ y+\frac{1}{4},\ \frac{1}{8}\right]$	[4,21,100,117]
5	$\left[y,\ y+\frac{3}{4},\ \frac{3}{8}\right]$	[5,23,101,119]
6	$\left[\frac{1}{4}-y,\ \frac{7}{8},\ \frac{1}{2}-y\right]$	[6,22,102,118]
7	$\left[y+\frac{1}{4},\ \frac{1}{8},\ -y\right]$	[7,24,103,120]
8	$\left[\frac{1}{8},\ -y,\ y+\frac{1}{4}\right]$	[8,13,104,109]
9	$\left[y+\frac{3}{4},\ \frac{3}{8},\ y\right]$	[11,20,107,116]
10	$\left[\frac{1}{4}-y,\ \frac{1}{8},\ y\right]$	[12,17,108,113]
11	$\left[\frac{1}{2}-y,\ \frac{1}{4}-y,\ \frac{7}{8}\right]$	[15,19,111,115]
12	$\left[y,\ \frac{1}{4}-y,\ \frac{1}{8}\right]$	[16,18,112,114]
13	$\left[\frac{7}{8},\ -y,\ y+\frac{3}{4}\right]$	[25,86,121,182]
14	$\left[\frac{1}{8},\ \frac{1}{2}-y,\ \frac{3}{4}-y\right]$	[26,81,122,177]
15	$\left[\frac{5}{8},\ y,\ y+\frac{1}{4}\right]$	[27,82,123,178]
16	$\left[y+\frac{1}{2},\ \frac{1}{4}-y,\ \frac{3}{8}\right]$	[28,93,124,189]
17	$\left[\frac{1}{2}-y,\ \frac{3}{4}-y,\ \frac{1}{8}\right]$	[29,95,125,191]
18	$\left[y+\frac{1}{4},\ \frac{5}{8},\ y\right]$	[30,94,126,190]
19	$\left[\frac{1}{4}-y,\ \frac{3}{8},\ y+\frac{1}{2}\right]$	[31,96,127,192]
20	$\left[\frac{7}{8},\ y,\ \frac{3}{4}-y\right]$	[32,85,128,181]
21	$\left[\frac{5}{8},\ -y,\ \frac{1}{4}-y\right]$	[33,74,129,170]
22	$\left[\frac{1}{8},\ y+\frac{1}{2},\ y+\frac{3}{4}\right]$	[34,75,130,171]
23	$\left[\frac{3}{4}-y,\ \frac{1}{8},\ \frac{1}{2}-y\right]$	[35,92,131,188]
24	$\left[y+\frac{1}{4},\ \frac{3}{8},\ \frac{1}{2}-y\right]$	[36,89,132,185]
25	$\left[\frac{3}{8},\ y+\frac{1}{2},\ \frac{1}{4}-y\right]$	[37,80,133,176]
26	$\left[\frac{3}{8},\ \frac{1}{2}-y,\ y+\frac{1}{4}\right]$	[38,73,134,169]
27	$\left[y,\ y+\frac{1}{4},\ \frac{5}{8}\right]$	[39,91,135,187]
28	$\left[\frac{1}{2}-y,\ y+\frac{1}{4},\ \frac{3}{8}\right]$	[40,90,136,186]
29	$\left[y+\frac{3}{4},\ \frac{7}{8},\ -y\right]$	[41,84,137,180]
30	$\left[-y,\ y+\frac{3}{4},\ \frac{7}{8}\right]$	[42,88,138,184]
31	$\left[y+\frac{1}{2},\ y+\frac{3}{4},\ \frac{1}{8}\right]$	[43,87,139,183]

continued ...

