MSG No. 225.116 $Fm\bar{3}m$ [Type I, cubic]

Table 1: Wyckoff site: `4a`, site symmetry: `m-3m`

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,
		25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]
2	$[0, \frac{1}{2}, \frac{1}{2}]$	[49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,
		73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96]
3	$[\frac{1}{2}, 0, \frac{1}{2}]$	[97,98,99,100,101,102,103,104,105,106,107,108,109,110,111,112,113,114,115,116,117,118,119,120,
		121,122,123,124,125,126,127,128,129,130,131,132,133,134,135,136,137,138,139,140,141,142,143,144]
4	$[\frac{1}{2}, \frac{1}{2}, 0]$	[145,146,147,148,149,150,151,152,153,154,155,156,157,158,159,160,161,162,163,164,165,166,167,168,
		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-3m`

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,
		25,26,27,28,29,30,31,32,33,34,35,36,37,38,39,40,41,42,43,44,45,46,47,48]
2	$[\frac{1}{2}, 0, 0]$	[49,50,51,52,53,54,55,56,57,58,59,60,61,62,63,64,65,66,67,68,69,70,71,72,
		73,74,75,76,77,78,79,80,81,82,83,84,85,86,87,88,89,90,91,92,93,94,95,96]
3	$[0, \frac{1}{2}, 0]$	[97,98,99,100,101,102,103,104,105,106,107,108,109,110,111,112,113,114,115,116,117,118,119,120,
		121,122,123,124,125,126,127,128,129,130,131,132,133,134,135,136,137,138,139,140,141,142,143,144]
4	$[0, 0, \frac{1}{2}]$	[145,146,147,148,149,150,151,152,153,154,155,156,157,158,159,160,161,162,163,164,165,166,167,168,
		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: `-43m`

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

Table 4: Wyckoff site: `24d`, site symmetry: `m.mm`

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

Table 5: Wyckoff site: `24e`, site symmetry: `4m.m`

No.	position	mapping
1	$[x, 0, 0]$	`[1,2,3,8,33,34,37,38]`
2	$[0, 0, -x]$	`[4,16,19,23,29,39,42,45]`
3	$[0, 0, x]$	`[5,15,18,21,28,40,43,47]`
4	$[0, x, 0]$	`[6,11,17,24,31,36,44,46]`
5	$[0, -x, 0]$	`[7,12,20,22,30,35,41,48]`
6	$[-x, 0, 0]$	`[9,10,13,14,25,26,27,32]`
7	$\left[x, \frac{1}{2}, \frac{1}{2}\right]$	`[49,50,51,56,81,82,85,86]`
8	$\left[0, \frac{1}{2}, \frac{1}{2} - x\right]$	`[52,64,67,71,77,87,90,93]`
9	$\left[0, \frac{1}{2}, x + \frac{1}{2}\right]$	`[53,63,66,69,76,88,91,95]`
10	$\left[0, x + \frac{1}{2}, \frac{1}{2}\right]$	`[54,59,65,72,79,84,92,94]`
11	$\left[0, \frac{1}{2} - x, \frac{1}{2}\right]$	`[55,60,68,70,78,83,89,96]`
12	$\left[-x, \frac{1}{2}, \frac{1}{2}\right]$	`[57,58,61,62,73,74,75,80]`
13	$\left[x + \frac{1}{2}, 0, \frac{1}{2}\right]$	`[97,98,99,104,129,130,133,134]`
14	$\left[\frac{1}{2}, 0, \frac{1}{2} - x\right]$	`[100,112,115,119,125,135,138,141]`
15	$\left[\frac{1}{2}, 0, x + \frac{1}{2}\right]$	`[101,111,114,117,124,136,139,143]`

continued ...

Table 5

No.	position	mapping
16	$\left[\frac{1}{2}, x, \frac{1}{2}\right]$	[102,107,113,120,127,132,140,142]
17	$\left[\frac{1}{2}, -x, \frac{1}{2}\right]$	[103,108,116,118,126,131,137,144]
18	$\left[\frac{1}{2} - x, 0, \frac{1}{2}\right]$	[105,106,109,110,121,122,123,128]
19	$\left[x + \frac{1}{2}, \frac{1}{2}, 0\right]$	[145,146,147,152,177,178,181,182]
20	$\left[\frac{1}{2}, \frac{1}{2}, -x\right]$	[148,160,163,167,173,183,186,189]
21	$\left[\frac{1}{2}, \frac{1}{2}, x\right]$	[149,159,162,165,172,184,187,191]
22	$\left[\frac{1}{2}, x + \frac{1}{2}, 0\right]$	[150,155,161,168,175,180,188,190]
23	$\left[\frac{1}{2}, \frac{1}{2} - x, 0\right]$	[151,156,164,166,174,179,185,192]
24	$\left[\frac{1}{2} - x, \frac{1}{2}, 0\right]$	[153,154,157,158,169,170,171,176]

Table 6: Wyckoff site: 32f, site symmetry: .3m

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

continued ...

Table 6

No.	position	mapping
32	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ -x\right]$	[156,158,160,169,185,186]

Table 7: Wyckoff site: 48g, site symmetry: 2.mm

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

continued ...

