

MSG No. 225.120 $Fm'\bar{3}'m'$ [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: $-4'3m'$

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: $m' \cdot m' m'$

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

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

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	$[x, \frac{1}{2}, \frac{1}{2}]$	$[49, 50, 51, 56, 81, 82, 85, 86]$
8	$[0, \frac{1}{2}, \frac{1}{2} - x]$	$[52, 64, 67, 71, 77, 87, 90, 93]$
9	$[0, \frac{1}{2}, x + \frac{1}{2}]$	$[53, 63, 66, 69, 76, 88, 91, 95]$
10	$[0, x + \frac{1}{2}, \frac{1}{2}]$	$[54, 59, 65, 72, 79, 84, 92, 94]$
11	$[0, \frac{1}{2} - x, \frac{1}{2}]$	$[55, 60, 68, 70, 78, 83, 89, 96]$
12	$[-x, \frac{1}{2}, \frac{1}{2}]$	$[57, 58, 61, 62, 73, 74, 75, 80]$
13	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	$[97, 98, 99, 104, 129, 130, 133, 134]$
14	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	$[100, 112, 115, 119, 125, 135, 138, 141]$
15	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	$[101, 111, 114, 117, 124, 136, 139, 143]$

continued ...

Table 5

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

continued ...

Table 6

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

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

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

continued ...

Table 7

No.	position	mapping
40	$[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[72, 79, 161, 180]
41	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[97, 134, 152, 181]
42	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[98, 129, 147, 178]
43	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[99, 130, 146, 177]
44	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[104, 133, 145, 182]
45	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[105, 122, 154, 171]
46	$[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$	[106, 123, 153, 170]
47	$[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$	[109, 128, 158, 169]
48	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]$	[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	$[0, y + \frac{1}{2}, y + \frac{1}{2}]$	[49, 61, 80, 86]
14	$[0, \frac{1}{2} - y, y + \frac{1}{2}]$	[50, 58, 75, 81]
15	$[0, y + \frac{1}{2}, \frac{1}{2} - y]$	[51, 57, 74, 82]
16	$[y, y + \frac{1}{2}, \frac{1}{2}]$	[52, 66, 88, 93]
17	$[-y, y + \frac{1}{2}, \frac{1}{2}]$	[53, 67, 87, 95]
18	$[-y, \frac{1}{2}, y + \frac{1}{2}]$	[54, 68, 83, 94]
19	$[y, \frac{1}{2}, y + \frac{1}{2}]$	[55, 65, 84, 96]
20	$[0, \frac{1}{2} - y, \frac{1}{2} - y]$	[56, 62, 73, 85]
21	$[y, \frac{1}{2}, \frac{1}{2} - y]$	[59, 70, 78, 92]
22	$[-y, \frac{1}{2}, \frac{1}{2} - y]$	[60, 72, 79, 89]
23	$[y, \frac{1}{2} - y, \frac{1}{2}]$	[63, 71, 77, 91]
24	$[-y, \frac{1}{2} - y, \frac{1}{2}]$	[64, 69, 76, 90]
25	$[\frac{1}{2}, y, y + \frac{1}{2}]$	[97, 109, 128, 134]
26	$[\frac{1}{2}, -y, y + \frac{1}{2}]$	[98, 106, 123, 129]
27	$[\frac{1}{2}, y, \frac{1}{2} - y]$	[99, 105, 122, 130]
28	$[y + \frac{1}{2}, y, \frac{1}{2}]$	[100, 114, 136, 141]
29	$[\frac{1}{2} - y, y, \frac{1}{2}]$	[101, 115, 135, 143]
30	$[\frac{1}{2} - y, 0, y + \frac{1}{2}]$	[102, 116, 131, 142]
31	$[y + \frac{1}{2}, 0, y + \frac{1}{2}]$	[103, 113, 132, 144]

continued ...

Table 8

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

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

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

continued ...

