

# MSG No. 225.119 $Fm\bar{3}m'$ [ Type III, cubic ]

Table 1: Wyckoff site: 4a, site symmetry:  $m\bar{3}m'$

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:  $m\bar{3}m'$

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:  $-4'3m'$

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

Table 4: Wyckoff site: 24d, site symmetry:  $\text{m.m'}$ 

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

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

No.	position	mapping
1	$[x, 0, 0]$	$[1, 2, 15, 16, 25, 26, 45, 46]$
2	$[-x, 0, 0]$	$[3, 4, 13, 14, 33, 34, 37, 38]$
3	$[0, x, 0]$	$[5, 12, 20, 22, 29, 31, 42, 44]$
4	$[0, 0, x]$	$[6, 9, 19, 23, 28, 35, 39, 48]$
5	$[0, 0, -x]$	$[7, 11, 18, 21, 27, 36, 40, 47]$
6	$[0, -x, 0]$	$[8, 10, 17, 24, 30, 32, 41, 43]$
7	$[x, \frac{1}{2}, \frac{1}{2}]$	$[49, 50, 63, 64, 73, 74, 93, 94]$
8	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[51, 52, 61, 62, 81, 82, 85, 86]$
9	$[0, x + \frac{1}{2}, \frac{1}{2}]$	$[53, 60, 68, 70, 77, 79, 90, 92]$
10	$[0, \frac{1}{2}, x + \frac{1}{2}]$	$[54, 57, 67, 71, 76, 83, 87, 96]$
11	$[0, \frac{1}{2}, \frac{1}{2} - x]$	$[55, 59, 66, 69, 75, 84, 88, 95]$
12	$[0, \frac{1}{2} - x, \frac{1}{2}]$	$[56, 58, 65, 72, 78, 80, 89, 91]$
13	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	$[97, 98, 111, 112, 121, 122, 141, 142]$
14	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	$[99, 100, 109, 110, 129, 130, 133, 134]$
15	$[\frac{1}{2}, x, \frac{1}{2}]$	$[101, 108, 116, 118, 125, 127, 138, 140]$

continued ...

Table 5

No.	position	mapping
16	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[102, 105, 115, 119, 124, 131, 135, 144]
17	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[103, 107, 114, 117, 123, 132, 136, 143]
18	$[\frac{1}{2}, -x, \frac{1}{2}]$	[104, 106, 113, 120, 126, 128, 137, 139]
19	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[145, 146, 159, 160, 169, 170, 189, 190]
20	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[147, 148, 157, 158, 177, 178, 181, 182]
21	$[\frac{1}{2}, x + \frac{1}{2}, 0]$	[149, 156, 164, 166, 173, 175, 186, 188]
22	$[\frac{1}{2}, \frac{1}{2}, x]$	[150, 153, 163, 167, 172, 179, 183, 192]
23	$[\frac{1}{2}, \frac{1}{2}, -x]$	[151, 155, 162, 165, 171, 180, 184, 191]
24	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	[152, 154, 161, 168, 174, 176, 185, 187]

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

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

continued ...

Table 6

No.	position	mapping
32	$[x + \frac{1}{2}, x + \frac{1}{2}, -x]$	[160, 164, 165, 170, 171, 175]

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

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

continued ...

Table 7

No.	position	mapping
40	$[\frac{1}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[72, 78, 161, 176]
41	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[97, 142, 146, 189]
42	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[98, 141, 145, 190]
43	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[99, 133, 148, 182]
44	$[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$	[100, 134, 147, 181]
45	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]$	[109, 130, 158, 177]
46	$[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$	[110, 129, 157, 178]
47	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[111, 121, 160, 170]
48	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[112, 122, 159, 169]