Table 7

No.	position	mapping
40	$\left[\frac{3}{4},\, x+\frac{1}{2},\, \frac{1}{4}\right]$	[72,79,161,180]
41	$\left[x+\frac{1}{2},\, \frac{1}{4},\, \frac{3}{4}\right]$	[97,134,152,181]
42	$\left[x+\frac{1}{2},\, \frac{3}{4},\, \frac{3}{4}\right]$	[98,129,147,178]
43	$\left[x+\frac{1}{2},\, \frac{1}{4},\, \frac{1}{4}\right]$	[99,130,146,177]
44	$\left[x+\frac{1}{2},\, \frac{3}{4},\, \frac{1}{4}\right]$	[104,133,145,182]
45	$\left[\frac{1}{2}-x,\, \frac{1}{4},\, \frac{1}{4}\right]$	[105,122,154,171]
46	$\left[\frac{1}{2}-x,\, \frac{3}{4},\, \frac{3}{4}\right]$	[106,123,153,170]
47	$\left[\frac{1}{2}-x,\, \frac{1}{4},\, \frac{3}{4}\right]$	[109,128,158,169]
48	$\left[\frac{1}{2}-x,\, \frac{3}{4},\, \frac{1}{4}\right]$	[110,121,157,176]

Table 8: Wyckoff site: 48h, site symmetry: m.2m

No.	position	mapping
1	$[0,\, y,\, y]$	[1,13,32,38]
2	$[0,\, -y,\, y]$	[2,10,27,33]
3	$[0,\, y,\, -y]$	[3,9,26,34]
4	$[y,\, y,\, 0]$	[4,18,40,45]
5	$[-y,\, y,\, 0]$	[5,19,39,47]
6	$[-y,\, 0,\, y]$	[6,20,35,46]
7	$[y,\, 0,\, y]$	[7,17,36,48]
8	$[0,\, -y,\, -y]$	[8,14,25,37]
9	$[y,\, 0,\, -y]$	[11,22,30,44]
10	$[-y,\, 0,\, -y]$	[12,24,31,41]
11	$[y,\, -y,\, 0]$	[15,23,29,43]
12	$[-y,\, -y,\, 0]$	[16,21,28,42]
13	$\left[0,\, y+\frac{1}{2},\, y+\frac{1}{2}\right]$	[49,61,80,86]
14	$\left[0,\, \frac{1}{2}-y,\, y+\frac{1}{2}\right]$	[50,58,75,81]
15	$\left[0,\, y+\frac{1}{2},\, \frac{1}{2}-y\right]$	[51,57,74,82]
16	$\left[y,\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[52,66,88,93]
17	$\left[-y,\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[53,67,87,95]
18	$\left[-y,\, \frac{1}{2},\, y+\frac{1}{2}\right]$	[54,68,83,94]
19	$\left[y,\, \frac{1}{2},\, y+\frac{1}{2}\right]$	[55,65,84,96]
20	$\left[0,\, \frac{1}{2}-y,\, \frac{1}{2}-y\right]$	[56,62,73,85]
21	$\left[y,\, \frac{1}{2},\, \frac{1}{2}-y\right]$	[59,70,78,92]
22	$\left[-y,\, \frac{1}{2},\, \frac{1}{2}-y\right]$	[60,72,79,89]
23	$\left[y,\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[63,71,77,91]
24	$\left[-y,\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[64,69,76,90]
25	$\left[\frac{1}{2},\, y,\, y+\frac{1}{2}\right]$	[97,109,128,134]
26	$\left[\frac{1}{2},\, -y,\, y+\frac{1}{2}\right]$	[98,106,123,129]
27	$\left[\frac{1}{2},\, y,\, \frac{1}{2}-y\right]$	[99,105,122,130]
28	$\left[y+\frac{1}{2},\, y,\, \frac{1}{2}\right]$	[100,114,136,141]
29	$\left[\frac{1}{2}-y,\, y,\, \frac{1}{2}\right]$	[101,115,135,143]
30	$\left[\frac{1}{2}-y,\, 0,\, y+\frac{1}{2}\right]$	[102,116,131,142]
31	$\left[y+\frac{1}{2},\, 0,\, y+\frac{1}{2}\right]$	[103,113,132,144]

continued ...

Table 8

No.	position	mapping
32	$\left[\frac{1}{2}, -y, \frac{1}{2}-y\right]$	[104,110,121,133]
33	$\left[y+\frac{1}{2}, 0, \frac{1}{2}-y\right]$	[107,118,126,140]
34	$\left[\frac{1}{2}-y, 0, \frac{1}{2}-y\right]$	[108,120,127,137]
35	$\left[y+\frac{1}{2}, -y, \frac{1}{2}\right]$	[111,119,125,139]
36	$\left[\frac{1}{2}-y, -y, \frac{1}{2}\right]$	[112,117,124,138]
37	$\left[\frac{1}{2}, y+\frac{1}{2}, y\right]$	[145,157,176,182]
38	$\left[\frac{1}{2}, \frac{1}{2}-y, y\right]$	[146,154,171,177]
39	$\left[\frac{1}{2}, y+\frac{1}{2}, -y\right]$	[147,153,170,178]
40	$\left[y+\frac{1}{2}, y+\frac{1}{2}, 0\right]$	[148,162,184,189]
41	$\left[\frac{1}{2}-y, y+\frac{1}{2}, 0\right]$	[149,163,183,191]
42	$\left[\frac{1}{2}-y, \frac{1}{2}, y\right]$	[150,164,179,190]
43	$\left[y+\frac{1}{2}, \frac{1}{2}, y\right]$	[151,161,180,192]
44	$\left[\frac{1}{2}, \frac{1}{2}-y, -y\right]$	[152,158,169,181]
45	$\left[y+\frac{1}{2}, \frac{1}{2}, -y\right]$	[155,166,174,188]
46	$\left[\frac{1}{2}-y, \frac{1}{2}, -y\right]$	[156,168,175,185]
47	$\left[y+\frac{1}{2}, \frac{1}{2}-y, 0\right]$	[159,167,173,187]
48	$\left[\frac{1}{2}-y, \frac{1}{2}-y, 0\right]$	[160,165,172,186]