Table 7

No.	position	mapping
32	$\left[\frac{1}{4}-y,\ \frac{5}{8},\ -y\right]$	[44,83,140,179]
33	$\left[y,\ \frac{3}{4}-y,\ \frac{7}{8}\right]$	[45,76,141,172]
34	$\left[y+\frac{3}{4},\ \frac{1}{8},\ y+\frac{1}{2}\right]$	[46,78,142,174]
35	$\left[-y,\ \frac{1}{4}-y,\ \frac{5}{8}\right]$	[47,77,143,173]
36	$\left[\frac{3}{4}-y,\ \frac{7}{8},\ y\right]$	[48,79,144,175]
37	$\left[\frac{5}{8},\ y+\frac{1}{2},\ \frac{3}{4}-y\right]$	[49,62,145,158]
38	$\left[\frac{7}{8},\ y+\frac{1}{2},\ y+\frac{1}{4}\right]$	[50,57,146,153]
39	$\left[\frac{3}{8},\ -y,\ \frac{3}{4}-y\right]$	[51,58,147,154]
40	$\left[\frac{1}{2}-y,\ y+\frac{3}{4},\ \frac{5}{8}\right]$	[52,69,148,165]
41	$\left[y+\frac{1}{2},\ y+\frac{1}{4},\ \frac{7}{8}\right]$	[53,71,149,167]
42	$\left[\frac{3}{4}-y,\ \frac{3}{8},\ -y\right]$	[54,70,150,166]
43	$\left[y+\frac{3}{4},\ \frac{5}{8},\ \frac{1}{2}-y\right]$	[55,72,151,168]
44	$\left[\frac{5}{8},\ \frac{1}{2}-y,\ y+\frac{3}{4}\right]$	[56,61,152,157]
45	$\left[y+\frac{1}{4},\ \frac{7}{8},\ y+\frac{1}{2}\right]$	[59,68,155,164]
46	$\left[\frac{3}{4}-y,\ \frac{5}{8},\ y+\frac{1}{2}\right]$	[60,65,156,161]
47	$\left[-y,\ \frac{3}{4}-y,\ \frac{3}{8}\right]$	[63,67,159,163]
48	$\left[y+\frac{1}{2},\ \frac{3}{4}-y,\ \frac{5}{8}\right]$	[64,66,160,162]

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

No.	position	mapping
1	$[x,\ y,\ z]$	[1,97]
2	$\left[x+\frac{1}{4},\ \frac{1}{4}-z,\ y+\frac{3}{4}\right]$	[2,98]
3	$\left[x+\frac{3}{4},\ z+\frac{1}{4},\ \frac{1}{4}-y\right]$	[3,99]
4	$\left[z+\frac{3}{4},\ y+\frac{1}{4},\ \frac{1}{4}-x\right]$	[4,100]
5	$\left[\frac{1}{4}-z,\ y+\frac{3}{4},\ x+\frac{1}{4}\right]$	[5,101]
6	$\left[\frac{1}{4}-y,\ x+\frac{3}{4},\ z+\frac{1}{4}\right]$	[6,102]
7	$\left[y+\frac{1}{4},\ \frac{1}{4}-x,\ z+\frac{3}{4}\right]$	[7,103]
8	$\left[x,\ -y,\ \frac{1}{2}-z\right]$	[8,104]
9	$\left[\frac{1}{2}-x,\ y,\ -z\right]$	[9,105]
10	$\left[-x,\ \frac{1}{2}-y,\ z\right]$	[10,106]
11	$\left[y+\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{4}-z\right]$	[11,107]
12	$\left[\frac{1}{4}-y,\ \frac{1}{4}-x,\ \frac{1}{4}-z\right]$	[12,108]
13	$\left[\frac{1}{4}-x,\ z+\frac{3}{4},\ y+\frac{1}{4}\right]$	[13,109]
14	$\left[\frac{1}{4}-x,\ \frac{1}{4}-z,\ \frac{1}{4}-y\right]$	[14,110]
15	$\left[z+\frac{1}{4},\ \frac{1}{4}-y,\ x+\frac{3}{4}\right]$	[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	$\left[\frac{1}{2}-y,\ z,\ -x\right]$	[19,115]
20	$\left[-z,\ \frac{1}{2}-x,\ y\right]$	[20,116]
21	$\left[-y,\ \frac{1}{2}-z,\ x\right]$	[21,117]
22	$\left[z,\ -x,\ \frac{1}{2}-y\right]$	[22,118]
23	$\left[y,\ -z,\ \frac{1}{2}-x\right]$	[23,119]

continued ...