Table 8: Wyckoff site: 48h, site symmetry:  $m\cdot 2'm'$ 

No.	position	mapping
1	$[0, y, y]$	[1, 14, 33, 46]
2	$[0, -y, -y]$	[2, 13, 34, 45]
3	$[0, y, -y]$	[3, 16, 26, 37]
4	$[0, -y, y]$	[4, 15, 25, 38]
5	$[y, 0, y]$	[5, 24, 30, 44]
6	$[y, y, 0]$	[6, 21, 27, 48]
7	$[-y, y, 0]$	[7, 23, 28, 47]
8	$[-y, 0, y]$	[8, 22, 29, 43]
9	$[-y, -y, 0]$	[9, 18, 36, 39]
10	$[y, 0, -y]$	[10, 20, 31, 41]
11	$[y, -y, 0]$	[11, 19, 35, 40]
12	$[-y, 0, -y]$	[12, 17, 32, 42]
13	$[0, y + \frac{1}{2}, y + \frac{1}{2}]$	[49, 62, 81, 94]
14	$[0, \frac{1}{2} - y, \frac{1}{2} - y]$	[50, 61, 82, 93]
15	$[0, y + \frac{1}{2}, \frac{1}{2} - y]$	[51, 64, 74, 85]
16	$[0, \frac{1}{2} - y, y + \frac{1}{2}]$	[52, 63, 73, 86]
17	$[y, \frac{1}{2}, y + \frac{1}{2}]$	[53, 72, 78, 92]
18	$[y, y + \frac{1}{2}, \frac{1}{2}]$	[54, 69, 75, 96]
19	$[-y, y + \frac{1}{2}, \frac{1}{2}]$	[55, 71, 76, 95]
20	$[-y, \frac{1}{2}, y + \frac{1}{2}]$	[56, 70, 77, 91]
21	$[-y, \frac{1}{2} - y, \frac{1}{2}]$	[57, 66, 84, 87]
22	$[y, \frac{1}{2}, \frac{1}{2} - y]$	[58, 68, 79, 89]
23	$[y, \frac{1}{2} - y, \frac{1}{2}]$	[59, 67, 83, 88]
24	$[-y, \frac{1}{2}, \frac{1}{2} - y]$	[60, 65, 80, 90]
25	$[\frac{1}{2}, y, y + \frac{1}{2}]$	[97, 110, 129, 142]
26	$[\frac{1}{2}, -y, \frac{1}{2} - y]$	[98, 109, 130, 141]
27	$[\frac{1}{2}, y, \frac{1}{2} - y]$	[99, 112, 122, 133]
28	$[\frac{1}{2}, -y, y + \frac{1}{2}]$	[100, 111, 121, 134]
29	$[y + \frac{1}{2}, 0, y + \frac{1}{2}]$	[101, 120, 126, 140]
30	$[y + \frac{1}{2}, y, \frac{1}{2}]$	[102, 117, 123, 144]
31	$[\frac{1}{2} - y, y, \frac{1}{2}]$	[103, 119, 124, 143]

continued ...

Table 8

No.	position	mapping
32	$[\frac{1}{2} - y, 0, y + \frac{1}{2}]$	[104, 118, 125, 139]
33	$[\frac{1}{2} - y, -y, \frac{1}{2}]$	[105, 114, 132, 135]
34	$[y + \frac{1}{2}, 0, \frac{1}{2} - y]$	[106, 116, 127, 137]
35	$[y + \frac{1}{2}, -y, \frac{1}{2}]$	[107, 115, 131, 136]
36	$[\frac{1}{2} - y, 0, \frac{1}{2} - y]$	[108, 113, 128, 138]
37	$[\frac{1}{2}, y + \frac{1}{2}, y]$	[145, 158, 177, 190]
38	$[\frac{1}{2}, \frac{1}{2} - y, -y]$	[146, 157, 178, 189]
39	$[\frac{1}{2}, y + \frac{1}{2}, -y]$	[147, 160, 170, 181]
40	$[\frac{1}{2}, \frac{1}{2} - y, y]$	[148, 159, 169, 182]
41	$[y + \frac{1}{2}, \frac{1}{2}, y]$	[149, 168, 174, 188]
42	$[y + \frac{1}{2}, y + \frac{1}{2}, 0]$	[150, 165, 171, 192]
43	$[\frac{1}{2} - y, y + \frac{1}{2}, 0]$	[151, 167, 172, 191]
44	$[\frac{1}{2} - y, \frac{1}{2}, y]$	[152, 166, 173, 187]
45	$[\frac{1}{2} - y, \frac{1}{2} - y, 0]$	[153, 162, 180, 183]
46	$[y + \frac{1}{2}, \frac{1}{2}, -y]$	[154, 164, 175, 185]
47	$[y + \frac{1}{2}, \frac{1}{2} - y, 0]$	[155, 163, 179, 184]
48	$[\frac{1}{2} - y, \frac{1}{2}, -y]$	[156, 161, 176, 186]