Table 9: Wyckoff site: 48i, site symmetry: m.2m

No.	position	mapping
1	$\left[\frac{1}{2}, y, y\right]$	[1,13,32,38]
2	$\left[\frac{1}{2}, -y, y\right]$	[2,10,27,33]
3	$\left[\frac{1}{2}, y, -y\right]$	[3,9,26,34]
4	$\left[y, y, \frac{1}{2}\right]$	[4,18,40,45]
5	$\left[-y, y, \frac{1}{2}\right]$	[5,19,39,47]
6	$\left[-y, \frac{1}{2}, y\right]$	[6,20,35,46]
7	$\left[y, \frac{1}{2}, y\right]$	[7,17,36,48]
8	$\left[\frac{1}{2}, -y, -y\right]$	[8,14,25,37]
9	$\left[y, \frac{1}{2}, -y\right]$	[11,22,30,44]
10	$\left[-y, \frac{1}{2}, -y\right]$	[12,24,31,41]
11	$\left[y, -y, \frac{1}{2}\right]$	[15,23,29,43]
12	$\left[-y, -y, \frac{1}{2}\right]$	[16,21,28,42]
13	$\left[\frac{1}{2}, y+\frac{1}{2}, y+\frac{1}{2}\right]$	[49,61,80,86]
14	$\left[\frac{1}{2}, \frac{1}{2}-y, y+\frac{1}{2}\right]$	[50,58,75,81]
15	$\left[\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}-y\right]$	[51,57,74,82]
16	$\left[y, y+\frac{1}{2}, 0\right]$	[52,66,88,93]
17	$\left[-y, y+\frac{1}{2}, 0\right]$	[53,67,87,95]
18	$\left[-y, 0, y+\frac{1}{2}\right]$	[54,68,83,94]
19	$\left[y, 0, y+\frac{1}{2}\right]$	[55,65,84,96]
20	$\left[\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}-y\right]$	[56,62,73,85]
21	$\left[y, 0, \frac{1}{2}-y\right]$	[59,70,78,92]
22	$\left[-y, 0, \frac{1}{2}-y\right]$	[60,72,79,89]
23	$\left[y, \frac{1}{2}-y, 0\right]$	[63,71,77,91]

continued ...

Table 9

No.	position	mapping
24	$\left[-y,\ \frac{1}{2}-y,\ 0\right]$	[64,69,76,90]
25	$\left[0,\ y,\ y+\frac{1}{2}\right]$	[97,109,128,134]
26	$\left[0,\ -y,\ y+\frac{1}{2}\right]$	[98,106,123,129]
27	$\left[0,\ y,\ \frac{1}{2}-y\right]$	[99,105,122,130]
28	$\left[y+\frac{1}{2},\ y,\ 0\right]$	[100,114,136,141]
29	$\left[\frac{1}{2}-y,\ y,\ 0\right]$	[101,115,135,143]
30	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[102,116,131,142]
31	$\left[y+\frac{1}{2},\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[103,113,132,144]
32	$\left[0,\ -y,\ \frac{1}{2}-y\right]$	[104,110,121,133]
33	$\left[y+\frac{1}{2},\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[107,118,126,140]
34	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[108,120,127,137]
35	$\left[y+\frac{1}{2},\ -y,\ 0\right]$	[111,119,125,139]
36	$\left[\frac{1}{2}-y,\ -y,\ 0\right]$	[112,117,124,138]
37	$\left[0,\ y+\frac{1}{2},\ y\right]$	[145,157,176,182]
38	$\left[0,\ \frac{1}{2}-y,\ y\right]$	[146,154,171,177]
39	$\left[0,\ y+\frac{1}{2},\ -y\right]$	[147,153,170,178]
40	$\left[y+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[148,162,184,189]
41	$\left[\frac{1}{2}-y,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[149,163,183,191]
42	$\left[\frac{1}{2}-y,\ 0,\ y\right]$	[150,164,179,190]
43	$\left[y+\frac{1}{2},\ 0,\ y\right]$	[151,161,180,192]
44	$\left[0,\ \frac{1}{2}-y,\ -y\right]$	[152,158,169,181]
45	$\left[y+\frac{1}{2},\ 0,\ -y\right]$	[155,166,174,188]
46	$\left[\frac{1}{2}-y,\ 0,\ -y\right]$	[156,168,175,185]
47	$\left[y+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[159,167,173,187]
48	$\left[\frac{1}{2}-y,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[160,165,172,186]

Table 10: Wyckoff site: 96j, site symmetry: m..

No.	position	mapping
1	$[0,\ y,\ z]$	[1,32]
2	$[0,\ -z,\ y]$	[2,27]
3	$[0,\ z,\ -y]$	[3,26]
4	$[z,\ y,\ 0]$	[4,40]
5	$[-z,\ y,\ 0]$	[5,39]
6	$[-y,\ 0,\ z]$	[6,35]
7	$[y,\ 0,\ z]$	[7,36]
8	$[0,\ -y,\ -z]$	[8,25]
9	$[0,\ y,\ -z]$	[9,34]
10	$[0,\ -y,\ z]$	[10,33]
11	$[y,\ 0,\ -z]$	[11,30]
12	$[-y,\ 0,\ -z]$	[12,31]
13	$[0,\ z,\ y]$	[13,38]
14	$[0,\ -z,\ -y]$	[14,37]
15	$[z,\ -y,\ 0]$	[15,29]

continued ...

