

MSG No. 225.118 $Fm\bar{3}'m$ [Type III, cubic]

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

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: $m'-3'm$

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: $-43m$

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

Table 4: Wyckoff site: 24d, site symmetry: $m' \cdot mm$

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

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

No.	position	mapping
1	$[x, 0, 0]$	$[1, 2, 21, 22, 25, 26, 39, 40]$
2	$[-x, 0, 0]$	$[3, 4, 13, 14, 33, 34, 37, 38]$
3	$[0, x, 0]$	$[5, 12, 18, 20, 29, 31, 44, 46]$
4	$[0, 0, x]$	$[6, 9, 15, 24, 28, 35, 43, 47]$
5	$[0, 0, -x]$	$[7, 11, 16, 23, 27, 36, 42, 45]$
6	$[0, -x, 0]$	$[8, 10, 17, 19, 30, 32, 41, 48]$
7	$[x, \frac{1}{2}, \frac{1}{2}]$	$[49, 50, 69, 70, 73, 74, 87, 88]$
8	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[51, 52, 61, 62, 81, 82, 85, 86]$
9	$[0, x + \frac{1}{2}, \frac{1}{2}]$	$[53, 60, 66, 68, 77, 79, 92, 94]$
10	$[0, \frac{1}{2}, x + \frac{1}{2}]$	$[54, 57, 63, 72, 76, 83, 91, 95]$
11	$[0, \frac{1}{2}, \frac{1}{2} - x]$	$[55, 59, 64, 71, 75, 84, 90, 93]$
12	$[0, \frac{1}{2} - x, \frac{1}{2}]$	$[56, 58, 65, 67, 78, 80, 89, 96]$
13	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	$[97, 98, 117, 118, 121, 122, 135, 136]$
14	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	$[99, 100, 109, 110, 129, 130, 133, 134]$
15	$[\frac{1}{2}, x, \frac{1}{2}]$	$[101, 108, 114, 116, 125, 127, 140, 142]$

continued ...

Table 5

No.	position	mapping
16	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[102, 105, 111, 120, 124, 131, 139, 143]
17	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[103, 107, 112, 119, 123, 132, 138, 141]
18	$[\frac{1}{2}, -x, \frac{1}{2}]$	[104, 106, 113, 115, 126, 128, 137, 144]
19	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[145, 146, 165, 166, 169, 170, 183, 184]
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, 162, 164, 173, 175, 188, 190]
22	$[\frac{1}{2}, \frac{1}{2}, x]$	[150, 153, 159, 168, 172, 179, 187, 191]
23	$[\frac{1}{2}, \frac{1}{2}, -x]$	[151, 155, 160, 167, 171, 180, 186, 189]
24	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	[152, 154, 161, 163, 174, 176, 185, 192]

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

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

continued ...

Table 6

No.	position	mapping
32	$[\frac{1}{2} - x, \frac{1}{2} - x, -x]$	[176, 178, 180, 181, 185, 186]

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

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

continued ...

Table 7

No.	position	mapping
40	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[84, 90, 123, 141]
41	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[97, 118, 146, 165]
42	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[98, 117, 145, 166]
43	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[99, 109, 148, 158]
44	$[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$	[100, 110, 147, 157]
45	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[121, 135, 170, 184]
46	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[122, 136, 169, 183]
47	$[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$	[129, 134, 178, 181]
48	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]$	[130, 133, 177, 182]