Table 8

No.	position	mapping
24	$\left[\frac{1}{2}-z,\, x,\, -y\right]$	[24,120]
25	$[-x,\, -y,\, -z]$	[25,121]
26	$\left[\frac{1}{4}-x,\, z+\frac{1}{4},\, \frac{3}{4}-y\right]$	[26,122]
27	$\left[\frac{3}{4}-x,\, \frac{1}{4}-z,\, y+\frac{1}{4}\right]$	[27,123]
28	$\left[\frac{3}{4}-z,\, \frac{1}{4}-y,\, x+\frac{1}{4}\right]$	[28,124]
29	$\left[z+\frac{1}{4},\, \frac{3}{4}-y,\, \frac{1}{4}-x\right]$	[29,125]
30	$\left[y+\frac{1}{4},\, \frac{3}{4}-x,\, \frac{1}{4}-z\right]$	[30,126]
31	$\left[\frac{1}{4}-y,\, x+\frac{1}{4},\, \frac{3}{4}-z\right]$	[31,127]
32	$\left[-x,\, y,\, z+\frac{1}{2}\right]$	[32,128]
33	$\left[x+\frac{1}{2},\, -y,\, z\right]$	[33,129]
34	$\left[x,\, y+\frac{1}{2},\, -z\right]$	[34,130]
35	$\left[\frac{3}{4}-y,\, \frac{1}{4}-x,\, z+\frac{1}{4}\right]$	[35,131]
36	$\left[y+\frac{1}{4},\, x+\frac{1}{4},\, z+\frac{1}{4}\right]$	[36,132]
37	$\left[x+\frac{1}{4},\, \frac{3}{4}-z,\, \frac{1}{4}-y\right]$	[37,133]
38	$\left[x+\frac{1}{4},\, z+\frac{1}{4},\, y+\frac{1}{4}\right]$	[38,134]
39	$\left[\frac{1}{4}-z,\, y+\frac{1}{4},\, \frac{3}{4}-x\right]$	[39,135]
40	$\left[z+\frac{1}{4},\, y+\frac{1}{4},\, x+\frac{1}{4}\right]$	[40,136]
41	$[-z,\, -x,\, -y]$	[41,137]
42	$[-y,\, -z,\, -x]$	[42,138]
43	$\left[y+\frac{1}{2},\, -z,\, x\right]$	[43,139]
44	$\left[z,\, x+\frac{1}{2},\, -y\right]$	[44,140]
45	$\left[y,\, z+\frac{1}{2},\, -x\right]$	[45,141]
46	$\left[-z,\, x,\, y+\frac{1}{2}\right]$	[46,142]
47	$\left[-y,\, z,\, x+\frac{1}{2}\right]$	[47,143]
48	$\left[z+\frac{1}{2},\, -x,\, y\right]$	[48,144]
49	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[49,145]
50	$\left[x+\frac{3}{4},\, \frac{3}{4}-z,\, y+\frac{1}{4}\right]$	[50,146]
51	$\left[x+\frac{1}{4},\, z+\frac{3}{4},\, \frac{3}{4}-y\right]$	[51,147]
52	$\left[z+\frac{1}{4},\, y+\frac{3}{4},\, \frac{3}{4}-x\right]$	[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	$\left[y+\frac{3}{4},\, \frac{3}{4}-x,\, z+\frac{1}{4}\right]$	[55,151]
56	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	[56,152]
57	$\left[-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[57,153]
58	$\left[\frac{1}{2}-x,\, -y,\, z+\frac{1}{2}\right]$	[58,154]
59	$\left[y+\frac{1}{4},\, x+\frac{3}{4},\, \frac{3}{4}-z\right]$	[59,155]
60	$\left[\frac{3}{4}-y,\, \frac{3}{4}-x,\, \frac{3}{4}-z\right]$	[60,156]
61	$\left[\frac{3}{4}-x,\, z+\frac{1}{4},\, y+\frac{3}{4}\right]$	[61,157]
62	$\left[\frac{3}{4}-x,\, \frac{3}{4}-z,\, \frac{3}{4}-y\right]$	[62,158]
63	$\left[z+\frac{3}{4},\, \frac{3}{4}-y,\, x+\frac{1}{4}\right]$	[63,159]
64	$\left[\frac{3}{4}-z,\, \frac{3}{4}-y,\, \frac{3}{4}-x\right]$	[64,160]
65	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[65,161]
66	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[66,162]
67	$\left[-y,\, z+\frac{1}{2},\, \frac{1}{2}-x\right]$	[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	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, -y\right]$	[70,166]

