

MSG No. 225.121 $F_S m \bar{3} m$ [Type IV, cubic]

Table 1: Wyckoff site: 8a, 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]
5	$[0, 0, \frac{1}{2}]$	[193, 194, 195, 196, 197, 198, 199, 200, 201, 202, 203, 204, 205, 206, 207, 208, 209, 210, 211, 212, 213, 214, 215, 216, 217, 218, 219, 220, 221, 222, 223, 224, 225, 226, 227, 228, 229, 230, 231, 232, 233, 234, 235, 236, 237, 238, 239, 240]
6	$[0, \frac{1}{2}, 0]$	[241, 242, 243, 244, 245, 246, 247, 248, 249, 250, 251, 252, 253, 254, 255, 256, 257, 258, 259, 260, 261, 262, 263, 264, 265, 266, 267, 268, 269, 270, 271, 272, 273, 274, 275, 276, 277, 278, 279, 280, 281, 282, 283, 284, 285, 286, 287, 288]
7	$[\frac{1}{2}, 0, 0]$	[289, 290, 291, 292, 293, 294, 295, 296, 297, 298, 299, 300, 301, 302, 303, 304, 305, 306, 307, 308, 309, 310, 311, 312, 313, 314, 315, 316, 317, 318, 319, 320, 321, 322, 323, 324, 325, 326, 327, 328, 329, 330, 331, 332, 333, 334, 335, 336]
8	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[337, 338, 339, 340, 341, 342, 343, 344, 345, 346, 347, 348, 349, 350, 351, 352, 353, 354, 355, 356, 357, 358, 359, 360, 361, 362, 363, 364, 365, 366, 367, 368, 369, 370, 371, 372, 373, 374, 375, 376, 377, 378, 379, 380, 381, 382, 383, 384]

Table 2: Wyckoff site: 8b, site symmetry: $m'\bar{3}'m$

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, 195, 196, 203, 226, 236, 237, 242, 247, 255, 273, 283, 288, 293, 294, 301, 320, 334, 335, 348, 350, 352, 361, 377, 378]
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, 200, 214, 215, 221, 222, 229, 241, 257, 258, 276, 278, 280, 298, 308, 309, 315, 316, 323, 345, 355, 360, 362, 367, 375]
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, 193, 209, 210, 228, 230, 232, 248, 262, 263, 269, 270, 277, 297, 307, 312, 314, 319, 327, 346, 356, 357, 363, 364, 371]
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, 201, 211, 216, 218, 223, 231, 250, 260, 261, 267, 268, 275, 289, 305, 306, 324, 326, 328, 344, 358, 359, 365, 366, 373]
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, 194, 199, 207, 225, 235, 240, 243, 244, 251, 274, 284, 285, 300, 302, 304, 313, 329, 330, 341, 342, 349, 368, 382, 383]
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, 197, 198, 205, 224, 238, 239, 252, 254, 256, 265, 281, 282, 291, 292, 299, 322, 332, 333, 338, 343, 351, 369, 379, 384]
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, 204, 206, 208, 217, 233, 234, 245, 246, 253, 272, 286, 287, 290, 295, 303, 321, 331, 336, 339, 340, 347, 370, 380, 381]
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, 202, 212, 213, 219, 220, 227, 249, 259, 264, 266, 271, 279, 296, 310, 311, 317, 318, 325, 337, 353, 354, 372, 374, 376]

