MSG No. 202.23 $Fm\bar{3}1'$ [Type II, cubic]

Table 1: Wyckoff site: `4a`, site symmetry: `m-3.1'`

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

Table 2: Wyckoff site: `4b`, site symmetry: `m-3.1'`

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

Table 3: Wyckoff site: `8c`, site symmetry: `23.1'`

No.	position	mapping
1	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}]$	[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	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[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	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[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	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[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	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[13,17,18,38,46,47,63,67,72,88,92,93,109,113,114,134,142,143,159,163,168,184,188,189]
6	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[14,22,23,37,41,42,64,68,69,87,91,96,110,118,119,133,137,138,160,164,165,183,187,192]
7	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[15,19,24,40,44,45,61,65,66,86,94,95,111,115,120,136,140,141,157,161,162,182,190,191]
8	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[16,20,21,39,43,48,62,70,71,85,89,90,112,116,117,135,139,144,158,166,167,181,185,186]

Table 4: Wyckoff site: `24d`, site symmetry: `2/m..1'`

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

Table 5: Wyckoff site: `24e`, site symmetry: `2mm..1'`

No.	position	mapping
1	$[x,\ 0,\ 0]$	`[1,2,15,16,97,98,111,112]`
2	$[-x,\ 0,\ 0]$	`[3,4,13,14,99,100,109,110]`
3	$[0,\ x,\ 0]$	`[5,12,20,22,101,108,116,118]`
4	$[0,\ 0,\ x]$	`[6,9,19,23,102,105,115,119]`
5	$[0,\ 0,\ -x]$	`[7,11,18,21,103,107,114,117]`
6	$[0,\ -x,\ 0]$	`[8,10,17,24,104,106,113,120]`
7	$\left[x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[25,26,39,40,121,122,135,136]`
8	$\left[-x,\ \frac{1}{2},\ \frac{1}{2}\right]$	`[27,28,37,38,123,124,133,134]`
9	$\left[0,\ x+\frac{1}{2},\ \frac{1}{2}\right]$	`[29,36,44,46,125,132,140,142]`
10	$\left[0,\ \frac{1}{2},\ x+\frac{1}{2}\right]$	`[30,33,43,47,126,129,139,143]`
11	$\left[0,\ \frac{1}{2},\ \frac{1}{2}-x\right]$	`[31,35,42,45,127,131,138,141]`
12	$\left[0,\ \frac{1}{2}-x,\ \frac{1}{2}\right]$	`[32,34,41,48,128,130,137,144]`
13	$\left[x+\frac{1}{2},\ 0,\ \frac{1}{2}\right]$	`[49,50,63,64,145,146,159,160]`
14	$\left[\frac{1}{2}-x,\ 0,\ \frac{1}{2}\right]$	`[51,52,61,62,147,148,157,158]`
15	$\left[\frac{1}{2},\ x,\ \frac{1}{2}\right]$	`[53,60,68,70,149,156,164,166]`

continued ...

Table 5

No.	position	mapping
16	$\left[\frac{1}{2}, 0, x+\frac{1}{2}\right]$	[54,57,67,71,150,153,163,167]
17	$\left[\frac{1}{2}, 0, \frac{1}{2}-x\right]$	[55,59,66,69,151,155,162,165]
18	$\left[\frac{1}{2}, -x, \frac{1}{2}\right]$	[56,58,65,72,152,154,161,168]
19	$\left[x+\frac{1}{2}, \frac{1}{2}, 0\right]$	[73,74,87,88,169,170,183,184]
20	$\left[\frac{1}{2}-x, \frac{1}{2}, 0\right]$	[75,76,85,86,171,172,181,182]
21	$\left[\frac{1}{2}, x+\frac{1}{2}, 0\right]$	[77,84,92,94,173,180,188,190]
22	$\left[\frac{1}{2}, \frac{1}{2}, x\right]$	[78,81,91,95,174,177,187,191]
23	$\left[\frac{1}{2}, \frac{1}{2}, -x\right]$	[79,83,90,93,175,179,186,189]
24	$\left[\frac{1}{2}, \frac{1}{2}-x, 0\right]$	[80,82,89,96,176,178,185,192]