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

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

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

No.	position	mapping
1	$[\frac{1}{2}, y, y]$	[1, 22, 33, 38]
2	$[\frac{1}{2}, -y, -y]$	[2, 21, 34, 37]
3	$[\frac{1}{2}, y, -y]$	[3, 13, 26, 40]
4	$[\frac{1}{2}, -y, y]$	[4, 14, 25, 39]
5	$[y, \frac{1}{2}, y]$	[5, 20, 30, 48]
6	$[y, y, \frac{1}{2}]$	[6, 24, 27, 45]
7	$[-y, y, \frac{1}{2}]$	[7, 23, 28, 47]
8	$[-y, \frac{1}{2}, y]$	[8, 19, 29, 46]
9	$[-y, -y, \frac{1}{2}]$	[9, 15, 36, 42]
10	$[y, \frac{1}{2}, -y]$	[10, 17, 31, 44]
11	$[y, -y, \frac{1}{2}]$	[11, 16, 35, 43]
12	$[-y, \frac{1}{2}, -y]$	[12, 18, 32, 41]
13	$[\frac{1}{2}, y + \frac{1}{2}, y + \frac{1}{2}]$	[49, 70, 81, 86]
14	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - y]$	[50, 69, 82, 85]
15	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - y]$	[51, 61, 74, 88]
16	$[\frac{1}{2}, \frac{1}{2} - y, y + \frac{1}{2}]$	[52, 62, 73, 87]
17	$[y, 0, y + \frac{1}{2}]$	[53, 68, 78, 96]
18	$[y, y + \frac{1}{2}, 0]$	[54, 72, 75, 93]
19	$[-y, y + \frac{1}{2}, 0]$	[55, 71, 76, 95]
20	$[-y, 0, y + \frac{1}{2}]$	[56, 67, 77, 94]
21	$[-y, \frac{1}{2} - y, 0]$	[57, 63, 84, 90]
22	$[y, 0, \frac{1}{2} - y]$	[58, 65, 79, 92]
23	$[y, \frac{1}{2} - y, 0]$	[59, 64, 83, 91]

continued ...

Table 9

No.	position	mapping
24	$[-y, 0, \frac{1}{2} - y]$	[60,66,80,89]
25	$[0, y, y + \frac{1}{2}]$	[97,118,129,134]
26	$[0, -y, \frac{1}{2} - y]$	[98,117,130,133]
27	$[0, y, \frac{1}{2} - y]$	[99,109,122,136]
28	$[0, -y, y + \frac{1}{2}]$	[100,110,121,135]
29	$[y + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}]$	[101,116,126,144]
30	$[y + \frac{1}{2}, y, 0]$	[102,120,123,141]
31	$[\frac{1}{2} - y, y, 0]$	[103,119,124,143]
32	$[\frac{1}{2} - y, \frac{1}{2}, y + \frac{1}{2}]$	[104,115,125,142]
33	$[\frac{1}{2} - y, -y, 0]$	[105,111,132,138]
34	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - y]$	[106,113,127,140]
35	$[y + \frac{1}{2}, -y, 0]$	[107,112,131,139]
36	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - y]$	[108,114,128,137]
37	$[0, y + \frac{1}{2}, y]$	[145,166,177,182]
38	$[0, \frac{1}{2} - y, -y]$	[146,165,178,181]
39	$[0, y + \frac{1}{2}, -y]$	[147,157,170,184]
40	$[0, \frac{1}{2} - y, y]$	[148,158,169,183]
41	$[y + \frac{1}{2}, 0, y]$	[149,164,174,192]
42	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[150,168,171,189]
43	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{2}]$	[151,167,172,191]
44	$[\frac{1}{2} - y, 0, y]$	[152,163,173,190]
45	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{2}]$	[153,159,180,186]
46	$[y + \frac{1}{2}, 0, -y]$	[154,161,175,188]
47	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[155,160,179,187]
48	$[\frac{1}{2} - y, 0, -y]$	[156,162,176,185]

Table 10: Wyckoff site: 96j, site symmetry: $m' \dots$

No.	position	mapping
1	$[0, y, z]$	[1,38]
2	$[0, -y, -z]$	[2,37]
3	$[0, y, -z]$	[3,40]
4	$[0, -y, z]$	[4,39]
5	$[z, 0, y]$	[5,48]
6	$[y, z, 0]$	[6,45]
7	$[-y, z, 0]$	[7,47]
8	$[-z, 0, y]$	[8,46]
9	$[-y, -z, 0]$	[9,42]
10	$[z, 0, -y]$	[10,44]
11	$[y, -z, 0]$	[11,43]
12	$[-z, 0, -y]$	[12,41]
13	$[0, z, -y]$	[13,26]
14	$[0, -z, y]$	[14,25]
15	$[-z, -y, 0]$	[15,36]

continued ...