Table 3: Wyckoff site: 24c, site symmetry: $4'/mm'.m$

No.	position	mapping
1	$[0, \frac{1}{4}, \frac{1}{4}]$	[1, 13, 32, 38, 56, 62, 73, 85, 195, 201, 218, 226, 242, 250, 267, 273]
2	$[0, \frac{3}{4}, \frac{1}{4}]$	[2, 10, 27, 33, 51, 57, 74, 82, 200, 206, 217, 229, 241, 253, 272, 278]
3	$[0, \frac{1}{4}, \frac{3}{4}]$	[3, 9, 26, 34, 50, 58, 75, 81, 193, 205, 224, 230, 248, 254, 265, 277]
4	$[\frac{1}{4}, \frac{1}{4}, 0]$	[4, 18, 40, 45, 160, 165, 172, 186, 255, 263, 269, 283, 293, 307, 327, 335]
5	$[\frac{3}{4}, \frac{1}{4}, 0]$	[5, 19, 39, 47, 159, 167, 173, 187, 256, 261, 268, 282, 292, 306, 328, 333]
6	$[\frac{3}{4}, 0, \frac{1}{4}]$	[6, 20, 35, 46, 107, 118, 126, 140, 204, 216, 223, 233, 295, 305, 324, 336]
7	$[\frac{1}{4}, 0, \frac{1}{4}]$	[7, 17, 36, 48, 108, 120, 127, 137, 203, 214, 222, 236, 294, 308, 323, 334]
8	$[0, \frac{3}{4}, \frac{3}{4}]$	[8, 14, 25, 37, 49, 61, 80, 86, 194, 202, 219, 225, 243, 249, 266, 274]
9	$[\frac{1}{4}, 0, \frac{3}{4}]$	[11, 22, 30, 44, 102, 116, 131, 142, 199, 209, 228, 240, 300, 312, 319, 329]
10	$[\frac{3}{4}, 0, \frac{3}{4}]$	[12, 24, 31, 41, 103, 113, 132, 144, 198, 212, 227, 238, 299, 310, 318, 332]
11	$[\frac{1}{4}, \frac{3}{4}, 0]$	[15, 23, 29, 43, 149, 163, 183, 191, 244, 258, 280, 285, 304, 309, 316, 330]
12	$[\frac{3}{4}, \frac{3}{4}, 0]$	[16, 21, 28, 42, 148, 162, 184, 189, 245, 259, 279, 287, 303, 311, 317, 331]
13	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	[52, 66, 88, 93, 112, 117, 124, 138, 207, 215, 221, 235, 341, 355, 375, 383]
14	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$	[53, 67, 87, 95, 111, 119, 125, 139, 208, 213, 220, 234, 340, 354, 376, 381]
15	$[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}]$	[54, 68, 83, 94, 155, 166, 174, 188, 252, 264, 271, 281, 343, 353, 372, 384]
16	$[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}]$	[55, 65, 84, 96, 156, 168, 175, 185, 251, 262, 270, 284, 342, 356, 371, 382]
17	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$	[59, 70, 78, 92, 150, 164, 179, 190, 247, 257, 276, 288, 348, 360, 367, 377]
18	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$	[60, 72, 79, 89, 151, 161, 180, 192, 246, 260, 275, 286, 347, 358, 366, 380]
19	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$	[63, 71, 77, 91, 101, 115, 135, 143, 196, 210, 232, 237, 352, 357, 364, 378]
20	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	[64, 69, 76, 90, 100, 114, 136, 141, 197, 211, 231, 239, 351, 359, 365, 379]
21	$[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[97, 109, 128, 134, 152, 158, 169, 181, 291, 297, 314, 322, 338, 346, 363, 369]
22	$[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[98, 106, 123, 129, 147, 153, 170, 178, 296, 302, 313, 325, 337, 349, 368, 374]
23	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[99, 105, 122, 130, 146, 154, 171, 177, 289, 301, 320, 326, 344, 350, 361, 373]
24	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[104, 110, 121, 133, 145, 157, 176, 182, 290, 298, 315, 321, 339, 345, 362, 370]

Table 4: Wyckoff site: 24d, site symmetry: $4/m'.m.m$

No.	position	mapping
1	$[\frac{1}{4}, 0, 0]$	[1, 2, 3, 8, 33, 34, 37, 38, 297, 298, 301, 302, 313, 314, 315, 320]
2	$[0, 0, \frac{3}{4}]$	[4, 16, 19, 23, 29, 39, 42, 45, 197, 207, 210, 213, 220, 232, 235, 239]
3	$[0, 0, \frac{1}{4}]$	[5, 15, 18, 21, 28, 40, 43, 47, 196, 208, 211, 215, 221, 231, 234, 237]
4	$[0, \frac{1}{4}, 0]$	[6, 11, 17, 24, 31, 36, 44, 46, 247, 252, 260, 262, 270, 275, 281, 288]
5	$[0, \frac{3}{4}, 0]$	[7, 12, 20, 22, 30, 35, 41, 48, 246, 251, 257, 264, 271, 276, 284, 286]
6	$[\frac{3}{4}, 0, 0]$	[9, 10, 13, 14, 25, 26, 27, 32, 289, 290, 291, 296, 321, 322, 325, 326]
7	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}]$	[49, 50, 51, 56, 81, 82, 85, 86, 345, 346, 349, 350, 361, 362, 363, 368]
8	$[0, \frac{1}{2}, \frac{1}{4}]$	[52, 64, 67, 71, 77, 87, 90, 93, 245, 255, 258, 261, 268, 280, 283, 287]
9	$[0, \frac{1}{2}, \frac{3}{4}]$	[53, 63, 66, 69, 76, 88, 91, 95, 244, 256, 259, 263, 269, 279, 282, 285]
10	$[0, \frac{3}{4}, \frac{1}{2}]$	[54, 59, 65, 72, 79, 84, 92, 94, 199, 204, 212, 214, 222, 227, 233, 240]
11	$[0, \frac{1}{4}, \frac{1}{2}]$	[55, 60, 68, 70, 78, 83, 89, 96, 198, 203, 209, 216, 223, 228, 236, 238]
12	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}]$	[57, 58, 61, 62, 73, 74, 75, 80, 337, 338, 339, 344, 369, 370, 373, 374]
13	$[\frac{3}{4}, 0, \frac{1}{2}]$	[97, 98, 99, 104, 129, 130, 133, 134, 201, 202, 205, 206, 217, 218, 219, 224]
14	$[\frac{1}{2}, 0, \frac{1}{4}]$	[100, 112, 115, 119, 125, 135, 138, 141, 293, 303, 306, 309, 316, 328, 331, 335]
15	$[\frac{1}{2}, 0, \frac{3}{4}]$	[101, 111, 114, 117, 124, 136, 139, 143, 292, 304, 307, 311, 317, 327, 330, 333]

continued ...

