MSG No. 219.86 $F\bar{4}3c1'$ [Type II, cubic]

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

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

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

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

Table 3: Wyckoff site: 24c, site symmetry: -4..1'

No.	position	mapping
1	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	[1,26,62,85,97,122,158,181]
2	$\left[0, \frac{3}{4}, \frac{3}{4}\right]$	[2,25,61,86,98,121,157,182]
3	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	[3,28,69,94,99,124,165,190]
4	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	[4,27,70,93,100,123,166,189]
5	$\left[\frac{1}{4}, 0, \frac{1}{4}\right]$	[5,43,60,89,101,139,156,185]
6	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	[6,47,64,81,102,143,160,177]
7	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[7,48,63,83,103,144,159,179]
8	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	[8,44,58,90,104,140,154,186]
9	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	[9,40,71,78,105,136,167,174]
10	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	[10,42,56,92,106,138,152,188]
11	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[11,39,72,79,107,135,168,175]
12	$\left[\frac{3}{4}, 0, \frac{3}{4}\right]$	[12,41,53,91,108,137,149,187]
13	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[13,38,50,73,109,134,146,169]
14	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[14,37,49,74,110,133,145,170]
15	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[15,35,55,96,111,131,151,192]

continued ...

Table 3

No.	position	mapping
16	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[16,33,54,95,112,129,150,191]
17	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[17,36,67,77,113,132,163,173]
18	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[18,34,68,80,114,130,164,176]
19	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[19,29,65,84,115,125,161,180]
20	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[20,32,66,82,116,128,162,178]
21	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[21,46,51,76,117,142,147,172]
22	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[22,45,52,75,118,141,148,171]
23	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[23,30,57,88,119,126,153,184]
24	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[24,31,59,87,120,127,155,183]

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

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

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

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

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

No.	position	mapping
1	$[x,\ 0,\ 0]$	`[1,2,97,98]`
2	$[-x,\ 0,\ 0]$	`[3,4,99,100]`
3	$[0,\ x,\ 0]$	`[5,12,101,108]`
4	$[0,\ 0,\ x]$	`[6,9,102,105]`
5	$[0,\ 0,\ -x]$	`[7,11,103,107]`
6	$[0,\ -x,\ 0]$	`[8,10,104,106]`
7	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[13,14,109,110]`

continued ...

Table 6

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

Table 7: Wyckoff site: `48g`, site symmetry: `2..1'`

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

continued ...

Table 7

No.	position	mapping
47	$\left[x,\ \frac{1}{4},\ \frac{3}{4}\right]$	[69,94,165,190]
48	$\left[x,\ \frac{3}{4},\ \frac{1}{4}\right]$	[70,93,166,189]