Table 6: Wyckoff site: 32f, 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	$[-x, -x, -x]$	[13,17,18,109,113,114]
6	$[-x, x, x]$	[14,22,23,110,118,119]
7	$[x, -x, x]$	[15,19,24,111,115,120]
8	$[x, x, -x]$	[16,20,21,112,116,117]
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	$\left[-x, \frac{1}{2}-x, \frac{1}{2}-x\right]$	[37,41,42,133,137,138]
14	$\left[-x, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[38,46,47,134,142,143]
15	$\left[x, \frac{1}{2}-x, x+\frac{1}{2}\right]$	[39,43,48,135,139,144]
16	$\left[x, x+\frac{1}{2}, \frac{1}{2}-x\right]$	[40,44,45,136,140,141]
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	$\left[\frac{1}{2}-x, -x, \frac{1}{2}-x\right]$	[61,65,66,157,161,162]
22	$\left[\frac{1}{2}-x, x, x+\frac{1}{2}\right]$	[62,70,71,158,166,167]
23	$\left[x+\frac{1}{2}, -x, x+\frac{1}{2}\right]$	[63,67,72,159,163,168]
24	$\left[x+\frac{1}{2}, x, \frac{1}{2}-x\right]$	[64,68,69,160,164,165]
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	$\left[\frac{1}{2}-x, \frac{1}{2}-x, -x\right]$	[85,89,90,181,185,186]
30	$\left[\frac{1}{2}-x, x+\frac{1}{2}, x\right]$	[86,94,95,182,190,191]
31	$\left[x+\frac{1}{2}, \frac{1}{2}-x, x\right]$	[87,91,96,183,187,192]

continued ...

Table 6

No.	position	mapping
32	$\left[x+\frac{1}{2}, x+\frac{1}{2}, -x\right]$	[88,92,93,184,188,189]

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	$\left[-x, \frac{3}{4}, \frac{3}{4}\right]$	[13,38,109,134]
14	$\left[-x, \frac{1}{4}, \frac{1}{4}\right]$	[14,37,110,133]
15	$\left[x, \frac{3}{4}, \frac{1}{4}\right]$	[15,40,111,136]
16	$\left[x, \frac{1}{4}, \frac{3}{4}\right]$	[16,39,112,135]
17	$\left[\frac{3}{4}, -x, \frac{3}{4}\right]$	[17,72,113,168]
18	$\left[\frac{3}{4}, \frac{3}{4}, -x\right]$	[18,93,114,189]
19	$\left[\frac{1}{4}, \frac{3}{4}, x\right]$	[19,95,115,191]
20	$\left[\frac{1}{4}, x, \frac{3}{4}\right]$	[20,70,116,166]
21	$\left[\frac{1}{4}, \frac{1}{4}, -x\right]$	[21,90,117,186]
22	$\left[\frac{3}{4}, x, \frac{1}{4}\right]$	[22,68,118,164]
23	$\left[\frac{3}{4}, \frac{1}{4}, x\right]$	[23,91,119,187]
24	$\left[\frac{1}{4}, -x, \frac{1}{4}\right]$	[24,65,120,161]
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	$\left[\frac{3}{4}, \frac{1}{2}-x, \frac{1}{4}\right]$	[41,96,137,192]
34	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}-x\right]$	[42,69,138,165]
35	$\left[\frac{1}{4}, \frac{1}{4}, x+\frac{1}{2}\right]$	[43,71,139,167]
36	$\left[\frac{1}{4}, x+\frac{1}{2}, \frac{1}{4}\right]$	[44,94,140,190]
37	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}-x\right]$	[45,66,141,162]
38	$\left[\frac{3}{4}, x+\frac{1}{2}, \frac{3}{4}\right]$	[46,92,142,188]
39	$\left[\frac{3}{4}, \frac{3}{4}, x+\frac{1}{2}\right]$	[47,67,143,163]

continued ...