Table 4

No.	position	mapping
16	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2}]$	[102, 107, 113, 120, 127, 132, 140, 142, 343, 348, 356, 358, 366, 371, 377, 384]
17	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{2}]$	[103, 108, 116, 118, 126, 131, 137, 144, 342, 347, 353, 360, 367, 372, 380, 382]
18	$[\frac{1}{4}, 0, \frac{1}{2}]$	[105, 106, 109, 110, 121, 122, 123, 128, 193, 194, 195, 200, 225, 226, 229, 230]
19	$[\frac{3}{4}, \frac{1}{2}, 0]$	[145, 146, 147, 152, 177, 178, 181, 182, 249, 250, 253, 254, 265, 266, 267, 272]
20	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[148, 160, 163, 167, 173, 183, 186, 189, 341, 351, 354, 357, 364, 376, 379, 383]
21	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[149, 159, 162, 165, 172, 184, 187, 191, 340, 352, 355, 359, 365, 375, 378, 381]
22	$[\frac{1}{2}, \frac{3}{4}, 0]$	[150, 155, 161, 168, 175, 180, 188, 190, 295, 300, 308, 310, 318, 323, 329, 336]
23	$[\frac{1}{2}, \frac{1}{4}, 0]$	[151, 156, 164, 166, 174, 179, 185, 192, 294, 299, 305, 312, 319, 324, 332, 334]
24	$[\frac{1}{4}, \frac{1}{2}, 0]$	[153, 154, 157, 158, 169, 170, 171, 176, 241, 242, 243, 248, 273, 274, 277, 278]

Table 5: Wyckoff site: 48e, site symmetry: 4m.m

No.	position	mapping
1	$[x, 0, 0]$	[1, 2, 3, 8, 33, 34, 37, 38]
2	$[0, 0, -x]$	[4, 16, 19, 23, 29, 39, 42, 45]
3	$[0, 0, x]$	[5, 15, 18, 21, 28, 40, 43, 47]
4	$[0, x, 0]$	[6, 11, 17, 24, 31, 36, 44, 46]
5	$[0, -x, 0]$	[7, 12, 20, 22, 30, 35, 41, 48]
6	$[-x, 0, 0]$	[9, 10, 13, 14, 25, 26, 27, 32]
7	$[x, \frac{1}{2}, \frac{1}{2}]$	[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]
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]
25	$[x, 0, \frac{1}{2}]$	[193, 194, 195, 200, 225, 226, 229, 230]
26	$[0, 0, \frac{1}{2} - x]$	[196, 208, 211, 215, 221, 231, 234, 237]
27	$[0, 0, x + \frac{1}{2}]$	[197, 207, 210, 213, 220, 232, 235, 239]
28	$[0, x, \frac{1}{2}]$	[198, 203, 209, 216, 223, 228, 236, 238]
29	$[0, -x, \frac{1}{2}]$	[199, 204, 212, 214, 222, 227, 233, 240]
30	$[-x, 0, \frac{1}{2}]$	[201, 202, 205, 206, 217, 218, 219, 224]
31	$[x, \frac{1}{2}, 0]$	[241, 242, 243, 248, 273, 274, 277, 278]

continued ...

Table 5

No.	position	mapping
32	$[0, \frac{1}{2}, -x]$	[244, 256, 259, 263, 269, 279, 282, 285]
33	$[0, \frac{1}{2}, x]$	[245, 255, 258, 261, 268, 280, 283, 287]
34	$[0, x + \frac{1}{2}, 0]$	[246, 251, 257, 264, 271, 276, 284, 286]
35	$[0, \frac{1}{2} - x, 0]$	[247, 252, 260, 262, 270, 275, 281, 288]
36	$[-x, \frac{1}{2}, 0]$	[249, 250, 253, 254, 265, 266, 267, 272]
37	$[x + \frac{1}{2}, 0, 0]$	[289, 290, 291, 296, 321, 322, 325, 326]
38	$[\frac{1}{2}, 0, -x]$	[292, 304, 307, 311, 317, 327, 330, 333]
39	$[\frac{1}{2}, 0, x]$	[293, 303, 306, 309, 316, 328, 331, 335]
40	$[\frac{1}{2}, x, 0]$	[294, 299, 305, 312, 319, 324, 332, 334]
41	$[\frac{1}{2}, -x, 0]$	[295, 300, 308, 310, 318, 323, 329, 336]
42	$[\frac{1}{2} - x, 0, 0]$	[297, 298, 301, 302, 313, 314, 315, 320]
43	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[337, 338, 339, 344, 369, 370, 373, 374]
44	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	[340, 352, 355, 359, 365, 375, 378, 381]
45	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	[341, 351, 354, 357, 364, 376, 379, 383]
46	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[342, 347, 353, 360, 367, 372, 380, 382]
47	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[343, 348, 356, 358, 366, 371, 377, 384]
48	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[345, 346, 349, 350, 361, 362, 363, 368]