Table 9

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

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

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	$[0, y + \frac{1}{2}, z + \frac{1}{2}]$	[49, 80]
26	$[0, \frac{1}{2} - z, y + \frac{1}{2}]$	[50, 75]
27	$[0, z + \frac{1}{2}, \frac{1}{2} - y]$	[51, 74]
28	$[z, y + \frac{1}{2}, \frac{1}{2}]$	[52, 88]
29	$[-z, y + \frac{1}{2}, \frac{1}{2}]$	[53, 87]
30	$[-y, \frac{1}{2}, z + \frac{1}{2}]$	[54, 83]
31	$[y, \frac{1}{2}, z + \frac{1}{2}]$	[55, 84]
32	$[0, \frac{1}{2} - y, \frac{1}{2} - z]$	[56, 73]
33	$[0, y + \frac{1}{2}, \frac{1}{2} - z]$	[57, 82]
34	$[0, \frac{1}{2} - y, z + \frac{1}{2}]$	[58, 81]
35	$[y, \frac{1}{2}, \frac{1}{2} - z]$	[59, 78]
36	$[-y, \frac{1}{2}, \frac{1}{2} - z]$	[60, 79]
37	$[0, z + \frac{1}{2}, y + \frac{1}{2}]$	[61, 86]
38	$[0, \frac{1}{2} - z, \frac{1}{2} - y]$	[62, 85]
39	$[z, \frac{1}{2} - y, \frac{1}{2}]$	[63, 77]
40	$[-z, \frac{1}{2} - y, \frac{1}{2}]$	[64, 76]
41	$[z, \frac{1}{2}, y + \frac{1}{2}]$	[65, 96]
42	$[y, z + \frac{1}{2}, \frac{1}{2}]$	[66, 93]
43	$[-y, z + \frac{1}{2}, \frac{1}{2}]$	[67, 95]
44	$[-z, \frac{1}{2}, y + \frac{1}{2}]$	[68, 94]
45	$[-y, \frac{1}{2} - z, \frac{1}{2}]$	[69, 90]
46	$[z, \frac{1}{2}, \frac{1}{2} - y]$	[70, 92]
47	$[y, \frac{1}{2} - z, \frac{1}{2}]$	[71, 91]
48	$[-z, \frac{1}{2}, \frac{1}{2} - y]$	[72, 89]
49	$[\frac{1}{2}, y, z + \frac{1}{2}]$	[97, 128]
50	$[\frac{1}{2}, -z, y + \frac{1}{2}]$	[98, 123]
51	$[\frac{1}{2}, z, \frac{1}{2} - y]$	[99, 122]
52	$[z + \frac{1}{2}, y, \frac{1}{2}]$	[100, 136]
53	$[\frac{1}{2} - z, y, \frac{1}{2}]$	[101, 135]
54	$[\frac{1}{2} - y, 0, z + \frac{1}{2}]$	[102, 131]
55	$[y + \frac{1}{2}, 0, z + \frac{1}{2}]$	[103, 132]
56	$[\frac{1}{2}, -y, \frac{1}{2} - z]$	[104, 121]
57	$[\frac{1}{2}, y, \frac{1}{2} - z]$	[105, 130]
58	$[\frac{1}{2}, -y, z + \frac{1}{2}]$	[106, 129]
59	$[y + \frac{1}{2}, 0, \frac{1}{2} - z]$	[107, 126]
60	$[\frac{1}{2} - y, 0, \frac{1}{2} - z]$	[108, 127]
61	$[\frac{1}{2}, z, y + \frac{1}{2}]$	[109, 134]
62	$[\frac{1}{2}, -z, \frac{1}{2} - y]$	[110, 133]

continued ...