Table 7

No.	position	mapping
40	$\left[\frac{1}{4},\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	[48,89,144,185]
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	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ \frac{1}{4}\right]$	[61,86,157,182]
46	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{3}{4}\right]$	[62,85,158,181]
47	$\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{3}{4}\right]$	[63,88,159,184]
48	$\left[x+\frac{1}{2},\ \frac{1}{4},\ \frac{1}{4}\right]$	[64,87,160,183]

Table 8: Wyckoff site: 48h, site symmetry: m..1'

No.	position	mapping
1	$[0,\ y,\ z]$	[1,14,97,110]
2	$[0,\ -y,\ -z]$	[2,13,98,109]
3	$[0,\ y,\ -z]$	[3,16,99,112]
4	$[0,\ -y,\ z]$	[4,15,100,111]
5	$[z,\ 0,\ y]$	[5,24,101,120]
6	$[y,\ z,\ 0]$	[6,21,102,117]
7	$[-y,\ z,\ 0]$	[7,23,103,119]
8	$[-z,\ 0,\ y]$	[8,22,104,118]
9	$[-y,\ -z,\ 0]$	[9,18,105,114]
10	$[z,\ 0,\ -y]$	[10,20,106,116]
11	$[y,\ -z,\ 0]$	[11,19,107,115]
12	$[-z,\ 0,\ -y]$	[12,17,108,113]
13	$\left[0,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[25,38,121,134]
14	$\left[0,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[26,37,122,133]
15	$\left[0,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[27,40,123,136]
16	$\left[0,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[28,39,124,135]
17	$\left[z,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[29,48,125,144]
18	$\left[y,\ z+\frac{1}{2},\ \frac{1}{2}\right]$	[30,45,126,141]
19	$\left[-y,\ z+\frac{1}{2},\ \frac{1}{2}\right]$	[31,47,127,143]
20	$\left[-z,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[32,46,128,142]
21	$\left[-y,\ \frac{1}{2}-z,\ \frac{1}{2}\right]$	[33,42,129,138]
22	$\left[z,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[34,44,130,140]
23	$\left[y,\ \frac{1}{2}-z,\ \frac{1}{2}\right]$	[35,43,131,139]
24	$\left[-z,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[36,41,132,137]
25	$\left[\frac{1}{2},\ y,\ z+\frac{1}{2}\right]$	[49,62,145,158]
26	$\left[\frac{1}{2},\ -y,\ \frac{1}{2}-z\right]$	[50,61,146,157]
27	$\left[\frac{1}{2},\ y,\ \frac{1}{2}-z\right]$	[51,64,147,160]
28	$\left[\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	[52,63,148,159]
29	$\left[z+\frac{1}{2},\ 0,\ y+\frac{1}{2}\right]$	[53,72,149,168]
30	$\left[y+\frac{1}{2},\ z,\ \frac{1}{2}\right]$	[54,69,150,165]
31	$\left[\frac{1}{2}-y,\ z,\ \frac{1}{2}\right]$	[55,71,151,167]

continued ...