Table 10

No.	position	mapping
16	$[z, -y, 0]$	[16,35]
17	$[y, 0, -z]$	[17,31]
18	$[-y, 0, -z]$	[18,32]
19	$[-y, 0, z]$	[19,29]
20	$[y, 0, z]$	[20,30]
21	$[0, -z, -y]$	[21,34]
22	$[0, z, y]$	[22,33]
23	$[-z, y, 0]$	[23,28]
24	$[z, y, 0]$	[24,27]
25	$[0, y + \frac{1}{2}, z + \frac{1}{2}]$	[49,86]
26	$[0, \frac{1}{2} - y, \frac{1}{2} - z]$	[50,85]
27	$[0, y + \frac{1}{2}, \frac{1}{2} - z]$	[51,88]
28	$[0, \frac{1}{2} - y, z + \frac{1}{2}]$	[52,87]
29	$[z, \frac{1}{2}, y + \frac{1}{2}]$	[53,96]
30	$[y, z + \frac{1}{2}, \frac{1}{2}]$	[54,93]
31	$[-y, z + \frac{1}{2}, \frac{1}{2}]$	[55,95]
32	$[-z, \frac{1}{2}, y + \frac{1}{2}]$	[56,94]
33	$[-y, \frac{1}{2} - z, \frac{1}{2}]$	[57,90]
34	$[z, \frac{1}{2}, \frac{1}{2} - y]$	[58,92]
35	$[y, \frac{1}{2} - z, \frac{1}{2}]$	[59,91]
36	$[-z, \frac{1}{2}, \frac{1}{2} - y]$	[60,89]
37	$[0, z + \frac{1}{2}, \frac{1}{2} - y]$	[61,74]
38	$[0, \frac{1}{2} - z, y + \frac{1}{2}]$	[62,73]
39	$[-z, \frac{1}{2} - y, \frac{1}{2}]$	[63,84]
40	$[z, \frac{1}{2} - y, \frac{1}{2}]$	[64,83]
41	$[y, \frac{1}{2}, \frac{1}{2} - z]$	[65,79]
42	$[-y, \frac{1}{2}, \frac{1}{2} - z]$	[66,80]
43	$[-y, \frac{1}{2}, z + \frac{1}{2}]$	[67,77]
44	$[y, \frac{1}{2}, z + \frac{1}{2}]$	[68,78]
45	$[0, \frac{1}{2} - z, \frac{1}{2} - y]$	[69,82]
46	$[0, z + \frac{1}{2}, y + \frac{1}{2}]$	[70,81]
47	$[-z, y + \frac{1}{2}, \frac{1}{2}]$	[71,76]
48	$[z, y + \frac{1}{2}, \frac{1}{2}]$	[72,75]
49	$[\frac{1}{2}, y, z + \frac{1}{2}]$	[97,134]
50	$[\frac{1}{2}, -y, \frac{1}{2} - z]$	[98,133]
51	$[\frac{1}{2}, y, \frac{1}{2} - z]$	[99,136]
52	$[\frac{1}{2}, -y, z + \frac{1}{2}]$	[100,135]
53	$[z + \frac{1}{2}, 0, y + \frac{1}{2}]$	[101,144]
54	$[y + \frac{1}{2}, z, \frac{1}{2}]$	[102,141]
55	$[\frac{1}{2} - y, z, \frac{1}{2}]$	[103,143]
56	$[\frac{1}{2} - z, 0, y + \frac{1}{2}]$	[104,142]
57	$[\frac{1}{2} - y, -z, \frac{1}{2}]$	[105,138]
58	$[z + \frac{1}{2}, 0, \frac{1}{2} - y]$	[106,140]
59	$[y + \frac{1}{2}, -z, \frac{1}{2}]$	[107,139]
60	$[\frac{1}{2} - z, 0, \frac{1}{2} - y]$	[108,137]
61	$[\frac{1}{2}, z, \frac{1}{2} - y]$	[109,122]
62	$[\frac{1}{2}, -z, y + \frac{1}{2}]$	[110,121]

continued ...