Table 9: Wyckoff site: 48i, site symmetry:  $m\cdot 2'm'$ 

No.	position	mapping
1	$[\frac{1}{2}, y, y]$	[1, 14, 33, 46]
2	$[\frac{1}{2}, -y, -y]$	[2, 13, 34, 45]
3	$[\frac{1}{2}, y, -y]$	[3, 16, 26, 37]
4	$[\frac{1}{2}, -y, y]$	[4, 15, 25, 38]
5	$[y, \frac{1}{2}, y]$	[5, 24, 30, 44]
6	$[y, y, \frac{1}{2}]$	[6, 21, 27, 48]
7	$[-y, y, \frac{1}{2}]$	[7, 23, 28, 47]
8	$[-y, \frac{1}{2}, y]$	[8, 22, 29, 43]
9	$[-y, -y, \frac{1}{2}]$	[9, 18, 36, 39]
10	$[y, \frac{1}{2}, -y]$	[10, 20, 31, 41]
11	$[y, -y, \frac{1}{2}]$	[11, 19, 35, 40]
12	$[-y, \frac{1}{2}, -y]$	[12, 17, 32, 42]
13	$[\frac{1}{2}, y + \frac{1}{2}, y + \frac{1}{2}]$	[49, 62, 81, 94]
14	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - y]$	[50, 61, 82, 93]
15	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - y]$	[51, 64, 74, 85]
16	$[\frac{1}{2}, \frac{1}{2} - y, y + \frac{1}{2}]$	[52, 63, 73, 86]
17	$[y, 0, y + \frac{1}{2}]$	[53, 72, 78, 92]
18	$[y, y + \frac{1}{2}, 0]$	[54, 69, 75, 96]
19	$[-y, y + \frac{1}{2}, 0]$	[55, 71, 76, 95]
20	$[-y, 0, y + \frac{1}{2}]$	[56, 70, 77, 91]
21	$[-y, \frac{1}{2} - y, 0]$	[57, 66, 84, 87]
22	$[y, 0, \frac{1}{2} - y]$	[58, 68, 79, 89]
23	$[y, \frac{1}{2} - y, 0]$	[59, 67, 83, 88]

continued ...

Table 9

No.	position	mapping
24	$[-y, 0, \frac{1}{2} - y]$	[60,65,80,90]
25	$[0, y, y + \frac{1}{2}]$	[97,110,129,142]
26	$[0, -y, \frac{1}{2} - y]$	[98,109,130,141]
27	$[0, y, \frac{1}{2} - y]$	[99,112,122,133]
28	$[0, -y, y + \frac{1}{2}]$	[100,111,121,134]
29	$[y + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}]$	[101,120,126,140]
30	$[y + \frac{1}{2}, y, 0]$	[102,117,123,144]
31	$[\frac{1}{2} - y, y, 0]$	[103,119,124,143]
32	$[\frac{1}{2} - y, \frac{1}{2}, y + \frac{1}{2}]$	[104,118,125,139]
33	$[\frac{1}{2} - y, -y, 0]$	[105,114,132,135]
34	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - y]$	[106,116,127,137]
35	$[y + \frac{1}{2}, -y, 0]$	[107,115,131,136]
36	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - y]$	[108,113,128,138]
37	$[0, y + \frac{1}{2}, y]$	[145,158,177,190]
38	$[0, \frac{1}{2} - y, -y]$	[146,157,178,189]
39	$[0, y + \frac{1}{2}, -y]$	[147,160,170,181]
40	$[0, \frac{1}{2} - y, y]$	[148,159,169,182]
41	$[y + \frac{1}{2}, 0, y]$	[149,168,174,188]
42	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[150,165,171,192]
43	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{2}]$	[151,167,172,191]
44	$[\frac{1}{2} - y, 0, y]$	[152,166,173,187]
45	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{2}]$	[153,162,180,183]
46	$[y + \frac{1}{2}, 0, -y]$	[154,164,175,185]
47	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[155,163,179,184]
48	$[\frac{1}{2} - y, 0, -y]$	[156,161,176,186]