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

No.	position	mapping
1	$[x,\ y,\ z]$	[1,97]
2	$[x,\ -y,\ -z]$	[2,98]
3	$[-x,\ y,\ -z]$	[3,99]
4	$[-x,\ -y,\ z]$	[4,100]
5	$[z,\ x,\ y]$	[5,101]
6	$[y,\ z,\ x]$	[6,102]
7	$[-y,\ z,\ -x]$	[7,103]
8	$[-z,\ -x,\ y]$	[8,104]
9	$[-y,\ -z,\ x]$	[9,105]
10	$[z,\ -x,\ -y]$	[10,106]
11	$[y,\ -z,\ -x]$	[11,107]
12	$[-z,\ x,\ -y]$	[12,108]
13	$\left[\frac{1}{2}-x,\ z+\frac{1}{2},\ \frac{1}{2}-y\right]$	[13,109]
14	$\left[\frac{1}{2}-x,\ \frac{1}{2}-z,\ y+\frac{1}{2}\right]$	[14,110]
15	$\left[\frac{1}{2}-z,\ \frac{1}{2}-y,\ x+\frac{1}{2}\right]$	[15,111]
16	$\left[z+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-x\right]$	[16,112]
17	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[17,113]
18	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[18,114]
19	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	[19,115]
20	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[20,116]
21	$\left[x+\frac{1}{2},\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[21,117]
22	$\left[x+\frac{1}{2},\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	[22,118]
23	$\left[\frac{1}{2}-z,\ y+\frac{1}{2},\ \frac{1}{2}-x\right]$	[23,119]
24	$\left[z+\frac{1}{2},\ y+\frac{1}{2},\ x+\frac{1}{2}\right]$	[24,120]
25	$\left[x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[25,121]
26	$\left[x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[26,122]
27	$\left[-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[27,123]
28	$\left[-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[28,124]
29	$\left[z,\ x+\frac{1}{2},\ y+\frac{1}{2}\right]$	[29,125]
30	$\left[y,\ z+\frac{1}{2},\ x+\frac{1}{2}\right]$	[30,126]
31	$\left[-y,\ z+\frac{1}{2},\ \frac{1}{2}-x\right]$	[31,127]
32	$\left[-z,\ \frac{1}{2}-x,\ y+\frac{1}{2}\right]$	[32,128]
33	$\left[-y,\ \frac{1}{2}-z,\ x+\frac{1}{2}\right]$	[33,129]
34	$\left[z,\ \frac{1}{2}-x,\ \frac{1}{2}-y\right]$	[34,130]
35	$\left[y,\ \frac{1}{2}-z,\ \frac{1}{2}-x\right]$	[35,131]
36	$\left[-z,\ x+\frac{1}{2},\ \frac{1}{2}-y\right]$	[36,132]
37	$\left[\frac{1}{2}-x,\ z,\ -y\right]$	[37,133]
38	$\left[\frac{1}{2}-x,\ -z,\ y\right]$	[38,134]

continued ...