Table 10

No.	position	mapping
63	$[z + \frac{1}{2}, -y, \frac{1}{2}]$	[111,125]
64	$[\frac{1}{2} - z, -y, \frac{1}{2}]$	[112,124]
65	$[z + \frac{1}{2}, 0, y + \frac{1}{2}]$	[113,144]
66	$[y + \frac{1}{2}, z, \frac{1}{2}]$	[114,141]
67	$[\frac{1}{2} - y, z, \frac{1}{2}]$	[115,143]
68	$[\frac{1}{2} - z, 0, y + \frac{1}{2}]$	[116,142]
69	$[\frac{1}{2} - y, -z, \frac{1}{2}]$	[117,138]
70	$[z + \frac{1}{2}, 0, \frac{1}{2} - y]$	[118,140]
71	$[y + \frac{1}{2}, -z, \frac{1}{2}]$	[119,139]
72	$[\frac{1}{2} - z, 0, \frac{1}{2} - y]$	[120,137]
73	$[\frac{1}{2}, y + \frac{1}{2}, z]$	[145,176]
74	$[\frac{1}{2}, \frac{1}{2} - z, y]$	[146,171]
75	$[\frac{1}{2}, z + \frac{1}{2}, -y]$	[147,170]
76	$[z + \frac{1}{2}, y + \frac{1}{2}, 0]$	[148,184]
77	$[\frac{1}{2} - z, y + \frac{1}{2}, 0]$	[149,183]
78	$[\frac{1}{2} - y, \frac{1}{2}, z]$	[150,179]
79	$[y + \frac{1}{2}, \frac{1}{2}, z]$	[151,180]
80	$[\frac{1}{2}, \frac{1}{2} - y, -z]$	[152,169]
81	$[\frac{1}{2}, y + \frac{1}{2}, -z]$	[153,178]
82	$[\frac{1}{2}, \frac{1}{2} - y, z]$	[154,177]
83	$[y + \frac{1}{2}, \frac{1}{2}, -z]$	[155,174]
84	$[\frac{1}{2} - y, \frac{1}{2}, -z]$	[156,175]
85	$[\frac{1}{2}, z + \frac{1}{2}, y]$	[157,182]
86	$[\frac{1}{2}, \frac{1}{2} - z, -y]$	[158,181]
87	$[z + \frac{1}{2}, \frac{1}{2} - y, 0]$	[159,173]
88	$[\frac{1}{2} - z, \frac{1}{2} - y, 0]$	[160,172]
89	$[z + \frac{1}{2}, \frac{1}{2}, y]$	[161,192]
90	$[y + \frac{1}{2}, z + \frac{1}{2}, 0]$	[162,189]
91	$[\frac{1}{2} - y, z + \frac{1}{2}, 0]$	[163,191]
92	$[\frac{1}{2} - z, \frac{1}{2}, y]$	[164,190]
93	$[\frac{1}{2} - y, \frac{1}{2} - z, 0]$	[165,186]
94	$[z + \frac{1}{2}, \frac{1}{2}, -y]$	[166,188]
95	$[y + \frac{1}{2}, \frac{1}{2} - z, 0]$	[167,187]
96	$[\frac{1}{2} - z, \frac{1}{2}, -y]$	[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	$[x, x + \frac{1}{2}, z + \frac{1}{2}]$	[49,84]
26	$[x, \frac{1}{2} - z, x + \frac{1}{2}]$	[50,91]
27	$[x, z + \frac{1}{2}, \frac{1}{2} - x]$	[51,93]
28	$[z, x + \frac{1}{2}, \frac{1}{2} - x]$	[52,92]
29	$[-z, x + \frac{1}{2}, x + \frac{1}{2}]$	[53,94]
30	$[-x, x + \frac{1}{2}, z + \frac{1}{2}]$	[54,80]
31	$[x, \frac{1}{2} - x, z + \frac{1}{2}]$	[55,81]
32	$[x, \frac{1}{2} - x, \frac{1}{2} - z]$	[56,78]
33	$[-x, x + \frac{1}{2}, \frac{1}{2} - z]$	[57,79]
34	$[-x, \frac{1}{2} - x, z + \frac{1}{2}]$	[58,83]
35	$[x, x + \frac{1}{2}, \frac{1}{2} - z]$	[59,82]
36	$[-x, \frac{1}{2} - x, \frac{1}{2} - z]$	[60,73]
37	$[-x, z + \frac{1}{2}, x + \frac{1}{2}]$	[61,95]
38	$[-x, \frac{1}{2} - z, \frac{1}{2} - x]$	[62,90]
39	$[z, \frac{1}{2} - x, x + \frac{1}{2}]$	[63,96]
40	$[-z, \frac{1}{2} - x, \frac{1}{2} - x]$	[64,89]
41	$[z, x + \frac{1}{2}, x + \frac{1}{2}]$	[65,88]
42	$[x, z + \frac{1}{2}, x + \frac{1}{2}]$	[66,86]
43	$[-x, z + \frac{1}{2}, \frac{1}{2} - x]$	[67,74]
44	$[-z, \frac{1}{2} - x, x + \frac{1}{2}]$	[68,76]
45	$[-x, \frac{1}{2} - z, x + \frac{1}{2}]$	[69,75]
46	$[z, \frac{1}{2} - x, \frac{1}{2} - x]$	[70,77]
47	$[x, \frac{1}{2} - z, \frac{1}{2} - x]$	[71,85]
48	$[-z, x + \frac{1}{2}, \frac{1}{2} - x]$	[72,87]
49	$[x + \frac{1}{2}, x, z + \frac{1}{2}]$	[97,132]
50	$[x + \frac{1}{2}, -z, x + \frac{1}{2}]$	[98,139]
51	$[x + \frac{1}{2}, z, \frac{1}{2} - x]$	[99,141]
52	$[z + \frac{1}{2}, x, \frac{1}{2} - x]$	[100,140]
53	$[\frac{1}{2} - z, x, x + \frac{1}{2}]$	[101,142]

continued ...