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

No.	position	mapping
1	$[0, y, z]$	[1,14]
2	$[0, -y, -z]$	[2,13]
3	$[0, y, -z]$	[3,16]
4	$[0, -y, z]$	[4,15]
5	$[z, 0, y]$	[5,24]
6	$[y, z, 0]$	[6,21]
7	$[-y, z, 0]$	[7,23]
8	$[-z, 0, y]$	[8,22]
9	$[-y, -z, 0]$	[9,18]
10	$[z, 0, -y]$	[10,20]
11	$[y, -z, 0]$	[11,19]
12	$[-z, 0, -y]$	[12,17]
13	$[0, -z, y]$	[25,38]
14	$[0, z, -y]$	[26,37]
15	$[z, y, 0]$	[27,48]

*continued ...*

Table 10

No.	position	mapping
16	$[-z, y, 0]$	[28,47]
17	$[-y, 0, z]$	[29,43]
18	$[y, 0, z]$	[30,44]
19	$[y, 0, -z]$	[31,41]
20	$[-y, 0, -z]$	[32,42]
21	$[0, z, y]$	[33,46]
22	$[0, -z, -y]$	[34,45]
23	$[z, -y, 0]$	[35,40]
24	$[-z, -y, 0]$	[36,39]
25	$[0, y + \frac{1}{2}, z + \frac{1}{2}]$	[49,62]
26	$[0, \frac{1}{2} - y, \frac{1}{2} - z]$	[50,61]
27	$[0, y + \frac{1}{2}, \frac{1}{2} - z]$	[51,64]
28	$[0, \frac{1}{2} - y, z + \frac{1}{2}]$	[52,63]
29	$[z, \frac{1}{2}, y + \frac{1}{2}]$	[53,72]
30	$[y, z + \frac{1}{2}, \frac{1}{2}]$	[54,69]
31	$[-y, z + \frac{1}{2}, \frac{1}{2}]$	[55,71]
32	$[-z, \frac{1}{2}, y + \frac{1}{2}]$	[56,70]
33	$[-y, \frac{1}{2} - z, \frac{1}{2}]$	[57,66]
34	$[z, \frac{1}{2}, \frac{1}{2} - y]$	[58,68]
35	$[y, \frac{1}{2} - z, \frac{1}{2}]$	[59,67]
36	$[-z, \frac{1}{2}, \frac{1}{2} - y]$	[60,65]
37	$[0, \frac{1}{2} - z, y + \frac{1}{2}]$	[73,86]
38	$[0, z + \frac{1}{2}, \frac{1}{2} - y]$	[74,85]
39	$[z, y + \frac{1}{2}, \frac{1}{2}]$	[75,96]
40	$[-z, y + \frac{1}{2}, \frac{1}{2}]$	[76,95]
41	$[-y, \frac{1}{2}, z + \frac{1}{2}]$	[77,91]
42	$[y, \frac{1}{2}, z + \frac{1}{2}]$	[78,92]
43	$[y, \frac{1}{2}, \frac{1}{2} - z]$	[79,89]
44	$[-y, \frac{1}{2}, \frac{1}{2} - z]$	[80,90]
45	$[0, z + \frac{1}{2}, y + \frac{1}{2}]$	[81,94]
46	$[0, \frac{1}{2} - z, \frac{1}{2} - y]$	[82,93]
47	$[z, \frac{1}{2} - y, \frac{1}{2}]$	[83,88]
48	$[-z, \frac{1}{2} - y, \frac{1}{2}]$	[84,87]
49	$[\frac{1}{2}, y, z + \frac{1}{2}]$	[97,110]
50	$[\frac{1}{2}, -y, \frac{1}{2} - z]$	[98,109]
51	$[\frac{1}{2}, y, \frac{1}{2} - z]$	[99,112]
52	$[\frac{1}{2}, -y, z + \frac{1}{2}]$	[100,111]
53	$[z + \frac{1}{2}, 0, y + \frac{1}{2}]$	[101,120]
54	$[y + \frac{1}{2}, z, \frac{1}{2}]$	[102,117]
55	$[\frac{1}{2} - y, z, \frac{1}{2}]$	[103,119]
56	$[\frac{1}{2} - z, 0, y + \frac{1}{2}]$	[104,118]
57	$[\frac{1}{2} - y, -z, \frac{1}{2}]$	[105,114]
58	$[z + \frac{1}{2}, 0, \frac{1}{2} - y]$	[106,116]
59	$[y + \frac{1}{2}, -z, \frac{1}{2}]$	[107,115]
60	$[\frac{1}{2} - z, 0, \frac{1}{2} - y]$	[108,113]
61	$[\frac{1}{2}, -z, y + \frac{1}{2}]$	[121,134]
62	$[\frac{1}{2}, z, \frac{1}{2} - y]$	[122,133]