Table 10

No.	position	mapping
16	$[-z,\ -y,\ 0]$	[16,28]
17	$[z,\ 0,\ y]$	[17,48]
18	$[y,\ z,\ 0]$	[18,45]
19	$[-y,\ z,\ 0]$	[19,47]
20	$[-z,\ 0,\ y]$	[20,46]
21	$[-y,\ -z,\ 0]$	[21,42]
22	$[z,\ 0,\ -y]$	[22,44]
23	$[y,\ -z,\ 0]$	[23,43]
24	$[-z,\ 0,\ -y]$	[24,41]
25	$\left[0,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[49,80]
26	$\left[0,\ \frac{1}{2}-z,\ y+\frac{1}{2}\right]$	[50,75]
27	$\left[0,\ z+\frac{1}{2},\ \frac{1}{2}-y\right]$	[51,74]
28	$\left[z,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[52,88]
29	$\left[-z,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[53,87]
30	$\left[-y,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[54,83]
31	$\left[y,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[55,84]
32	$\left[0,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[56,73]
33	$\left[0,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[57,82]
34	$\left[0,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[58,81]
35	$\left[y,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[59,78]
36	$\left[-y,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[60,79]
37	$\left[0,\ z+\frac{1}{2},\ y+\frac{1}{2}\right]$	[61,86]
38	$\left[0,\ \frac{1}{2}-z,\ \frac{1}{2}-y\right]$	[62,85]
39	$\left[z,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[63,77]
40	$\left[-z,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[64,76]
41	$\left[z,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[65,96]
42	$\left[y,\ z+\frac{1}{2},\ \frac{1}{2}\right]$	[66,93]
43	$\left[-y,\ z+\frac{1}{2},\ \frac{1}{2}\right]$	[67,95]
44	$\left[-z,\ \frac{1}{2},\ y+\frac{1}{2}\right]$	[68,94]
45	$\left[-y,\ \frac{1}{2}-z,\ \frac{1}{2}\right]$	[69,90]
46	$\left[z,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[70,92]
47	$\left[y,\ \frac{1}{2}-z,\ \frac{1}{2}\right]$	[71,91]
48	$\left[-z,\ \frac{1}{2},\ \frac{1}{2}-y\right]$	[72,89]
49	$\left[\frac{1}{2},\ y,\ z+\frac{1}{2}\right]$	[97,128]
50	$\left[\frac{1}{2},\ -z,\ y+\frac{1}{2}\right]$	[98,123]
51	$\left[\frac{1}{2},\ z,\ \frac{1}{2}-y\right]$	[99,122]
52	$\left[z+\frac{1}{2},\ y,\ \frac{1}{2}\right]$	[100,136]
53	$\left[\frac{1}{2}-z,\ y,\ \frac{1}{2}\right]$	[101,135]
54	$\left[\frac{1}{2}-y,\ 0,\ z+\frac{1}{2}\right]$	[102,131]
55	$\left[y+\frac{1}{2},\ 0,\ z+\frac{1}{2}\right]$	[103,132]
56	$\left[\frac{1}{2},\ -y,\ \frac{1}{2}-z\right]$	[104,121]
57	$\left[\frac{1}{2},\ y,\ \frac{1}{2}-z\right]$	[105,130]
58	$\left[\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	[106,129]
59	$\left[y+\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	[107,126]
60	$\left[\frac{1}{2}-y,\ 0,\ \frac{1}{2}-z\right]$	[108,127]
61	$\left[\frac{1}{2},\ z,\ y+\frac{1}{2}\right]$	[109,134]
62	$\left[\frac{1}{2},\ -z,\ \frac{1}{2}-y\right]$	[110,133]

continued ...

Table 10

No.	position	mapping
63	$\left[z+\frac{1}{2},\,-y,\,\frac{1}{2}\right]$	[111,125]
64	$\left[\frac{1}{2}-z,\,-y,\,\frac{1}{2}\right]$	[112,124]
65	$\left[z+\frac{1}{2},\,0,\,y+\frac{1}{2}\right]$	[113,144]
66	$\left[y+\frac{1}{2},\,z,\,\frac{1}{2}\right]$	[114,141]
67	$\left[\frac{1}{2}-y,\,z,\,\frac{1}{2}\right]$	[115,143]
68	$\left[\frac{1}{2}-z,\,0,\,y+\frac{1}{2}\right]$	[116,142]
69	$\left[\frac{1}{2}-y,\,-z,\,\frac{1}{2}\right]$	[117,138]
70	$\left[z+\frac{1}{2},\,0,\,\frac{1}{2}-y\right]$	[118,140]
71	$\left[y+\frac{1}{2},\,-z,\,\frac{1}{2}\right]$	[119,139]
72	$\left[\frac{1}{2}-z,\,0,\,\frac{1}{2}-y\right]$	[120,137]
73	$\left[\frac{1}{2},\,y+\frac{1}{2},\,z\right]$	[145,176]
74	$\left[\frac{1}{2},\,\frac{1}{2}-z,\,y\right]$	[146,171]
75	$\left[\frac{1}{2},\,z+\frac{1}{2},\,-y\right]$	[147,170]
76	$\left[z+\frac{1}{2},\,y+\frac{1}{2},\,0\right]$	[148,184]
77	$\left[\frac{1}{2}-z,\,y+\frac{1}{2},\,0\right]$	[149,183]
78	$\left[\frac{1}{2}-y,\,\frac{1}{2},\,z\right]$	[150,179]
79	$\left[y+\frac{1}{2},\,\frac{1}{2},\,z\right]$	[151,180]
80	$\left[\frac{1}{2},\,\frac{1}{2}-y,\,-z\right]$	[152,169]
81	$\left[\frac{1}{2},\,y+\frac{1}{2},\,-z\right]$	[153,178]
82	$\left[\frac{1}{2},\,\frac{1}{2}-y,\,z\right]$	[154,177]
83	$\left[y+\frac{1}{2},\,\frac{1}{2},\,-z\right]$	[155,174]
84	$\left[\frac{1}{2}-y,\,\frac{1}{2},\,-z\right]$	[156,175]
85	$\left[\frac{1}{2},\,z+\frac{1}{2},\,y\right]$	[157,182]
86	$\left[\frac{1}{2},\,\frac{1}{2}-z,\,-y\right]$	[158,181]
87	$\left[z+\frac{1}{2},\,\frac{1}{2}-y,\,0\right]$	[159,173]
88	$\left[\frac{1}{2}-z,\,\frac{1}{2}-y,\,0\right]$	[160,172]
89	$\left[z+\frac{1}{2},\,\frac{1}{2},\,y\right]$	[161,192]
90	$\left[y+\frac{1}{2},\,z+\frac{1}{2},\,0\right]$	[162,189]
91	$\left[\frac{1}{2}-y,\,z+\frac{1}{2},\,0\right]$	[163,191]
92	$\left[\frac{1}{2}-z,\,\frac{1}{2},\,y\right]$	[164,190]
93	$\left[\frac{1}{2}-y,\,\frac{1}{2}-z,\,0\right]$	[165,186]
94	$\left[z+\frac{1}{2},\,\frac{1}{2},\,-y\right]$	[166,188]
95	$\left[y+\frac{1}{2},\,\frac{1}{2}-z,\,0\right]$	[167,187]
96	$\left[\frac{1}{2}-z,\,\frac{1}{2},\,-y\right]$	[168,185]