Table 6: Wyckoff site: 48f, site symmetry: $4'm'.m$

No.	position	mapping
1	$[x, \frac{1}{4}, \frac{1}{4}]$	[1, 38, 56, 85, 195, 226, 242, 273]
2	$[x, \frac{3}{4}, \frac{1}{4}]$	[2, 33, 51, 82, 200, 229, 241, 278]
3	$[x, \frac{1}{4}, \frac{3}{4}]$	[3, 34, 50, 81, 193, 230, 248, 277]
4	$[\frac{1}{4}, \frac{1}{4}, -x]$	[4, 45, 160, 186, 263, 269, 307, 327]
5	$[\frac{3}{4}, \frac{1}{4}, x]$	[5, 47, 159, 187, 261, 268, 306, 328]
6	$[\frac{3}{4}, x, \frac{1}{4}]$	[6, 46, 107, 140, 216, 223, 305, 324]
7	$[\frac{1}{4}, -x, \frac{1}{4}]$	[7, 48, 108, 137, 214, 222, 308, 323]
8	$[x, \frac{3}{4}, \frac{3}{4}]$	[8, 37, 49, 86, 194, 225, 243, 274]
9	$[-x, \frac{1}{4}, \frac{3}{4}]$	[9, 26, 58, 75, 205, 224, 254, 265]
10	$[-x, \frac{3}{4}, \frac{1}{4}]$	[10, 27, 57, 74, 206, 217, 253, 272]
11	$[\frac{1}{4}, x, \frac{3}{4}]$	[11, 44, 102, 142, 209, 228, 312, 319]
12	$[\frac{3}{4}, -x, \frac{3}{4}]$	[12, 41, 103, 144, 212, 227, 310, 318]
13	$[-x, \frac{1}{4}, \frac{1}{4}]$	[13, 32, 62, 73, 201, 218, 250, 267]
14	$[-x, \frac{3}{4}, \frac{3}{4}]$	[14, 25, 61, 80, 202, 219, 249, 266]
15	$[\frac{1}{4}, \frac{3}{4}, x]$	[15, 43, 149, 191, 258, 280, 309, 316]
16	$[\frac{3}{4}, \frac{3}{4}, -x]$	[16, 42, 148, 189, 259, 279, 311, 317]
17	$[\frac{1}{4}, x, \frac{1}{4}]$	[17, 36, 120, 127, 203, 236, 294, 334]
18	$[\frac{1}{4}, \frac{1}{4}, x]$	[18, 40, 165, 172, 255, 283, 293, 335]
19	$[\frac{3}{4}, \frac{1}{4}, -x]$	[19, 39, 167, 173, 256, 282, 292, 333]
20	$[\frac{3}{4}, -x, \frac{1}{4}]$	[20, 35, 118, 126, 204, 233, 295, 336]
21	$[\frac{3}{4}, \frac{3}{4}, x]$	[21, 28, 162, 184, 245, 287, 303, 331]
22	$[\frac{1}{4}, -x, \frac{3}{4}]$	[22, 30, 116, 131, 199, 240, 300, 329]
23	$[\frac{1}{4}, \frac{3}{4}, -x]$	[23, 29, 163, 183, 244, 285, 304, 330]

continued ...

Table 6

No.	position	mapping
24	$[\frac{3}{4}, x, \frac{3}{4}]$	[24, 31, 113, 132, 198, 238, 299, 332]
25	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[52, 93, 112, 138, 215, 221, 355, 375]
26	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[53, 95, 111, 139, 213, 220, 354, 376]
27	$[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[54, 94, 155, 188, 264, 271, 353, 372]
28	$[\frac{1}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[55, 96, 156, 185, 262, 270, 356, 371]
29	$[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[59, 92, 150, 190, 257, 276, 360, 367]
30	$[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[60, 89, 151, 192, 260, 275, 358, 366]
31	$[\frac{1}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[63, 91, 101, 143, 210, 232, 357, 364]
32	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[64, 90, 100, 141, 211, 231, 359, 365]
33	$[\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[65, 84, 168, 175, 251, 284, 342, 382]
34	$[\frac{1}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[66, 88, 117, 124, 207, 235, 341, 383]
35	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[67, 87, 119, 125, 208, 234, 340, 381]
36	$[\frac{3}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[68, 83, 166, 174, 252, 281, 343, 384]
37	$[\frac{3}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[69, 76, 114, 136, 197, 239, 351, 379]
38	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[70, 78, 164, 179, 247, 288, 348, 377]
39	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[71, 77, 115, 135, 196, 237, 352, 378]
40	$[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[72, 79, 161, 180, 246, 286, 347, 380]
41	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[97, 134, 152, 181, 291, 322, 338, 369]
42	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[98, 129, 147, 178, 296, 325, 337, 374]
43	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[99, 130, 146, 177, 289, 326, 344, 373]
44	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[104, 133, 145, 182, 290, 321, 339, 370]
45	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[105, 122, 154, 171, 301, 320, 350, 361]
46	$[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$	[106, 123, 153, 170, 302, 313, 349, 368]
47	$[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$	[109, 128, 158, 169, 297, 314, 346, 363]
48	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]$	[110, 121, 157, 176, 298, 315, 345, 362]

Table 7: Wyckoff site: 64g, site symmetry: $\cdot 3m$

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]

continued ...