*continued ...*

Table 10

No.	position	mapping
63	$[z + \frac{1}{2}, y, \frac{1}{2}]$	[123,144]
64	$[\frac{1}{2} - z, y, \frac{1}{2}]$	[124,143]
65	$[\frac{1}{2} - y, 0, z + \frac{1}{2}]$	[125,139]
66	$[y + \frac{1}{2}, 0, z + \frac{1}{2}]$	[126,140]
67	$[y + \frac{1}{2}, 0, \frac{1}{2} - z]$	[127,137]
68	$[\frac{1}{2} - y, 0, \frac{1}{2} - z]$	[128,138]
69	$[\frac{1}{2}, z, y + \frac{1}{2}]$	[129,142]
70	$[\frac{1}{2}, -z, \frac{1}{2} - y]$	[130,141]
71	$[z + \frac{1}{2}, -y, \frac{1}{2}]$	[131,136]
72	$[\frac{1}{2} - z, -y, \frac{1}{2}]$	[132,135]
73	$[\frac{1}{2}, y + \frac{1}{2}, z]$	[145,158]
74	$[\frac{1}{2}, \frac{1}{2} - y, -z]$	[146,157]
75	$[\frac{1}{2}, y + \frac{1}{2}, -z]$	[147,160]
76	$[\frac{1}{2}, \frac{1}{2} - y, z]$	[148,159]
77	$[z + \frac{1}{2}, \frac{1}{2}, y]$	[149,168]
78	$[y + \frac{1}{2}, z + \frac{1}{2}, 0]$	[150,165]
79	$[\frac{1}{2} - y, z + \frac{1}{2}, 0]$	[151,167]
80	$[\frac{1}{2} - z, \frac{1}{2}, y]$	[152,166]
81	$[\frac{1}{2} - y, \frac{1}{2} - z, 0]$	[153,162]
82	$[z + \frac{1}{2}, \frac{1}{2}, -y]$	[154,164]
83	$[y + \frac{1}{2}, \frac{1}{2} - z, 0]$	[155,163]
84	$[\frac{1}{2} - z, \frac{1}{2}, -y]$	[156,161]
85	$[\frac{1}{2}, \frac{1}{2} - z, y]$	[169,182]
86	$[\frac{1}{2}, z + \frac{1}{2}, -y]$	[170,181]
87	$[z + \frac{1}{2}, y + \frac{1}{2}, 0]$	[171,192]
88	$[\frac{1}{2} - z, y + \frac{1}{2}, 0]$	[172,191]
89	$[\frac{1}{2} - y, \frac{1}{2}, z]$	[173,187]
90	$[y + \frac{1}{2}, \frac{1}{2}, z]$	[174,188]
91	$[y + \frac{1}{2}, \frac{1}{2}, -z]$	[175,185]
92	$[\frac{1}{2} - y, \frac{1}{2}, -z]$	[176,186]
93	$[\frac{1}{2}, z + \frac{1}{2}, y]$	[177,190]
94	$[\frac{1}{2}, \frac{1}{2} - z, -y]$	[178,189]
95	$[z + \frac{1}{2}, \frac{1}{2} - y, 0]$	[179,184]
96	$[\frac{1}{2} - z, \frac{1}{2} - y, 0]$	[180,183]

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

No.	position	mapping
1	$[x, x, z]$	[1,44]
2	$[x, -x, -z]$	[2,41]
3	$[-x, x, -z]$	[3,42]
4	$[-x, -x, z]$	[4,43]
5	$[z, x, x]$	[5,48]
6	$[x, z, x]$	[6,46]

continued ...