Table 11

No.	position	mapping
54	$[\frac{1}{2} - x, x, z + \frac{1}{2}]$	[102,128]
55	$[x + \frac{1}{2}, -x, z + \frac{1}{2}]$	[103,129]
56	$[x + \frac{1}{2}, -x, \frac{1}{2} - z]$	[104,126]
57	$[\frac{1}{2} - x, x, \frac{1}{2} - z]$	[105,127]
58	$[\frac{1}{2} - x, -x, z + \frac{1}{2}]$	[106,131]
59	$[x + \frac{1}{2}, x, \frac{1}{2} - z]$	[107,130]
60	$[\frac{1}{2} - x, -x, \frac{1}{2} - z]$	[108,121]
61	$[\frac{1}{2} - x, z, x + \frac{1}{2}]$	[109,143]
62	$[\frac{1}{2} - x, -z, \frac{1}{2} - x]$	[110,138]
63	$[z + \frac{1}{2}, -x, x + \frac{1}{2}]$	[111,144]
64	$[\frac{1}{2} - z, -x, \frac{1}{2} - x]$	[112,137]
65	$[z + \frac{1}{2}, x, x + \frac{1}{2}]$	[113,136]
66	$[x + \frac{1}{2}, z, x + \frac{1}{2}]$	[114,134]
67	$[\frac{1}{2} - x, z, \frac{1}{2} - x]$	[115,122]
68	$[\frac{1}{2} - z, -x, x + \frac{1}{2}]$	[116,124]
69	$[\frac{1}{2} - x, -z, x + \frac{1}{2}]$	[117,123]
70	$[z + \frac{1}{2}, -x, \frac{1}{2} - x]$	[118,125]
71	$[x + \frac{1}{2}, -z, \frac{1}{2} - x]$	[119,133]
72	$[\frac{1}{2} - z, x, \frac{1}{2} - x]$	[120,135]
73	$[x + \frac{1}{2}, x + \frac{1}{2}, z]$	[145,180]
74	$[x + \frac{1}{2}, \frac{1}{2} - z, x]$	[146,187]
75	$[x + \frac{1}{2}, z + \frac{1}{2}, -x]$	[147,189]
76	$[z + \frac{1}{2}, x + \frac{1}{2}, -x]$	[148,188]
77	$[\frac{1}{2} - z, x + \frac{1}{2}, x]$	[149,190]
78	$[\frac{1}{2} - x, x + \frac{1}{2}, z]$	[150,176]
79	$[x + \frac{1}{2}, \frac{1}{2} - x, z]$	[151,177]
80	$[x + \frac{1}{2}, \frac{1}{2} - x, -z]$	[152,174]
81	$[\frac{1}{2} - x, x + \frac{1}{2}, -z]$	[153,175]
82	$[\frac{1}{2} - x, \frac{1}{2} - x, z]$	[154,179]
83	$[x + \frac{1}{2}, x + \frac{1}{2}, -z]$	[155,178]
84	$[\frac{1}{2} - x, \frac{1}{2} - x, -z]$	[156,169]
85	$[\frac{1}{2} - x, z + \frac{1}{2}, x]$	[157,191]
86	$[\frac{1}{2} - x, \frac{1}{2} - z, -x]$	[158,186]
87	$[z + \frac{1}{2}, \frac{1}{2} - x, x]$	[159,192]
88	$[\frac{1}{2} - z, \frac{1}{2} - x, -x]$	[160,185]
89	$[z + \frac{1}{2}, x + \frac{1}{2}, x]$	[161,184]
90	$[x + \frac{1}{2}, z + \frac{1}{2}, x]$	[162,182]
91	$[\frac{1}{2} - x, z + \frac{1}{2}, -x]$	[163,170]
92	$[\frac{1}{2} - z, \frac{1}{2} - x, x]$	[164,172]
93	$[\frac{1}{2} - x, \frac{1}{2} - z, x]$	[165,171]
94	$[z + \frac{1}{2}, \frac{1}{2} - x, -x]$	[166,173]
95	$[x + \frac{1}{2}, \frac{1}{2} - z, -x]$	[167,181]
96	$[\frac{1}{2} - z, x + \frac{1}{2}, -x]$	[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	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[49]
50	$[x, \frac{1}{2} - z, y + \frac{1}{2}]$	[50]
51	$[x, z + \frac{1}{2}, \frac{1}{2} - y]$	[51]
52	$[z, y + \frac{1}{2}, \frac{1}{2} - x]$	[52]
53	$[-z, y + \frac{1}{2}, x + \frac{1}{2}]$	[53]
54	$[-y, x + \frac{1}{2}, z + \frac{1}{2}]$	[54]
55	$[y, \frac{1}{2} - x, z + \frac{1}{2}]$	[55]
56	$[x, \frac{1}{2} - y, \frac{1}{2} - z]$	[56]
57	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[57]
58	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[58]