Table 7

No.	position	mapping
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]
32	$[\frac{1}{2} - x, \frac{1}{2} - x, -x]$	[156, 158, 160, 169, 185, 186]
33	$[x, x, x + \frac{1}{2}]$	[193, 209, 210, 228, 230, 232]
34	$[x, -x, x + \frac{1}{2}]$	[194, 199, 207, 225, 235, 240]
35	$[x, x, \frac{1}{2} - x]$	[195, 196, 203, 226, 236, 237]
36	$[-x, x, x + \frac{1}{2}]$	[197, 198, 205, 224, 238, 239]
37	$[x, -x, \frac{1}{2} - x]$	[200, 214, 215, 221, 222, 229]
38	$[-x, x, \frac{1}{2} - x]$	[201, 211, 216, 218, 223, 231]
39	$[-x, -x, x + \frac{1}{2}]$	[202, 212, 213, 219, 220, 227]
40	$[-x, -x, \frac{1}{2} - x]$	[204, 206, 208, 217, 233, 234]
41	$[x, x + \frac{1}{2}, x]$	[241, 257, 258, 276, 278, 280]
42	$[x, \frac{1}{2} - x, x]$	[242, 247, 255, 273, 283, 288]
43	$[x, x + \frac{1}{2}, -x]$	[243, 244, 251, 274, 284, 285]
44	$[-x, x + \frac{1}{2}, x]$	[245, 246, 253, 272, 286, 287]
45	$[x, \frac{1}{2} - x, -x]$	[248, 262, 263, 269, 270, 277]
46	$[-x, x + \frac{1}{2}, -x]$	[249, 259, 264, 266, 271, 279]
47	$[-x, \frac{1}{2} - x, x]$	[250, 260, 261, 267, 268, 275]
48	$[-x, \frac{1}{2} - x, -x]$	[252, 254, 256, 265, 281, 282]
49	$[x + \frac{1}{2}, x, x]$	[289, 305, 306, 324, 326, 328]
50	$[x + \frac{1}{2}, -x, x]$	[290, 295, 303, 321, 331, 336]
51	$[x + \frac{1}{2}, x, -x]$	[291, 292, 299, 322, 332, 333]
52	$[\frac{1}{2} - x, x, x]$	[293, 294, 301, 320, 334, 335]
53	$[x + \frac{1}{2}, -x, -x]$	[296, 310, 311, 317, 318, 325]
54	$[\frac{1}{2} - x, x, -x]$	[297, 307, 312, 314, 319, 327]
55	$[\frac{1}{2} - x, -x, x]$	[298, 308, 309, 315, 316, 323]
56	$[\frac{1}{2} - x, -x, -x]$	[300, 302, 304, 313, 329, 330]
57	$[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[337, 353, 354, 372, 374, 376]
58	$[x + \frac{1}{2}, \frac{1}{2} - x, x + \frac{1}{2}]$	[338, 343, 351, 369, 379, 384]
59	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - x]$	[339, 340, 347, 370, 380, 381]
60	$[\frac{1}{2} - x, x + \frac{1}{2}, x + \frac{1}{2}]$	[341, 342, 349, 368, 382, 383]
61	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x]$	[344, 358, 359, 365, 366, 373]
62	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - x]$	[345, 355, 360, 362, 367, 375]

continued ...

Table 7

No.	position	mapping
63	$[\frac{1}{2} - x, \frac{1}{2} - x, x + \frac{1}{2}]$	[346, 356, 357, 363, 364, 371]
64	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x]$	[348, 350, 352, 361, 377, 378]

Table 8: Wyckoff site: 96h, site symmetry: $2'm'm..$

No.	position	mapping
1	$[x, \frac{1}{4}, 0]$	[1, 34, 248, 273]
2	$[x, 0, \frac{1}{4}]$	[2, 38, 195, 229]
3	$[x, 0, \frac{3}{4}]$	[3, 37, 194, 230]
4	$[0, \frac{1}{4}, -x]$	[4, 39, 256, 269]
5	$[0, \frac{1}{4}, x]$	[5, 40, 255, 268]
6	$[\frac{3}{4}, x, 0]$	[6, 31, 299, 324]
7	$[\frac{1}{4}, -x, 0]$	[7, 30, 300, 323]
8	$[x, \frac{3}{4}, 0]$	[8, 33, 241, 274]
9	$[-x, \frac{1}{4}, 0]$	[9, 32, 250, 265]
10	$[-x, \frac{3}{4}, 0]$	[10, 25, 249, 272]
11	$[\frac{1}{4}, x, 0]$	[11, 36, 294, 319]
12	$[\frac{3}{4}, -x, 0]$	[12, 35, 295, 318]
13	$[-x, 0, \frac{1}{4}]$	[13, 27, 206, 218]
14	$[-x, 0, \frac{3}{4}]$	[14, 26, 205, 219]
15	$[0, \frac{3}{4}, x]$	[15, 28, 245, 280]
16	$[0, \frac{3}{4}, -x]$	[16, 29, 244, 279]
17	$[0, x, \frac{1}{4}]$	[17, 46, 216, 236]
18	$[\frac{1}{4}, 0, x]$	[18, 43, 309, 335]
19	$[\frac{3}{4}, 0, -x]$	[19, 42, 311, 333]
20	$[0, -x, \frac{1}{4}]$	[20, 48, 214, 233]
21	$[\frac{3}{4}, 0, x]$	[21, 47, 306, 331]
22	$[0, -x, \frac{3}{4}]$	[22, 41, 212, 240]
23	$[\frac{1}{4}, 0, -x]$	[23, 45, 307, 330]
24	$[0, x, \frac{3}{4}]$	[24, 44, 209, 238]
25	$[x, \frac{3}{4}, \frac{1}{2}]$	[49, 82, 200, 225]
26	$[x, \frac{1}{2}, \frac{3}{4}]$	[50, 86, 243, 277]
27	$[x, \frac{1}{2}, \frac{1}{4}]$	[51, 85, 242, 278]
28	$[0, \frac{3}{4}, \frac{1}{2} - x]$	[52, 87, 208, 221]
29	$[0, \frac{3}{4}, x + \frac{1}{2}]$	[53, 88, 207, 220]
30	$[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{2}]$	[54, 79, 347, 372]
31	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{2}]$	[55, 78, 348, 371]
32	$[x, \frac{1}{4}, \frac{1}{2}]$	[56, 81, 193, 226]
33	$[-x, \frac{3}{4}, \frac{1}{2}]$	[57, 80, 202, 217]
34	$[-x, \frac{1}{4}, \frac{1}{2}]$	[58, 73, 201, 224]
35	$[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{2}]$	[59, 84, 342, 367]
36	$[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{2}]$	[60, 83, 343, 366]
37	$[-x, \frac{1}{2}, \frac{3}{4}]$	[61, 75, 254, 266]
38	$[-x, \frac{1}{2}, \frac{1}{4}]$	[62, 74, 253, 267]