Table 8

No.	position	mapping
39	$\left[\frac{1}{2}-z,\,-y,\,x\right]$	[39,135]
40	$\left[z+\frac{1}{2},\,-y,\,-x\right]$	[40,136]
41	$\left[y+\frac{1}{2},\,-x,\,-z\right]$	[41,137]
42	$\left[\frac{1}{2}-y,\,x,\,-z\right]$	[42,138]
43	$\left[\frac{1}{2}-y,\,-x,\,z\right]$	[43,139]
44	$\left[y+\frac{1}{2},\,x,\,z\right]$	[44,140]
45	$\left[x+\frac{1}{2},\,-z,\,-y\right]$	[45,141]
46	$\left[x+\frac{1}{2},\,z,\,y\right]$	[46,142]
47	$\left[\frac{1}{2}-z,\,y,\,-x\right]$	[47,143]
48	$\left[z+\frac{1}{2},\,y,\,x\right]$	[48,144]
49	$\left[x+\frac{1}{2},\,y,\,z+\frac{1}{2}\right]$	[49,145]
50	$\left[x+\frac{1}{2},\,-y,\,\frac{1}{2}-z\right]$	[50,146]
51	$\left[\frac{1}{2}-x,\,y,\,\frac{1}{2}-z\right]$	[51,147]
52	$\left[\frac{1}{2}-x,\,-y,\,z+\frac{1}{2}\right]$	[52,148]
53	$\left[z+\frac{1}{2},\,x,\,y+\frac{1}{2}\right]$	[53,149]
54	$\left[y+\frac{1}{2},\,z,\,x+\frac{1}{2}\right]$	[54,150]
55	$\left[\frac{1}{2}-y,\,z,\,\frac{1}{2}-x\right]$	[55,151]
56	$\left[\frac{1}{2}-z,\,-x,\,y+\frac{1}{2}\right]$	[56,152]
57	$\left[\frac{1}{2}-y,\,-z,\,x+\frac{1}{2}\right]$	[57,153]
58	$\left[z+\frac{1}{2},\,-x,\,\frac{1}{2}-y\right]$	[58,154]
59	$\left[y+\frac{1}{2},\,-z,\,\frac{1}{2}-x\right]$	[59,155]
60	$\left[\frac{1}{2}-z,\,x,\,\frac{1}{2}-y\right]$	[60,156]
61	$\left[-x,\,z+\frac{1}{2},\,-y\right]$	[61,157]
62	$\left[-x,\,\frac{1}{2}-z,\,y\right]$	[62,158]
63	$\left[-z,\,\frac{1}{2}-y,\,x\right]$	[63,159]
64	$\left[z,\,\frac{1}{2}-y,\,-x\right]$	[64,160]
65	$\left[y,\,\frac{1}{2}-x,\,-z\right]$	[65,161]
66	$\left[-y,\,x+\frac{1}{2},\,-z\right]$	[66,162]
67	$\left[-y,\,\frac{1}{2}-x,\,z\right]$	[67,163]
68	$\left[y,\,x+\frac{1}{2},\,z\right]$	[68,164]
69	$\left[x,\,\frac{1}{2}-z,\,-y\right]$	[69,165]
70	$\left[x,\,z+\frac{1}{2},\,y\right]$	[70,166]
71	$\left[-z,\,y+\frac{1}{2},\,-x\right]$	[71,167]
72	$\left[z,\,y+\frac{1}{2},\,x\right]$	[72,168]
73	$\left[x+\frac{1}{2},\,y+\frac{1}{2},\,z\right]$	[73,169]
74	$\left[x+\frac{1}{2},\,\frac{1}{2}-y,\,-z\right]$	[74,170]
75	$\left[\frac{1}{2}-x,\,y+\frac{1}{2},\,-z\right]$	[75,171]
76	$\left[\frac{1}{2}-x,\,\frac{1}{2}-y,\,z\right]$	[76,172]
77	$\left[z+\frac{1}{2},\,x+\frac{1}{2},\,y\right]$	[77,173]
78	$\left[y+\frac{1}{2},\,z+\frac{1}{2},\,x\right]$	[78,174]
79	$\left[\frac{1}{2}-y,\,z+\frac{1}{2},\,-x\right]$	[79,175]
80	$\left[\frac{1}{2}-z,\,\frac{1}{2}-x,\,y\right]$	[80,176]
81	$\left[\frac{1}{2}-y,\,\frac{1}{2}-z,\,x\right]$	[81,177]
82	$\left[z+\frac{1}{2},\,\frac{1}{2}-x,\,-y\right]$	[82,178]
83	$\left[y+\frac{1}{2},\,\frac{1}{2}-z,\,-x\right]$	[83,179]
84	$\left[\frac{1}{2}-z,\,x+\frac{1}{2},\,-y\right]$	[84,180]
85	$\left[-x,\,z,\,\frac{1}{2}-y\right]$	[85,181]

continued ...

Table 8

No.	position	mapping
86	$\left[-x,\, -z,\, y+\frac{1}{2}\right]$	[86,182]
87	$\left[-z,\, -y,\, x+\frac{1}{2}\right]$	[87,183]
88	$\left[z,\, -y,\, \frac{1}{2}-x\right]$	[88,184]
89	$\left[y,\, -x,\, \frac{1}{2}-z\right]$	[89,185]
90	$\left[-y,\, x,\, \frac{1}{2}-z\right]$	[90,186]
91	$\left[-y,\, -x,\, z+\frac{1}{2}\right]$	[91,187]
92	$\left[y,\, x,\, z+\frac{1}{2}\right]$	[92,188]
93	$\left[x,\, -z,\, \frac{1}{2}-y\right]$	[93,189]
94	$\left[x,\, z,\, y+\frac{1}{2}\right]$	[94,190]
95	$\left[-z,\, y,\, \frac{1}{2}-x\right]$	[95,191]
96	$\left[z,\, y,\, x+\frac{1}{2}\right]$	[96,192]