Table 10

No.	position	mapping
63	$[\frac{1}{2} - z, -y, \frac{1}{2}]$	[111,132]
64	$[z + \frac{1}{2}, -y, \frac{1}{2}]$	[112,131]
65	$[y + \frac{1}{2}, 0, \frac{1}{2} - z]$	[113,127]
66	$[\frac{1}{2} - y, 0, \frac{1}{2} - z]$	[114,128]
67	$[\frac{1}{2} - y, 0, z + \frac{1}{2}]$	[115,125]
68	$[y + \frac{1}{2}, 0, z + \frac{1}{2}]$	[116,126]
69	$[\frac{1}{2}, -z, \frac{1}{2} - y]$	[117,130]
70	$[\frac{1}{2}, z, y + \frac{1}{2}]$	[118,129]
71	$[\frac{1}{2} - z, y, \frac{1}{2}]$	[119,124]
72	$[z + \frac{1}{2}, y, \frac{1}{2}]$	[120,123]
73	$[\frac{1}{2}, y + \frac{1}{2}, z]$	[145,182]
74	$[\frac{1}{2}, \frac{1}{2} - y, -z]$	[146,181]
75	$[\frac{1}{2}, y + \frac{1}{2}, -z]$	[147,184]
76	$[\frac{1}{2}, \frac{1}{2} - y, z]$	[148,183]
77	$[z + \frac{1}{2}, \frac{1}{2}, y]$	[149,192]
78	$[y + \frac{1}{2}, z + \frac{1}{2}, 0]$	[150,189]
79	$[\frac{1}{2} - y, z + \frac{1}{2}, 0]$	[151,191]
80	$[\frac{1}{2} - z, \frac{1}{2}, y]$	[152,190]
81	$[\frac{1}{2} - y, \frac{1}{2} - z, 0]$	[153,186]
82	$[z + \frac{1}{2}, \frac{1}{2}, -y]$	[154,188]
83	$[y + \frac{1}{2}, \frac{1}{2} - z, 0]$	[155,187]
84	$[\frac{1}{2} - z, \frac{1}{2}, -y]$	[156,185]
85	$[\frac{1}{2}, z + \frac{1}{2}, -y]$	[157,170]
86	$[\frac{1}{2}, \frac{1}{2} - z, y]$	[158,169]
87	$[\frac{1}{2} - z, \frac{1}{2} - y, 0]$	[159,180]
88	$[z + \frac{1}{2}, \frac{1}{2} - y, 0]$	[160,179]
89	$[y + \frac{1}{2}, \frac{1}{2}, -z]$	[161,175]
90	$[\frac{1}{2} - y, \frac{1}{2}, -z]$	[162,176]
91	$[\frac{1}{2} - y, \frac{1}{2}, z]$	[163,173]
92	$[y + \frac{1}{2}, \frac{1}{2}, z]$	[164,174]
93	$[\frac{1}{2}, \frac{1}{2} - z, -y]$	[165,178]
94	$[\frac{1}{2}, z + \frac{1}{2}, y]$	[166,177]
95	$[\frac{1}{2} - z, y + \frac{1}{2}, 0]$	[167,172]
96	$[z + \frac{1}{2}, y + \frac{1}{2}, 0]$	[168,171]

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

No.	position	mapping
1	$[x, x, z]$	[1,20]
2	$[x, -x, -z]$	[2,17]
3	$[-x, x, -z]$	[3,18]
4	$[-x, -x, z]$	[4,19]
5	$[z, x, x]$	[5,24]
6	$[x, z, x]$	[6,22]

continued ...