continued ...

Table 8

No.	position	mapping
39	$[0, \frac{1}{4}, x + \frac{1}{2}]$	[63, 76, 197, 232]
40	$[0, \frac{1}{4}, \frac{1}{2} - x]$	[64, 77, 196, 231]
41	$[0, x + \frac{1}{2}, \frac{3}{4}]$	[65, 94, 264, 284]
42	$[\frac{1}{4}, \frac{1}{2}, x + \frac{1}{2}]$	[66, 91, 357, 383]
43	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{2} - x]$	[67, 90, 359, 381]
44	$[0, \frac{1}{2} - x, \frac{3}{4}]$	[68, 96, 262, 281]
45	$[\frac{3}{4}, \frac{1}{2}, x + \frac{1}{2}]$	[69, 95, 354, 379]
46	$[0, \frac{1}{2} - x, \frac{1}{4}]$	[70, 89, 260, 288]
47	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{2} - x]$	[71, 93, 355, 378]
48	$[0, x + \frac{1}{2}, \frac{1}{4}]$	[72, 92, 257, 286]
49	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{2}]$	[97, 130, 344, 369]
50	$[x + \frac{1}{2}, 0, \frac{3}{4}]$	[98, 134, 291, 325]
51	$[x + \frac{1}{2}, 0, \frac{1}{4}]$	[99, 133, 290, 326]
52	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2} - x]$	[100, 135, 352, 365]
53	$[\frac{1}{2}, \frac{1}{4}, x + \frac{1}{2}]$	[101, 136, 351, 364]
54	$[\frac{1}{4}, x, \frac{1}{2}]$	[102, 127, 203, 228]
55	$[\frac{3}{4}, -x, \frac{1}{2}]$	[103, 126, 204, 227]
56	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{2}]$	[104, 129, 337, 370]
57	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{2}]$	[105, 128, 346, 361]
58	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{2}]$	[106, 121, 345, 368]
59	$[\frac{3}{4}, x, \frac{1}{2}]$	[107, 132, 198, 223]
60	$[\frac{1}{4}, -x, \frac{1}{2}]$	[108, 131, 199, 222]
61	$[\frac{1}{2} - x, 0, \frac{3}{4}]$	[109, 123, 302, 314]
62	$[\frac{1}{2} - x, 0, \frac{1}{4}]$	[110, 122, 301, 315]
63	$[\frac{1}{2}, \frac{3}{4}, x + \frac{1}{2}]$	[111, 124, 341, 376]
64	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{2} - x]$	[112, 125, 340, 375]
65	$[\frac{1}{2}, x, \frac{3}{4}]$	[113, 142, 312, 332]
66	$[\frac{3}{4}, 0, x + \frac{1}{2}]$	[114, 139, 213, 239]
67	$[\frac{1}{4}, 0, \frac{1}{2} - x]$	[115, 138, 215, 237]
68	$[\frac{1}{2}, -x, \frac{3}{4}]$	[116, 144, 310, 329]
69	$[\frac{1}{4}, 0, x + \frac{1}{2}]$	[117, 143, 210, 235]
70	$[\frac{1}{2}, -x, \frac{1}{4}]$	[118, 137, 308, 336]
71	$[\frac{3}{4}, 0, \frac{1}{2} - x]$	[119, 141, 211, 234]
72	$[\frac{1}{2}, x, \frac{1}{4}]$	[120, 140, 305, 334]
73	$[x + \frac{1}{2}, \frac{3}{4}, 0]$	[145, 178, 296, 321]
74	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[146, 182, 339, 373]
75	$[x + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[147, 181, 338, 374]
76	$[\frac{1}{2}, \frac{3}{4}, -x]$	[148, 183, 304, 317]
77	$[\frac{1}{2}, \frac{3}{4}, x]$	[149, 184, 303, 316]
78	$[\frac{1}{4}, x + \frac{1}{2}, 0]$	[150, 175, 251, 276]
79	$[\frac{3}{4}, \frac{1}{2} - x, 0]$	[151, 174, 252, 275]
80	$[x + \frac{1}{2}, \frac{1}{4}, 0]$	[152, 177, 289, 322]
81	$[\frac{1}{2} - x, \frac{3}{4}, 0]$	[153, 176, 298, 313]
82	$[\frac{1}{2} - x, \frac{1}{4}, 0]$	[154, 169, 297, 320]
83	$[\frac{3}{4}, x + \frac{1}{2}, 0]$	[155, 180, 246, 271]
84	$[\frac{1}{4}, \frac{1}{2} - x, 0]$	[156, 179, 247, 270]
85	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{4}]$	[157, 171, 350, 362]