continued ...

Table 8

No.	position	mapping
71	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ -x\right]$	[71,167]
72	$\left[-z,\ x+\frac{1}{2},\ \frac{1}{2}-y\right]$	[72,168]
73	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[73,169]
74	$\left[\frac{3}{4}-x,\ z+\frac{3}{4},\ \frac{1}{4}-y\right]$	[74,170]
75	$\left[\frac{1}{4}-x,\ \frac{3}{4}-z,\ y+\frac{3}{4}\right]$	[75,171]
76	$\left[\frac{1}{4}-z,\ \frac{3}{4}-y,\ x+\frac{3}{4}\right]$	[76,172]
77	$\left[z+\frac{3}{4},\ \frac{1}{4}-y,\ \frac{3}{4}-x\right]$	[77,173]
78	$\left[y+\frac{3}{4},\ \frac{1}{4}-x,\ \frac{3}{4}-z\right]$	[78,174]
79	$\left[\frac{3}{4}-y,\ x+\frac{3}{4},\ \frac{1}{4}-z\right]$	[79,175]
80	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z\right]$	[80,176]
81	$\left[x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[81,177]
82	$\left[x+\frac{1}{2},\ y,\ \frac{1}{2}-z\right]$	[82,178]
83	$\left[\frac{1}{4}-y,\ \frac{3}{4}-x,\ z+\frac{3}{4}\right]$	[83,179]
84	$\left[y+\frac{3}{4},\ x+\frac{3}{4},\ z+\frac{3}{4}\right]$	[84,180]
85	$\left[x+\frac{3}{4},\ \frac{1}{4}-z,\ \frac{3}{4}-y\right]$	[85,181]
86	$\left[x+\frac{3}{4},\ z+\frac{3}{4},\ y+\frac{3}{4}\right]$	[86,182]
87	$\left[\frac{3}{4}-z,\ y+\frac{3}{4},\ \frac{1}{4}-x\right]$	[87,183]
88	$\left[z+\frac{3}{4},\ y+\frac{3}{4},\ x+\frac{3}{4}\right]$	[88,184]
89	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ \frac{1}{2}-y\right]$	[89,185]
90	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[90,186]
91	$\left[y,\ \frac{1}{2}-z,\ x+\frac{1}{2}\right]$	[91,187]
92	$\left[z+\frac{1}{2},\ x,\ \frac{1}{2}-y\right]$	[92,188]
93	$\left[y+\frac{1}{2},\ z,\ \frac{1}{2}-x\right]$	[93,189]
94	$\left[\frac{1}{2}-z,\ x+\frac{1}{2},\ y\right]$	[94,190]
95	$\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ x\right]$	[95,191]
96	$\left[z,\ \frac{1}{2}-x,\ y+\frac{1}{2}\right]$	[96,192]