Table 8

No.	position	mapping
32	$\left[\frac{1}{2}-z,\ 0,\ y+\frac{1}{2}\right]$	[56,70,152,166]
33	$\left[\frac{1}{2}-y,\ -z,\ \frac{1}{2}\right]$	[57,66,153,162]
34	$\left[z+\frac{1}{2},\ 0,\ \frac{1}{2}-y\right]$	[58,68,154,164]
35	$\left[y+\frac{1}{2},\ -z,\ \frac{1}{2}\right]$	[59,67,155,163]
36	$\left[\frac{1}{2}-z,\ 0,\ \frac{1}{2}-y\right]$	[60,65,156,161]
37	$\left[\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[73,86,169,182]
38	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[74,85,170,181]
39	$\left[\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	[75,88,171,184]
40	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$	[76,87,172,183]
41	$\left[z+\frac{1}{2},\ \frac{1}{2},\ y\right]$	[77,96,173,192]
42	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ 0\right]$	[78,93,174,189]
43	$\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ 0\right]$	[79,95,175,191]
44	$\left[\frac{1}{2}-z,\ \frac{1}{2},\ y\right]$	[80,94,176,190]
45	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ 0\right]$	[81,90,177,186]
46	$\left[z+\frac{1}{2},\ \frac{1}{2},\ -y\right]$	[82,92,178,188]
47	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ 0\right]$	[83,91,179,187]
48	$\left[\frac{1}{2}-z,\ \frac{1}{2},\ -y\right]$	[84,89,180,185]

Table 9: Wyckoff site: 96i, 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	$[-x,\ -y,\ -z]$	[13,109]
14	$[-x,\ y,\ z]$	[14,110]
15	$[x,\ -y,\ z]$	[15,111]
16	$[x,\ y,\ -z]$	[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]

continued ...

Table 9

No.	position	mapping
24	$[z, -x, y]$	[24,120]
25	$\left[x, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[25,121]
26	$\left[x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[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	$\left[-x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[37,133]
38	$\left[-x, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[38,134]
39	$\left[x, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[39,135]
40	$\left[x, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[40,136]
41	$\left[-z, \frac{1}{2}-x, \frac{1}{2}-y\right]$	[41,137]
42	$\left[-y, \frac{1}{2}-z, \frac{1}{2}-x\right]$	[42,138]
43	$\left[y, \frac{1}{2}-z, x+\frac{1}{2}\right]$	[43,139]
44	$\left[z, x+\frac{1}{2}, \frac{1}{2}-y\right]$	[44,140]
45	$\left[y, z+\frac{1}{2}, \frac{1}{2}-x\right]$	[45,141]
46	$\left[-z, x+\frac{1}{2}, y+\frac{1}{2}\right]$	[46,142]
47	$\left[-y, z+\frac{1}{2}, x+\frac{1}{2}\right]$	[47,143]
48	$\left[z, \frac{1}{2}-x, y+\frac{1}{2}\right]$	[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	$\left[\frac{1}{2}-x, -y, \frac{1}{2}-z\right]$	[61,157]
62	$\left[\frac{1}{2}-x, y, z+\frac{1}{2}\right]$	[62,158]
63	$\left[x+\frac{1}{2}, -y, z+\frac{1}{2}\right]$	[63,159]
64	$\left[x+\frac{1}{2}, y, \frac{1}{2}-z\right]$	[64,160]
65	$\left[\frac{1}{2}-z, -x, \frac{1}{2}-y\right]$	[65,161]
66	$\left[\frac{1}{2}-y, -z, \frac{1}{2}-x\right]$	[66,162]
67	$\left[y+\frac{1}{2}, -z, x+\frac{1}{2}\right]$	[67,163]
68	$\left[z+\frac{1}{2}, x, \frac{1}{2}-y\right]$	[68,164]
69	$\left[y+\frac{1}{2}, z, \frac{1}{2}-x\right]$	[69,165]
70	$\left[\frac{1}{2}-z, x, y+\frac{1}{2}\right]$	[70,166]

continued ...

Table 9

No.	position	mapping
71	$\left[\frac{1}{2}-y,\, z,\, x+\frac{1}{2}\right]$	[71,167]
72	$\left[z+\frac{1}{2},\, -x,\, y+\frac{1}{2}\right]$	[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	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, -z\right]$	[85,181]
86	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z\right]$	[86,182]
87	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z\right]$	[87,183]
88	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, -z\right]$	[88,184]
89	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, -y\right]$	[89,185]
90	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, -x\right]$	[90,186]
91	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, x\right]$	[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	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, y\right]$	[96,192]