Table 11: Wyckoff site: 96k, site symmetry: ..m

No.	position	mapping
1	$[x,\,x,\,z]$	[1,36]
2	$[x,\,-z,\,x]$	[2,43]
3	$[x,\,z,\,-x]$	[3,45]
4	$[z,\,x,\,-x]$	[4,44]
5	$[-z,\,x,\,x]$	[5,46]
6	$[-x,\,x,\,z]$	[6,32]

continued ...

Table 11

No.	position	mapping
7	$[x, -x, z]$	[7,33]
8	$[x, -x, -z]$	[8,30]
9	$[-x, x, -z]$	[9,31]
10	$[-x, -x, z]$	[10,35]
11	$[x, x, -z]$	[11,34]
12	$[-x, -x, -z]$	[12,25]
13	$[-x, z, x]$	[13,47]
14	$[-x, -z, -x]$	[14,42]
15	$[z, -x, x]$	[15,48]
16	$[-z, -x, -x]$	[16,41]
17	$[z, x, x]$	[17,40]
18	$[x, z, x]$	[18,38]
19	$[-x, z, -x]$	[19,26]
20	$[-z, -x, x]$	[20,28]
21	$[-x, -z, x]$	[21,27]
22	$[z, -x, -x]$	[22,29]
23	$[x, -z, -x]$	[23,37]
24	$[-z, x, -x]$	[24,39]
25	$\left[x, x+\frac{1}{2}, z+\frac{1}{2}\right]$	[49,84]
26	$\left[x, \frac{1}{2}-z, x+\frac{1}{2}\right]$	[50,91]
27	$\left[x, z+\frac{1}{2}, \frac{1}{2}-x\right]$	[51,93]
28	$\left[z, x+\frac{1}{2}, \frac{1}{2}-x\right]$	[52,92]
29	$\left[-z, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[53,94]
30	$\left[-x, x+\frac{1}{2}, z+\frac{1}{2}\right]$	[54,80]
31	$\left[x, \frac{1}{2}-x, z+\frac{1}{2}\right]$	[55,81]
32	$\left[x, \frac{1}{2}-x, \frac{1}{2}-z\right]$	[56,78]
33	$\left[-x, x+\frac{1}{2}, \frac{1}{2}-z\right]$	[57,79]
34	$\left[-x, \frac{1}{2}-x, z+\frac{1}{2}\right]$	[58,83]
35	$\left[x, x+\frac{1}{2}, \frac{1}{2}-z\right]$	[59,82]
36	$\left[-x, \frac{1}{2}-x, \frac{1}{2}-z\right]$	[60,73]
37	$\left[-x, z+\frac{1}{2}, x+\frac{1}{2}\right]$	[61,95]
38	$\left[-x, \frac{1}{2}-z, \frac{1}{2}-x\right]$	[62,90]
39	$\left[z, \frac{1}{2}-x, x+\frac{1}{2}\right]$	[63,96]
40	$\left[-z, \frac{1}{2}-x, \frac{1}{2}-x\right]$	[64,89]
41	$\left[z, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[65,88]
42	$\left[x, z+\frac{1}{2}, x+\frac{1}{2}\right]$	[66,86]
43	$\left[-x, z+\frac{1}{2}, \frac{1}{2}-x\right]$	[67,74]
44	$\left[-z, \frac{1}{2}-x, x+\frac{1}{2}\right]$	[68,76]
45	$\left[-x, \frac{1}{2}-z, x+\frac{1}{2}\right]$	[69,75]
46	$\left[z, \frac{1}{2}-x, \frac{1}{2}-x\right]$	[70,77]
47	$\left[x, \frac{1}{2}-z, \frac{1}{2}-x\right]$	[71,85]
48	$\left[-z, x+\frac{1}{2}, \frac{1}{2}-x\right]$	[72,87]
49	$\left[x+\frac{1}{2}, x, z+\frac{1}{2}\right]$	[97,132]
50	$\left[x+\frac{1}{2}, -z, x+\frac{1}{2}\right]$	[98,139]
51	$\left[x+\frac{1}{2}, z, \frac{1}{2}-x\right]$	[99,141]
52	$\left[z+\frac{1}{2}, x, \frac{1}{2}-x\right]$	[100,140]
53	$\left[\frac{1}{2}-z, x, x+\frac{1}{2}\right]$	[101,142]

continued ...