Table 11

No.	position	mapping
7	$[-x, z, -x]$	[7,13]
8	$[-z, -x, x]$	[8,15]
9	$[-x, -z, x]$	[9,14]
10	$[z, -x, -x]$	[10,16]
11	$[x, -z, -x]$	[11,21]
12	$[-z, x, -x]$	[12,23]
13	$[x, -z, x]$	[25,43]
14	$[x, z, -x]$	[26,45]
15	$[z, x, -x]$	[27,44]
16	$[-z, x, x]$	[28,46]
17	$[-x, x, z]$	[29,38]
18	$[x, -x, z]$	[30,39]
19	$[x, x, -z]$	[31,40]
20	$[-x, -x, -z]$	[32,37]
21	$[-x, z, x]$	[33,47]
22	$[-x, -z, -x]$	[34,42]
23	$[z, -x, x]$	[35,48]
24	$[-z, -x, -x]$	[36,41]
25	$[x, x + \frac{1}{2}, z + \frac{1}{2}]$	[49,68]
26	$[x, \frac{1}{2} - x, \frac{1}{2} - z]$	[50,65]
27	$[-x, x + \frac{1}{2}, \frac{1}{2} - z]$	[51,66]
28	$[-x, \frac{1}{2} - x, z + \frac{1}{2}]$	[52,67]
29	$[z, x + \frac{1}{2}, x + \frac{1}{2}]$	[53,72]
30	$[x, z + \frac{1}{2}, x + \frac{1}{2}]$	[54,70]
31	$[-x, z + \frac{1}{2}, \frac{1}{2} - x]$	[55,61]
32	$[-z, \frac{1}{2} - x, x + \frac{1}{2}]$	[56,63]
33	$[-x, \frac{1}{2} - z, x + \frac{1}{2}]$	[57,62]
34	$[z, \frac{1}{2} - x, \frac{1}{2} - x]$	[58,64]
35	$[x, \frac{1}{2} - z, \frac{1}{2} - x]$	[59,69]
36	$[-z, x + \frac{1}{2}, \frac{1}{2} - x]$	[60,71]
37	$[x, \frac{1}{2} - z, x + \frac{1}{2}]$	[73,91]
38	$[x, z + \frac{1}{2}, \frac{1}{2} - x]$	[74,93]
39	$[z, x + \frac{1}{2}, \frac{1}{2} - x]$	[75,92]
40	$[-z, x + \frac{1}{2}, x + \frac{1}{2}]$	[76,94]
41	$[-x, x + \frac{1}{2}, z + \frac{1}{2}]$	[77,86]
42	$[x, \frac{1}{2} - x, z + \frac{1}{2}]$	[78,87]
43	$[x, x + \frac{1}{2}, \frac{1}{2} - z]$	[79,88]
44	$[-x, \frac{1}{2} - x, \frac{1}{2} - z]$	[80,85]
45	$[-x, z + \frac{1}{2}, x + \frac{1}{2}]$	[81,95]
46	$[-x, \frac{1}{2} - z, \frac{1}{2} - x]$	[82,90]
47	$[z, \frac{1}{2} - x, x + \frac{1}{2}]$	[83,96]
48	$[-z, \frac{1}{2} - x, \frac{1}{2} - x]$	[84,89]
49	$[x + \frac{1}{2}, x, z + \frac{1}{2}]$	[97,116]
50	$[x + \frac{1}{2}, -x, \frac{1}{2} - z]$	[98,113]
51	$[\frac{1}{2} - x, x, \frac{1}{2} - z]$	[99,114]
52	$[\frac{1}{2} - x, -x, z + \frac{1}{2}]$	[100,115]
53	$[z + \frac{1}{2}, x, x + \frac{1}{2}]$	[101,120]

continued ...