continued ...

Table 8

No.	position	mapping
86	$[\frac{1}{2} - x, \frac{1}{2}, \frac{3}{4}]$	[158, 170, 349, 363]
87	$[\frac{1}{2}, \frac{1}{4}, x]$	[159, 172, 293, 328]
88	$[\frac{1}{2}, \frac{1}{4}, -x]$	[160, 173, 292, 327]
89	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[161, 190, 360, 380]
90	$[\frac{3}{4}, \frac{1}{2}, x]$	[162, 187, 261, 287]
91	$[\frac{1}{4}, \frac{1}{2}, -x]$	[163, 186, 263, 285]
92	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}]$	[164, 192, 358, 377]
93	$[\frac{1}{4}, \frac{1}{2}, x]$	[165, 191, 258, 283]
94	$[\frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}]$	[166, 185, 356, 384]
95	$[\frac{3}{4}, \frac{1}{2}, -x]$	[167, 189, 259, 282]
96	$[\frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}]$	[168, 188, 353, 382]

Table 9: Wyckoff site: 96i, 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]

continued ...

Table 9

No.	position	mapping
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]
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]
49	$[0, y, y + \frac{1}{2}]$	[193, 205, 224, 230]
50	$[0, -y, y + \frac{1}{2}]$	[194, 202, 219, 225]
51	$[0, y, \frac{1}{2} - y]$	[195, 201, 218, 226]
52	$[y, y, \frac{1}{2}]$	[196, 210, 232, 237]
53	$[-y, y, \frac{1}{2}]$	[197, 211, 231, 239]
54	$[-y, 0, y + \frac{1}{2}]$	[198, 212, 227, 238]
55	$[y, 0, y + \frac{1}{2}]$	[199, 209, 228, 240]
56	$[0, -y, \frac{1}{2} - y]$	[200, 206, 217, 229]
57	$[y, 0, \frac{1}{2} - y]$	[203, 214, 222, 236]
58	$[-y, 0, \frac{1}{2} - y]$	[204, 216, 223, 233]
59	$[y, -y, \frac{1}{2}]$	[207, 215, 221, 235]
60	$[-y, -y, \frac{1}{2}]$	[208, 213, 220, 234]
61	$[0, y + \frac{1}{2}, y]$	[241, 253, 272, 278]
62	$[0, \frac{1}{2} - y, y]$	[242, 250, 267, 273]
63	$[0, y + \frac{1}{2}, -y]$	[243, 249, 266, 274]
64	$[y, y + \frac{1}{2}, 0]$	[244, 258, 280, 285]
65	$[-y, y + \frac{1}{2}, 0]$	[245, 259, 279, 287]
66	$[-y, \frac{1}{2}, y]$	[246, 260, 275, 286]
67	$[y, \frac{1}{2}, y]$	[247, 257, 276, 288]
68	$[0, \frac{1}{2} - y, -y]$	[248, 254, 265, 277]
69	$[y, \frac{1}{2}, -y]$	[251, 262, 270, 284]
70	$[-y, \frac{1}{2}, -y]$	[252, 264, 271, 281]
71	$[y, \frac{1}{2} - y, 0]$	[255, 263, 269, 283]
72	$[-y, \frac{1}{2} - y, 0]$	[256, 261, 268, 282]
73	$[\frac{1}{2}, y, y]$	[289, 301, 320, 326]
74	$[\frac{1}{2}, -y, y]$	[290, 298, 315, 321]
75	$[\frac{1}{2}, y, -y]$	[291, 297, 314, 322]
76	$[y + \frac{1}{2}, y, 0]$	[292, 306, 328, 333]

continued ...