Table 11

No.	position	mapping
54	$\left[\frac{1}{2}-x,\, x,\, z+\frac{1}{2}\right]$	[102,128]
55	$\left[x+\frac{1}{2},\, -x,\, z+\frac{1}{2}\right]$	[103,129]
56	$\left[x+\frac{1}{2},\, -x,\, \frac{1}{2}-z\right]$	[104,126]
57	$\left[\frac{1}{2}-x,\, x,\, \frac{1}{2}-z\right]$	[105,127]
58	$\left[\frac{1}{2}-x,\, -x,\, z+\frac{1}{2}\right]$	[106,131]
59	$\left[x+\frac{1}{2},\, x,\, \frac{1}{2}-z\right]$	[107,130]
60	$\left[\frac{1}{2}-x,\, -x,\, \frac{1}{2}-z\right]$	[108,121]
61	$\left[\frac{1}{2}-x,\, z,\, x+\frac{1}{2}\right]$	[109,143]
62	$\left[\frac{1}{2}-x,\, -z,\, \frac{1}{2}-x\right]$	[110,138]
63	$\left[z+\frac{1}{2},\, -x,\, x+\frac{1}{2}\right]$	[111,144]
64	$\left[\frac{1}{2}-z,\, -x,\, \frac{1}{2}-x\right]$	[112,137]
65	$\left[z+\frac{1}{2},\, x,\, x+\frac{1}{2}\right]$	[113,136]
66	$\left[x+\frac{1}{2},\, z,\, x+\frac{1}{2}\right]$	[114,134]
67	$\left[\frac{1}{2}-x,\, z,\, \frac{1}{2}-x\right]$	[115,122]
68	$\left[\frac{1}{2}-z,\, -x,\, x+\frac{1}{2}\right]$	[116,124]
69	$\left[\frac{1}{2}-x,\, -z,\, x+\frac{1}{2}\right]$	[117,123]
70	$\left[z+\frac{1}{2},\, -x,\, \frac{1}{2}-x\right]$	[118,125]
71	$\left[x+\frac{1}{2},\, -z,\, \frac{1}{2}-x\right]$	[119,133]
72	$\left[\frac{1}{2}-z,\, x,\, \frac{1}{2}-x\right]$	[120,135]
73	$\left[x+\frac{1}{2},\, x+\frac{1}{2},\, z\right]$	[145,180]
74	$\left[x+\frac{1}{2},\, \frac{1}{2}-z,\, x\right]$	[146,187]
75	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, -x\right]$	[147,189]
76	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, -x\right]$	[148,188]
77	$\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, x\right]$	[149,190]
78	$\left[\frac{1}{2}-x,\, x+\frac{1}{2},\, z\right]$	[150,176]
79	$\left[x+\frac{1}{2},\, \frac{1}{2}-x,\, z\right]$	[151,177]
80	$\left[x+\frac{1}{2},\, \frac{1}{2}-x,\, -z\right]$	[152,174]
81	$\left[\frac{1}{2}-x,\, x+\frac{1}{2},\, -z\right]$	[153,175]
82	$\left[\frac{1}{2}-x,\, \frac{1}{2}-x,\, z\right]$	[154,179]
83	$\left[x+\frac{1}{2},\, x+\frac{1}{2},\, -z\right]$	[155,178]
84	$\left[\frac{1}{2}-x,\, \frac{1}{2}-x,\, -z\right]$	[156,169]
85	$\left[\frac{1}{2}-x,\, z+\frac{1}{2},\, x\right]$	[157,191]
86	$\left[\frac{1}{2}-x,\, \frac{1}{2}-z,\, -x\right]$	[158,186]
87	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, x\right]$	[159,192]
88	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, -x\right]$	[160,185]
89	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, x\right]$	[161,184]
90	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, x\right]$	[162,182]
91	$\left[\frac{1}{2}-x,\, z+\frac{1}{2},\, -x\right]$	[163,170]
92	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, x\right]$	[164,172]
93	$\left[\frac{1}{2}-x,\, \frac{1}{2}-z,\, x\right]$	[165,171]
94	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, -x\right]$	[166,173]
95	$\left[x+\frac{1}{2},\, \frac{1}{2}-z,\, -x\right]$	[167,181]
96	$\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, -x\right]$	[168,183]

Table 12: Wyckoff site: 1921, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, -z, y]$	[2]
3	$[x, z, -y]$	[3]
4	$[z, y, -x]$	[4]
5	$[-z, y, x]$	[5]
6	$[-y, x, z]$	[6]
7	$[y, -x, z]$	[7]
8	$[x, -y, -z]$	[8]
9	$[-x, y, -z]$	[9]
10	$[-x, -y, z]$	[10]
11	$[y, x, -z]$	[11]
12	$[-y, -x, -z]$	[12]
13	$[-x, z, y]$	[13]
14	$[-x, -z, -y]$	[14]
15	$[z, -y, x]$	[15]
16	$[-z, -y, -x]$	[16]
17	$[z, x, y]$	[17]
18	$[y, z, x]$	[18]
19	$[-y, z, -x]$	[19]
20	$[-z, -x, y]$	[20]
21	$[-y, -z, x]$	[21]
22	$[z, -x, -y]$	[22]
23	$[y, -z, -x]$	[23]
24	$[-z, x, -y]$	[24]
25	$[-x, -y, -z]$	[25]
26	$[-x, z, -y]$	[26]
27	$[-x, -z, y]$	[27]
28	$[-z, -y, x]$	[28]
29	$[z, -y, -x]$	[29]
30	$[y, -x, -z]$	[30]
31	$[-y, x, -z]$	[31]
32	$[-x, y, z]$	[32]
33	$[x, -y, z]$	[33]
34	$[x, y, -z]$	[34]
35	$[-y, -x, z]$	[35]
36	$[y, x, z]$	[36]
37	$[x, -z, -y]$	[37]
38	$[x, z, y]$	[38]
39	$[-z, y, -x]$	[39]
40	$[z, y, x]$	[40]
41	$[-z, -x, -y]$	[41]
42	$[-y, -z, -x]$	[42]
43	$[y, -z, x]$	[43]
44	$[z, x, -y]$	[44]
45	$[y, z, -x]$	[45]
46	$[-z, x, y]$	[46]

continued ...