59	$[y, x + \frac{1}{2}, \frac{1}{2} - z]$	[59]
60	$[-y, \frac{1}{2} - x, \frac{1}{2} - z]$	[60]
61	$[-x, z + \frac{1}{2}, y + \frac{1}{2}]$	[61]
62	$[-x, \frac{1}{2} - z, \frac{1}{2} - y]$	[62]
63	$[z, \frac{1}{2} - y, x + \frac{1}{2}]$	[63]
64	$[-z, \frac{1}{2} - y, \frac{1}{2} - x]$	[64]
65	$[z, x + \frac{1}{2}, y + \frac{1}{2}]$	[65]
66	$[y, z + \frac{1}{2}, x + \frac{1}{2}]$	[66]
67	$[-y, z + \frac{1}{2}, \frac{1}{2} - x]$	[67]
68	$[-z, \frac{1}{2} - x, y + \frac{1}{2}]$	[68]
69	$[-y, \frac{1}{2} - z, x + \frac{1}{2}]$	[69]
70	$[z, \frac{1}{2} - x, \frac{1}{2} - y]$	[70]
71	$[y, \frac{1}{2} - z, \frac{1}{2} - x]$	[71]
72	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[72]
73	$[-x, \frac{1}{2} - y, \frac{1}{2} - z]$	[73]
74	$[-x, z + \frac{1}{2}, \frac{1}{2} - y]$	[74]
75	$[-x, \frac{1}{2} - z, y + \frac{1}{2}]$	[75]
76	$[-z, \frac{1}{2} - y, x + \frac{1}{2}]$	[76]
77	$[z, \frac{1}{2} - y, \frac{1}{2} - x]$	[77]
78	$[y, \frac{1}{2} - x, \frac{1}{2} - z]$	[78]
79	$[-y, x + \frac{1}{2}, \frac{1}{2} - z]$	[79]
80	$[-x, y + \frac{1}{2}, z + \frac{1}{2}]$	[80]
81	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[81]
82	$[x, y + \frac{1}{2}, \frac{1}{2} - z]$	[82]
83	$[-y, \frac{1}{2} - x, z + \frac{1}{2}]$	[83]
84	$[y, x + \frac{1}{2}, z + \frac{1}{2}]$	[84]
85	$[x, \frac{1}{2} - z, \frac{1}{2} - y]$	[85]
86	$[x, z + \frac{1}{2}, y + \frac{1}{2}]$	[86]
87	$[-z, y + \frac{1}{2}, \frac{1}{2} - x]$	[87]
88	$[z, y + \frac{1}{2}, x + \frac{1}{2}]$	[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	$[x + \frac{1}{2}, -z, y + \frac{1}{2}]$	[98]
99	$[x + \frac{1}{2}, z, \frac{1}{2} - y]$	[99]
100	$[z + \frac{1}{2}, y, \frac{1}{2} - x]$	[100]
101	$[\frac{1}{2} - z, y, x + \frac{1}{2}]$	[101]
102	$[\frac{1}{2} - y, x, z + \frac{1}{2}]$	[102]
103	$[y + \frac{1}{2}, -x, z + \frac{1}{2}]$	[103]
104	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[104]
105	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[105]
106	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[106]
107	$[y + \frac{1}{2}, x, \frac{1}{2} - z]$	[107]
108	$[\frac{1}{2} - y, -x, \frac{1}{2} - z]$	[108]
109	$[\frac{1}{2} - x, z, y + \frac{1}{2}]$	[109]
110	$[\frac{1}{2} - x, -z, \frac{1}{2} - y]$	[110]
111	$[z + \frac{1}{2}, -y, x + \frac{1}{2}]$	[111]
112	$[\frac{1}{2} - z, -y, \frac{1}{2} - x]$	[112]
113	$[z + \frac{1}{2}, x, y + \frac{1}{2}]$	[113]
114	$[y + \frac{1}{2}, z, x + \frac{1}{2}]$	[114]
115	$[\frac{1}{2} - y, z, \frac{1}{2} - x]$	[115]
116	$[\frac{1}{2} - z, -x, y + \frac{1}{2}]$	[116]
117	$[\frac{1}{2} - y, -z, x + \frac{1}{2}]$	[117]
118	$[z + \frac{1}{2}, -x, \frac{1}{2} - y]$	[118]
119	$[y + \frac{1}{2}, -z, \frac{1}{2} - x]$	[119]
120	$[\frac{1}{2} - z, x, \frac{1}{2} - y]$	[120]
121	$[\frac{1}{2} - x, -y, \frac{1}{2} - z]$	[121]
122	$[\frac{1}{2} - x, z, \frac{1}{2} - y]$	[122]
123	$[\frac{1}{2} - x, -z, y + \frac{1}{2}]$	[123]