Table 11

No.	position	mapping
7	$[-x, z, -x]$	[7,37]
8	$[-z, -x, x]$	[8,39]
9	$[-x, -z, x]$	[9,38]
10	$[z, -x, -x]$	[10,40]
11	$[x, -z, -x]$	[11,45]
12	$[-z, x, -x]$	[12,47]
13	$[-x, -x, -z]$	[13,32]
14	$[-x, x, z]$	[14,29]
15	$[x, -x, z]$	[15,30]
16	$[x, x, -z]$	[16,31]
17	$[-z, -x, -x]$	[17,36]
18	$[-x, -z, -x]$	[18,34]
19	$[x, -z, x]$	[19,25]
20	$[z, x, -x]$	[20,27]
21	$[x, z, -x]$	[21,26]
22	$[-z, x, x]$	[22,28]
23	$[-x, z, x]$	[23,33]
24	$[z, -x, x]$	[24,35]
25	$[x, x + \frac{1}{2}, z + \frac{1}{2}]$	[49,92]
26	$[x, \frac{1}{2} - x, \frac{1}{2} - z]$	[50,89]
27	$[-x, x + \frac{1}{2}, \frac{1}{2} - z]$	[51,90]
28	$[-x, \frac{1}{2} - x, z + \frac{1}{2}]$	[52,91]
29	$[z, x + \frac{1}{2}, x + \frac{1}{2}]$	[53,96]
30	$[x, z + \frac{1}{2}, x + \frac{1}{2}]$	[54,94]
31	$[-x, z + \frac{1}{2}, \frac{1}{2} - x]$	[55,85]
32	$[-z, \frac{1}{2} - x, x + \frac{1}{2}]$	[56,87]
33	$[-x, \frac{1}{2} - z, x + \frac{1}{2}]$	[57,86]
34	$[z, \frac{1}{2} - x, \frac{1}{2} - x]$	[58,88]
35	$[x, \frac{1}{2} - z, \frac{1}{2} - x]$	[59,93]
36	$[-z, x + \frac{1}{2}, \frac{1}{2} - x]$	[60,95]
37	$[-x, \frac{1}{2} - x, \frac{1}{2} - z]$	[61,80]
38	$[-x, x + \frac{1}{2}, z + \frac{1}{2}]$	[62,77]
39	$[x, \frac{1}{2} - x, z + \frac{1}{2}]$	[63,78]
40	$[x, x + \frac{1}{2}, \frac{1}{2} - z]$	[64,79]
41	$[-z, \frac{1}{2} - x, \frac{1}{2} - x]$	[65,84]
42	$[-x, \frac{1}{2} - z, \frac{1}{2} - x]$	[66,82]
43	$[x, \frac{1}{2} - z, x + \frac{1}{2}]$	[67,73]
44	$[z, x + \frac{1}{2}, \frac{1}{2} - x]$	[68,75]
45	$[x, z + \frac{1}{2}, \frac{1}{2} - x]$	[69,74]
46	$[-z, x + \frac{1}{2}, x + \frac{1}{2}]$	[70,76]
47	$[-x, z + \frac{1}{2}, x + \frac{1}{2}]$	[71,81]
48	$[z, \frac{1}{2} - x, x + \frac{1}{2}]$	[72,83]
49	$[x + \frac{1}{2}, x, z + \frac{1}{2}]$	[97,140]
50	$[x + \frac{1}{2}, -x, \frac{1}{2} - z]$	[98,137]
51	$[\frac{1}{2} - x, x, \frac{1}{2} - z]$	[99,138]
52	$[\frac{1}{2} - x, -x, z + \frac{1}{2}]$	[100,139]
53	$[z + \frac{1}{2}, x, x + \frac{1}{2}]$	[101,144]

continued ...