Table 12

No.	position	mapping
47	$[-y,\, z,\, x]$	[47]
48	$[z,\, -x,\, y]$	[48]
49	$\left[x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[49]
50	$\left[x,\, \frac{1}{2}-z,\, y+\frac{1}{2}\right]$	[50]
51	$\left[x,\, z+\frac{1}{2},\, \frac{1}{2}-y\right]$	[51]
52	$\left[z,\, y+\frac{1}{2},\, \frac{1}{2}-x\right]$	[52]
53	$\left[-z,\, y+\frac{1}{2},\, x+\frac{1}{2}\right]$	[53]
54	$\left[-y,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[54]
55	$\left[y,\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$	[55]
56	$\left[x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[56]
57	$\left[-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[57]
58	$\left[-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[58]
59	$\left[y,\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[59]
60	$\left[-y,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[60]
61	$\left[-x,\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[61]
62	$\left[-x,\, \frac{1}{2}-z,\, \frac{1}{2}-y\right]$	[62]
63	$\left[z,\, \frac{1}{2}-y,\, x+\frac{1}{2}\right]$	[63]
64	$\left[-z,\, \frac{1}{2}-y,\, \frac{1}{2}-x\right]$	[64]
65	$\left[z,\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[65]
66	$\left[y,\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[66]
67	$\left[-y,\, z+\frac{1}{2},\, \frac{1}{2}-x\right]$	[67]
68	$\left[-z,\, \frac{1}{2}-x,\, y+\frac{1}{2}\right]$	[68]
69	$\left[-y,\, \frac{1}{2}-z,\, x+\frac{1}{2}\right]$	[69]
70	$\left[z,\, \frac{1}{2}-x,\, \frac{1}{2}-y\right]$	[70]
71	$\left[y,\, \frac{1}{2}-z,\, \frac{1}{2}-x\right]$	[71]
72	$\left[-z,\, x+\frac{1}{2},\, \frac{1}{2}-y\right]$	[72]
73	$\left[-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[73]
74	$\left[-x,\, z+\frac{1}{2},\, \frac{1}{2}-y\right]$	[74]
75	$\left[-x,\, \frac{1}{2}-z,\, y+\frac{1}{2}\right]$	[75]
76	$\left[-z,\, \frac{1}{2}-y,\, x+\frac{1}{2}\right]$	[76]
77	$\left[z,\, \frac{1}{2}-y,\, \frac{1}{2}-x\right]$	[77]
78	$\left[y,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[78]
79	$\left[-y,\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[79]
80	$\left[-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[80]
81	$\left[x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[81]
82	$\left[x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[82]
83	$\left[-y,\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$	[83]
84	$\left[y,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[84]
85	$\left[x,\, \frac{1}{2}-z,\, \frac{1}{2}-y\right]$	[85]
86	$\left[x,\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[86]
87	$\left[-z,\, y+\frac{1}{2},\, \frac{1}{2}-x\right]$	[87]
88	$\left[z,\, y+\frac{1}{2},\, x+\frac{1}{2}\right]$	[88]
89	$\left[-z,\, \frac{1}{2}-x,\, \frac{1}{2}-y\right]$	[89]
90	$\left[-y,\, \frac{1}{2}-z,\, \frac{1}{2}-x\right]$	[90]
91	$\left[y,\, \frac{1}{2}-z,\, x+\frac{1}{2}\right]$	[91]
92	$\left[z,\, x+\frac{1}{2},\, \frac{1}{2}-y\right]$	[92]
93	$\left[y,\, z+\frac{1}{2},\, \frac{1}{2}-x\right]$	[93]

continued ...

Table 12

No.	position	mapping
94	$\left[-z,\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[94]
95	$\left[-y,\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[95]
96	$\left[z,\, \frac{1}{2}-x,\, y+\frac{1}{2}\right]$	[96]
97	$\left[x+\frac{1}{2},\, y,\, z+\frac{1}{2}\right]$	[97]
98	$\left[x+\frac{1}{2},\, -z,\, y+\frac{1}{2}\right]$	[98]
99	$\left[x+\frac{1}{2},\, z,\, \frac{1}{2}-y\right]$	[99]
100	$\left[z+\frac{1}{2},\, y,\, \frac{1}{2}-x\right]$	[100]
101	$\left[\frac{1}{2}-z,\, y,\, x+\frac{1}{2}\right]$	[101]
102	$\left[\frac{1}{2}-y,\, x,\, z+\frac{1}{2}\right]$	[102]
103	$\left[y+\frac{1}{2},\, -x,\, z+\frac{1}{2}\right]$	[103]
104	$\left[x+\frac{1}{2},\, -y,\, \frac{1}{2}-z\right]$	[104]
105	$\left[\frac{1}{2}-x,\, y,\, \frac{1}{2}-z\right]$	[105]
106	$\left[\frac{1}{2}-x,\, -y,\, z+\frac{1}{2}\right]$	[106]
107	$\left[y+\frac{1}{2},\, x,\, \frac{1}{2}-z\right]$	[107]
108	$\left[\frac{1}{2}-y,\, -x,\, \frac{1}{2}-z\right]$	[108]
109	$\left[\frac{1}{2}-x,\, z,\, y+\frac{1}{2}\right]$	[109]
110	$\left[\frac{1}{2}-x,\, -z,\, \frac{1}{2}-y\right]$	[110]
111	$\left[z+\frac{1}{2},\, -y,\, x+\frac{1}{2}\right]$	[111]
112	$\left[\frac{1}{2}-z,\, -y,\, \frac{1}{2}-x\right]$	[112]
113	$\left[z+\frac{1}{2},\, x,\, y+\frac{1}{2}\right]$	[113]
114	$\left[y+\frac{1}{2},\, z,\, x+\frac{1}{2}\right]$	[114]
115	$\left[\frac{1}{2}-y,\, z,\, \frac{1}{2}-x\right]$	[115]
116	$\left[\frac{1}{2}-z,\, -x,\, y+\frac{1}{2}\right]$	[116]
117	$\left[\frac{1}{2}-y,\, -z,\, x+\frac{1}{2}\right]$	[117]
118	$\left[z+\frac{1}{2},\, -x,\, \frac{1}{2}-y\right]$	[118]
119	$\left[y+\frac{1}{2},\, -z,\, \frac{1}{2}-x\right]$	[119]
120	$\left[\frac{1}{2}-z,\, x,\, \frac{1}{2}-y\right]$	[120]
121	$\left[\frac{1}{2}-x,\, -y,\, \frac{1}{2}-z\right]$	[121]
122	$\left[\frac{1}{2}-x,\, z,\, \frac{1}{2}-y\right]$	[122]
123	$\left[\frac{1}{2}-x,\, -z,\, y+\frac{1}{2}\right]$	[123]
124	$\left[\frac{1}{2}-z,\, -y,\, x+\frac{1}{2}\right]$	[124]
125	$\left[z+\frac{1}{2},\, -y,\, \frac{1}{2}-x\right]$	[125]
126	$\left[y+\frac{1}{2},\, -x,\, \frac{1}{2}-z\right]$	[126]
127	$\left[\frac{1}{2}-y,\, x,\, \frac{1}{2}-z\right]$	[127]
128	$\left[\frac{1}{2}-x,\, y,\, z+\frac{1}{2}\right]$	[128]
129	$\left[x+\frac{1}{2},\, -y,\, z+\frac{1}{2}\right]$	[129]
130	$\left[x+\frac{1}{2},\, y,\, \frac{1}{2}-z\right]$	[130]
131	$\left[\frac{1}{2}-y,\, -x,\, z+\frac{1}{2}\right]$	[131]
132	$\left[y+\frac{1}{2},\, x,\, z+\frac{1}{2}\right]$	[132]
133	$\left[x+\frac{1}{2},\, -z,\, \frac{1}{2}-y\right]$	[133]
134	$\left[x+\frac{1}{2},\, z,\, y+\frac{1}{2}\right]$	[134]
135	$\left[\frac{1}{2}-z,\, y,\, \frac{1}{2}-x\right]$	[135]
136	$\left[z+\frac{1}{2},\, y,\, x+\frac{1}{2}\right]$	[136]
137	$\left[\frac{1}{2}-z,\, -x,\, \frac{1}{2}-y\right]$	[137]
138	$\left[\frac{1}{2}-y,\, -z,\, \frac{1}{2}-x\right]$	[138]
139	$\left[y+\frac{1}{2},\, -z,\, x+\frac{1}{2}\right]$	[139]
140	$\left[z+\frac{1}{2},\, x,\, \frac{1}{2}-y\right]$	[140]