124	$[\frac{1}{2} - z, -y, x + \frac{1}{2}]$	[124]
125	$[z + \frac{1}{2}, -y, \frac{1}{2} - x]$	[125]
126	$[y + \frac{1}{2}, -x, \frac{1}{2} - z]$	[126]
127	$[\frac{1}{2} - y, x, \frac{1}{2} - z]$	[127]
128	$[\frac{1}{2} - x, y, z + \frac{1}{2}]$	[128]
129	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[129]
130	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[130]
131	$[\frac{1}{2} - y, -x, z + \frac{1}{2}]$	[131]
132	$[y + \frac{1}{2}, x, z + \frac{1}{2}]$	[132]
133	$[x + \frac{1}{2}, -z, \frac{1}{2} - y]$	[133]
134	$[x + \frac{1}{2}, z, y + \frac{1}{2}]$	[134]
135	$[\frac{1}{2} - z, y, \frac{1}{2} - x]$	[135]
136	$[z + \frac{1}{2}, y, x + \frac{1}{2}]$	[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	$[x + \frac{1}{2}, \frac{1}{2} - z, y]$	[146]
147	$[x + \frac{1}{2}, z + \frac{1}{2}, -y]$	[147]
148	$[z + \frac{1}{2}, y + \frac{1}{2}, -x]$	[148]
149	$[\frac{1}{2} - z, y + \frac{1}{2}, x]$	[149]
150	$[\frac{1}{2} - y, x + \frac{1}{2}, z]$	[150]
151	$[y + \frac{1}{2}, \frac{1}{2} - x, z]$	[151]
152	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[152]
153	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[153]
154	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[154]
155	$[y + \frac{1}{2}, x + \frac{1}{2}, -z]$	[155]
156	$[\frac{1}{2} - y, \frac{1}{2} - x, -z]$	[156]
157	$[\frac{1}{2} - x, z + \frac{1}{2}, y]$	[157]
158	$[\frac{1}{2} - x, \frac{1}{2} - z, -y]$	[158]
159	$[z + \frac{1}{2}, \frac{1}{2} - y, x]$	[159]
160	$[\frac{1}{2} - z, \frac{1}{2} - y, -x]$	[160]
161	$[z + \frac{1}{2}, x + \frac{1}{2}, y]$	[161]
162	$[y + \frac{1}{2}, z + \frac{1}{2}, x]$	[162]
163	$[\frac{1}{2} - y, z + \frac{1}{2}, -x]$	[163]
164	$[\frac{1}{2} - z, \frac{1}{2} - x, y]$	[164]
165	$[\frac{1}{2} - y, \frac{1}{2} - z, x]$	[165]
166	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[166]
167	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[167]
168	$[\frac{1}{2} - z, x + \frac{1}{2}, -y]$	[168]
169	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[169]
170	$[\frac{1}{2} - x, z + \frac{1}{2}, -y]$	[170]
171	$[\frac{1}{2} - x, \frac{1}{2} - z, y]$	[171]
172	$[\frac{1}{2} - z, \frac{1}{2} - y, x]$	[172]
173	$[z + \frac{1}{2}, \frac{1}{2} - y, -x]$	[173]
174	$[y + \frac{1}{2}, \frac{1}{2} - x, -z]$	[174]
175	$[\frac{1}{2} - y, x + \frac{1}{2}, -z]$	[175]
176	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[176]
177	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[177]
178	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[178]
179	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[179]
180	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[180]
181	$[x + \frac{1}{2}, \frac{1}{2} - z, -y]$	[181]
182	$[x + \frac{1}{2}, z + \frac{1}{2}, y]$	[182]
183	$[\frac{1}{2} - z, y + \frac{1}{2}, -x]$	[183]
184	$[z + \frac{1}{2}, y + \frac{1}{2}, x]$	[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]