Table 11

No.	position	mapping
54	$[x + \frac{1}{2}, z, x + \frac{1}{2}]$	[102,142]
55	$[\frac{1}{2} - x, z, \frac{1}{2} - x]$	[103,133]
56	$[\frac{1}{2} - z, -x, x + \frac{1}{2}]$	[104,135]
57	$[\frac{1}{2} - x, -z, x + \frac{1}{2}]$	[105,134]
58	$[z + \frac{1}{2}, -x, \frac{1}{2} - x]$	[106,136]
59	$[x + \frac{1}{2}, -z, \frac{1}{2} - x]$	[107,141]
60	$[\frac{1}{2} - z, x, \frac{1}{2} - x]$	[108,143]
61	$[\frac{1}{2} - x, -x, \frac{1}{2} - z]$	[109,128]
62	$[\frac{1}{2} - x, x, z + \frac{1}{2}]$	[110,125]
63	$[x + \frac{1}{2}, -x, z + \frac{1}{2}]$	[111,126]
64	$[x + \frac{1}{2}, x, \frac{1}{2} - z]$	[112,127]
65	$[\frac{1}{2} - z, -x, \frac{1}{2} - x]$	[113,132]
66	$[\frac{1}{2} - x, -z, \frac{1}{2} - x]$	[114,130]
67	$[x + \frac{1}{2}, -z, x + \frac{1}{2}]$	[115,121]
68	$[z + \frac{1}{2}, x, \frac{1}{2} - x]$	[116,123]
69	$[x + \frac{1}{2}, z, \frac{1}{2} - x]$	[117,122]
70	$[\frac{1}{2} - z, x, x + \frac{1}{2}]$	[118,124]
71	$[\frac{1}{2} - x, z, x + \frac{1}{2}]$	[119,129]
72	$[z + \frac{1}{2}, -x, x + \frac{1}{2}]$	[120,131]
73	$[x + \frac{1}{2}, x + \frac{1}{2}, z]$	[145,188]
74	$[x + \frac{1}{2}, \frac{1}{2} - x, -z]$	[146,185]
75	$[\frac{1}{2} - x, x + \frac{1}{2}, -z]$	[147,186]
76	$[\frac{1}{2} - x, \frac{1}{2} - x, z]$	[148,187]
77	$[z + \frac{1}{2}, x + \frac{1}{2}, x]$	[149,192]
78	$[x + \frac{1}{2}, z + \frac{1}{2}, x]$	[150,190]
79	$[\frac{1}{2} - x, z + \frac{1}{2}, -x]$	[151,181]
80	$[\frac{1}{2} - z, \frac{1}{2} - x, x]$	[152,183]
81	$[\frac{1}{2} - x, \frac{1}{2} - z, x]$	[153,182]
82	$[z + \frac{1}{2}, \frac{1}{2} - x, -x]$	[154,184]
83	$[x + \frac{1}{2}, \frac{1}{2} - z, -x]$	[155,189]
84	$[\frac{1}{2} - z, x + \frac{1}{2}, -x]$	[156,191]
85	$[\frac{1}{2} - x, \frac{1}{2} - x, -z]$	[157,176]
86	$[\frac{1}{2} - x, x + \frac{1}{2}, z]$	[158,173]
87	$[x + \frac{1}{2}, \frac{1}{2} - x, z]$	[159,174]
88	$[x + \frac{1}{2}, x + \frac{1}{2}, -z]$	[160,175]
89	$[\frac{1}{2} - z, \frac{1}{2} - x, -x]$	[161,180]
90	$[\frac{1}{2} - x, \frac{1}{2} - z, -x]$	[162,178]
91	$[x + \frac{1}{2}, \frac{1}{2} - z, x]$	[163,169]
92	$[z + \frac{1}{2}, x + \frac{1}{2}, -x]$	[164,171]
93	$[x + \frac{1}{2}, z + \frac{1}{2}, -x]$	[165,170]
94	$[\frac{1}{2} - z, x + \frac{1}{2}, x]$	[166,172]
95	$[\frac{1}{2} - x, z + \frac{1}{2}, x]$	[167,177]
96	$[z + \frac{1}{2}, \frac{1}{2} - x, x]$	[168,179]

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

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

*continued ...*

Table 12

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

*continued ...*

Table 12

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

*continued ...*

Table 12

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

*continued ...*

Table 12

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