Table 11

No.	position	mapping
54	$[x + \frac{1}{2}, z, x + \frac{1}{2}]$	[102,118]
55	$[\frac{1}{2} - x, z, \frac{1}{2} - x]$	[103,109]
56	$[\frac{1}{2} - z, -x, x + \frac{1}{2}]$	[104,111]
57	$[\frac{1}{2} - x, -z, x + \frac{1}{2}]$	[105,110]
58	$[z + \frac{1}{2}, -x, \frac{1}{2} - x]$	[106,112]
59	$[x + \frac{1}{2}, -z, \frac{1}{2} - x]$	[107,117]
60	$[\frac{1}{2} - z, x, \frac{1}{2} - x]$	[108,119]
61	$[x + \frac{1}{2}, -z, x + \frac{1}{2}]$	[121,139]
62	$[x + \frac{1}{2}, z, \frac{1}{2} - x]$	[122,141]
63	$[z + \frac{1}{2}, x, \frac{1}{2} - x]$	[123,140]
64	$[\frac{1}{2} - z, x, x + \frac{1}{2}]$	[124,142]
65	$[\frac{1}{2} - x, x, z + \frac{1}{2}]$	[125,134]
66	$[x + \frac{1}{2}, -x, z + \frac{1}{2}]$	[126,135]
67	$[x + \frac{1}{2}, x, \frac{1}{2} - z]$	[127,136]
68	$[\frac{1}{2} - x, -x, \frac{1}{2} - z]$	[128,133]
69	$[\frac{1}{2} - x, z, x + \frac{1}{2}]$	[129,143]
70	$[\frac{1}{2} - x, -z, \frac{1}{2} - x]$	[130,138]
71	$[z + \frac{1}{2}, -x, x + \frac{1}{2}]$	[131,144]
72	$[\frac{1}{2} - z, -x, \frac{1}{2} - x]$	[132,137]
73	$[x + \frac{1}{2}, x + \frac{1}{2}, z]$	[145,164]
74	$[x + \frac{1}{2}, \frac{1}{2} - x, -z]$	[146,161]
75	$[\frac{1}{2} - x, x + \frac{1}{2}, -z]$	[147,162]
76	$[\frac{1}{2} - x, \frac{1}{2} - x, z]$	[148,163]
77	$[z + \frac{1}{2}, x + \frac{1}{2}, x]$	[149,168]
78	$[x + \frac{1}{2}, z + \frac{1}{2}, x]$	[150,166]
79	$[\frac{1}{2} - x, z + \frac{1}{2}, -x]$	[151,157]
80	$[\frac{1}{2} - z, \frac{1}{2} - x, x]$	[152,159]
81	$[\frac{1}{2} - x, \frac{1}{2} - z, x]$	[153,158]
82	$[z + \frac{1}{2}, \frac{1}{2} - x, -x]$	[154,160]
83	$[x + \frac{1}{2}, \frac{1}{2} - z, -x]$	[155,165]
84	$[\frac{1}{2} - z, x + \frac{1}{2}, -x]$	[156,167]
85	$[x + \frac{1}{2}, \frac{1}{2} - z, x]$	[169,187]
86	$[x + \frac{1}{2}, z + \frac{1}{2}, -x]$	[170,189]
87	$[z + \frac{1}{2}, x + \frac{1}{2}, -x]$	[171,188]
88	$[\frac{1}{2} - z, x + \frac{1}{2}, x]$	[172,190]
89	$[\frac{1}{2} - x, x + \frac{1}{2}, z]$	[173,182]
90	$[x + \frac{1}{2}, \frac{1}{2} - x, z]$	[174,183]
91	$[x + \frac{1}{2}, x + \frac{1}{2}, -z]$	[175,184]
92	$[\frac{1}{2} - x, \frac{1}{2} - x, -z]$	[176,181]
93	$[\frac{1}{2} - x, z + \frac{1}{2}, x]$	[177,191]
94	$[\frac{1}{2} - x, \frac{1}{2} - z, -x]$	[178,186]
95	$[z + \frac{1}{2}, \frac{1}{2} - x, x]$	[179,192]
96	$[\frac{1}{2} - z, \frac{1}{2} - x, -x]$	[180,185]

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	$[-x, z, -y]$	[13]
14	$[-x, -z, y]$	[14]
15	$[-z, -y, x]$	[15]
16	$[z, -y, -x]$	[16]
17	$[y, -x, -z]$	[17]
18	$[-y, x, -z]$	[18]
19	$[-y, -x, z]$	[19]
20	$[y, x, z]$	[20]
21	$[x, -z, -y]$	[21]
22	$[x, z, y]$	[22]
23	$[-z, y, -x]$	[23]
24	$[z, y, x]$	[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	$[-x, -y, -z]$	[37]
38	$[-x, y, z]$	[38]
39	$[x, -y, z]$	[39]
40	$[x, y, -z]$	[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	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[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	$[-x, z + \frac{1}{2}, \frac{1}{2} - y]$	[61]
62	$[-x, \frac{1}{2} - z, y + \frac{1}{2}]$	[62]
63	$[-z, \frac{1}{2} - y, x + \frac{1}{2}]$	[63]
64	$[z, \frac{1}{2} - y, \frac{1}{2} - x]$	[64]
65	$[y, \frac{1}{2} - x, \frac{1}{2} - z]$	[65]
66	$[-y, x + \frac{1}{2}, \frac{1}{2} - z]$	[66]
67	$[-y, \frac{1}{2} - x, z + \frac{1}{2}]$	[67]
68	$[y, x + \frac{1}{2}, z + \frac{1}{2}]$	[68]
69	$[x, \frac{1}{2} - z, \frac{1}{2} - y]$	[69]
70	$[x, z + \frac{1}{2}, y + \frac{1}{2}]$	[70]
71	$[-z, y + \frac{1}{2}, \frac{1}{2} - x]$	[71]
72	$[z, y + \frac{1}{2}, x + \frac{1}{2}]$	[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	$[-x, \frac{1}{2} - y, \frac{1}{2} - z]$	[85]
86	$[-x, y + \frac{1}{2}, z + \frac{1}{2}]$	[86]
87	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[87]
88	$[x, y + \frac{1}{2}, \frac{1}{2} - z]$	[88]
89	$[-z, \frac{1}{2} - x, \frac{1}{2} - y]$	[89]
90	$[-y, \frac{1}{2} - z, \frac{1}{2} - x]$	[90]
91	$[y, \frac{1}{2} - z, x + \frac{1}{2}]$	[91]
92	$[z, x + \frac{1}{2}, \frac{1}{2} - y]$	[92]
93	$[y, z + \frac{1}{2}, \frac{1}{2} - x]$	[93]

continued ...