continued ...

Table 12

No.	position	mapping
141	$\left[y+\frac{1}{2},\, z,\, \frac{1}{2}-x\right]$	[141]
142	$\left[\frac{1}{2}-z,\, x,\, y+\frac{1}{2}\right]$	[142]
143	$\left[\frac{1}{2}-y,\, z,\, x+\frac{1}{2}\right]$	[143]
144	$\left[z+\frac{1}{2},\, -x,\, y+\frac{1}{2}\right]$	[144]
145	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z\right]$	[145]
146	$\left[x+\frac{1}{2},\, \frac{1}{2}-z,\, y\right]$	[146]
147	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, -y\right]$	[147]
148	$\left[z+\frac{1}{2},\, y+\frac{1}{2},\, -x\right]$	[148]
149	$\left[\frac{1}{2}-z,\, y+\frac{1}{2},\, x\right]$	[149]
150	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, z\right]$	[150]
151	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, z\right]$	[151]
152	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	[152]
153	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, -z\right]$	[153]
154	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z\right]$	[154]
155	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, -z\right]$	[155]
156	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, -z\right]$	[156]
157	$\left[\frac{1}{2}-x,\, z+\frac{1}{2},\, y\right]$	[157]
158	$\left[\frac{1}{2}-x,\, \frac{1}{2}-z,\, -y\right]$	[158]
159	$\left[z+\frac{1}{2},\, \frac{1}{2}-y,\, x\right]$	[159]
160	$\left[\frac{1}{2}-z,\, \frac{1}{2}-y,\, -x\right]$	[160]
161	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, y\right]$	[161]
162	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, x\right]$	[162]
163	$\left[\frac{1}{2}-y,\, z+\frac{1}{2},\, -x\right]$	[163]
164	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, y\right]$	[164]
165	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, x\right]$	[165]
166	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, -y\right]$	[166]
167	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, -x\right]$	[167]
168	$\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, -y\right]$	[168]
169	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, -z\right]$	[169]
170	$\left[\frac{1}{2}-x,\, z+\frac{1}{2},\, -y\right]$	[170]
171	$\left[\frac{1}{2}-x,\, \frac{1}{2}-z,\, y\right]$	[171]
172	$\left[\frac{1}{2}-z,\, \frac{1}{2}-y,\, x\right]$	[172]
173	$\left[z+\frac{1}{2},\, \frac{1}{2}-y,\, -x\right]$	[173]
174	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, -z\right]$	[174]
175	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, -z\right]$	[175]
176	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z\right]$	[176]
177	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z\right]$	[177]
178	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, -z\right]$	[178]
179	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, z\right]$	[179]
180	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z\right]$	[180]
181	$\left[x+\frac{1}{2},\, \frac{1}{2}-z,\, -y\right]$	[181]
182	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, y\right]$	[182]
183	$\left[\frac{1}{2}-z,\, y+\frac{1}{2},\, -x\right]$	[183]
184	$\left[z+\frac{1}{2},\, y+\frac{1}{2},\, x\right]$	[184]
185	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, -y\right]$	[185]
186	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, -x\right]$	[186]
187	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, x\right]$	[187]

continued ...

Table 12

No.	position	mapping
188	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, -y\right]$	[188]
189	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, -x\right]$	[189]
190	$\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, y\right]$	[190]
191	$\left[\frac{1}{2}-y,\, z+\frac{1}{2},\, x\right]$	[191]
192	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, y\right]$	[192]