Table 12

No.	position	mapping
94	$[-z, x + \frac{1}{2}, y + \frac{1}{2}]$	[94]
95	$[-y, z + \frac{1}{2}, x + \frac{1}{2}]$	[95]
96	$[z, \frac{1}{2} - x, y + \frac{1}{2}]$	[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	$[\frac{1}{2} - x, z, \frac{1}{2} - y]$	[109]
110	$[\frac{1}{2} - x, -z, y + \frac{1}{2}]$	[110]
111	$[\frac{1}{2} - z, -y, x + \frac{1}{2}]$	[111]
112	$[z + \frac{1}{2}, -y, \frac{1}{2} - x]$	[112]
113	$[y + \frac{1}{2}, -x, \frac{1}{2} - z]$	[113]
114	$[\frac{1}{2} - y, x, \frac{1}{2} - z]$	[114]
115	$[\frac{1}{2} - y, -x, z + \frac{1}{2}]$	[115]
116	$[y + \frac{1}{2}, x, z + \frac{1}{2}]$	[116]
117	$[x + \frac{1}{2}, -z, \frac{1}{2} - y]$	[117]
118	$[x + \frac{1}{2}, z, y + \frac{1}{2}]$	[118]
119	$[\frac{1}{2} - z, y, \frac{1}{2} - x]$	[119]
120	$[z + \frac{1}{2}, y, x + \frac{1}{2}]$	[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	$[\frac{1}{2} - x, -y, \frac{1}{2} - z]$	[133]
134	$[\frac{1}{2} - x, y, z + \frac{1}{2}]$	[134]
135	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[135]
136	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[136]
137	$[\frac{1}{2} - z, -x, \frac{1}{2} - y]$	[137]
138	$[\frac{1}{2} - y, -z, \frac{1}{2} - x]$	[138]
139	$[y + \frac{1}{2}, -z, x + \frac{1}{2}]$	[139]
140	$[z + \frac{1}{2}, x, \frac{1}{2} - y]$	[140]

continued ...

Table 12

No.	position	mapping
141	$[y + \frac{1}{2}, z, \frac{1}{2} - x]$	[141]
142	$[\frac{1}{2} - z, x, y + \frac{1}{2}]$	[142]
143	$[\frac{1}{2} - y, z, x + \frac{1}{2}]$	[143]
144	$[z + \frac{1}{2}, -x, y + \frac{1}{2}]$	[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	$[\frac{1}{2} - x, z + \frac{1}{2}, -y]$	[157]
158	$[\frac{1}{2} - x, \frac{1}{2} - z, y]$	[158]
159	$[\frac{1}{2} - z, \frac{1}{2} - y, x]$	[159]
160	$[z + \frac{1}{2}, \frac{1}{2} - y, -x]$	[160]
161	$[y + \frac{1}{2}, \frac{1}{2} - x, -z]$	[161]
162	$[\frac{1}{2} - y, x + \frac{1}{2}, -z]$	[162]
163	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[163]
164	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[164]
165	$[x + \frac{1}{2}, \frac{1}{2} - z, -y]$	[165]
166	$[x + \frac{1}{2}, z + \frac{1}{2}, y]$	[166]
167	$[\frac{1}{2} - z, y + \frac{1}{2}, -x]$	[167]
168	$[z + \frac{1}{2}, y + \frac{1}{2}, x]$	[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	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[181]
182	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[182]
183	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[183]
184	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[184]
185	$[\frac{1}{2} - z, \frac{1}{2} - x, -y]$	[185]
186	$[\frac{1}{2} - y, \frac{1}{2} - z, -x]$	[186]
187	$[y + \frac{1}{2}, \frac{1}{2} - z, x]$	[187]

continued ...

Table 12

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