Table 9

No.	position	mapping
77	$[\frac{1}{2} - y, y, 0]$	[293, 307, 327, 335]
78	$[\frac{1}{2} - y, 0, y]$	[294, 308, 323, 334]
79	$[y + \frac{1}{2}, 0, y]$	[295, 305, 324, 336]
80	$[\frac{1}{2}, -y, -y]$	[296, 302, 313, 325]
81	$[y + \frac{1}{2}, 0, -y]$	[299, 310, 318, 332]
82	$[\frac{1}{2} - y, 0, -y]$	[300, 312, 319, 329]
83	$[y + \frac{1}{2}, -y, 0]$	[303, 311, 317, 331]
84	$[\frac{1}{2} - y, -y, 0]$	[304, 309, 316, 330]
85	$[\frac{1}{2}, y + \frac{1}{2}, y + \frac{1}{2}]$	[337, 349, 368, 374]
86	$[\frac{1}{2}, \frac{1}{2} - y, y + \frac{1}{2}]$	[338, 346, 363, 369]
87	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - y]$	[339, 345, 362, 370]
88	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[340, 354, 376, 381]
89	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{2}]$	[341, 355, 375, 383]
90	$[\frac{1}{2} - y, \frac{1}{2}, y + \frac{1}{2}]$	[342, 356, 371, 382]
91	$[y + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}]$	[343, 353, 372, 384]
92	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - y]$	[344, 350, 361, 373]
93	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - y]$	[347, 358, 366, 380]
94	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - y]$	[348, 360, 367, 377]
95	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[351, 359, 365, 379]
96	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{2}]$	[352, 357, 364, 378]

Table 10: Wyckoff site: 96j, site symmetry: $m' . 2'm$

No.	position	mapping
1	$[\frac{1}{4}, y, y]$	[1, 38, 301, 320]
2	$[\frac{1}{4}, -y, y]$	[2, 33, 298, 315]
3	$[\frac{1}{4}, y, -y]$	[3, 34, 297, 314]
4	$[y, y, \frac{3}{4}]$	[4, 45, 210, 232]
5	$[-y, y, \frac{1}{4}]$	[5, 47, 211, 231]
6	$[-y, \frac{1}{4}, y]$	[6, 46, 260, 275]
7	$[y, \frac{3}{4}, y]$	[7, 48, 257, 276]
8	$[\frac{1}{4}, -y, -y]$	[8, 37, 302, 313]
9	$[\frac{3}{4}, y, -y]$	[9, 26, 291, 322]
10	$[\frac{3}{4}, -y, y]$	[10, 27, 290, 321]
11	$[y, \frac{1}{4}, -y]$	[11, 44, 262, 270]
12	$[-y, \frac{3}{4}, -y]$	[12, 41, 264, 271]
13	$[\frac{3}{4}, y, y]$	[13, 32, 289, 326]
14	$[\frac{3}{4}, -y, -y]$	[14, 25, 296, 325]
15	$[y, -y, \frac{1}{4}]$	[15, 43, 215, 221]
16	$[-y, -y, \frac{3}{4}]$	[16, 42, 213, 220]
17	$[y, \frac{1}{4}, y]$	[17, 36, 247, 288]
18	$[y, y, \frac{1}{4}]$	[18, 40, 196, 237]
19	$[-y, y, \frac{3}{4}]$	[19, 39, 197, 239]
20	$[-y, \frac{3}{4}, y]$	[20, 35, 246, 286]

continued ...

Table 10

No.	position	mapping
21	$[-y, -y, \frac{1}{4}]$	[21, 28, 208, 234]
22	$[y, \frac{3}{4}, -y]$	[22, 30, 251, 284]
23	$[y, -y, \frac{3}{4}]$	[23, 29, 207, 235]
24	$[-y, \frac{1}{4}, -y]$	[24, 31, 252, 281]
25	$[\frac{1}{4}, y + \frac{1}{2}, y + \frac{1}{2}]$	[49, 86, 349, 368]
26	$[\frac{1}{4}, \frac{1}{2} - y, y + \frac{1}{2}]$	[50, 81, 346, 363]
27	$[\frac{1}{4}, y + \frac{1}{2}, \frac{1}{2} - y]$	[51, 82, 345, 362]
28	$[y, y + \frac{1}{2}, \frac{1}{4}]$	[52, 93, 258, 280]
29	$[-y, y + \frac{1}{2}, \frac{3}{4}]$	[53, 95, 259, 279]
30	$[-y, \frac{3}{4}, y + \frac{1}{2}]$	[54, 94, 212, 227]
31	$[y, \frac{1}{4}, y + \frac{1}{2}]$	[55, 96, 209, 228]
32	$[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{2} - y]$	[56, 85, 350, 361]
33	$[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{2} - y]$	[57, 74, 339, 370]
34	$[\frac{3}{4}, \frac{1}{2} - y, y + \frac{1}{2}]$	[58, 75, 338, 369]
35	$[y, \frac{3}{4}, \frac{1}{2} - y]$	[59, 92, 214, 222]
36	$[-y, \frac{1}{4}, \frac{1}{2} - y]$	[60, 89, 216, 223]
37	$[\frac{3}{4}, y + \frac{1}{2}, y + \frac{1}{2}]$	[61, 80, 337, 374]
38	$[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{2} - y]$	[62, 73, 344, 373]
39	$[y, \frac{1}{2} - y, \frac{3}{4}]$	[63, 91, 263, 269]
40	$[-y, \frac{1}{2} - y, \frac{1}{4}]$	[64, 90, 261, 268]
41	$[y, \frac{3}{4}, y + \frac{1}{2}]$	[65, 84, 199, 240]
42	$[y, y + \frac{1}{2}, \frac{3}{4}]$	[66, 88, 244, 285]
43	$[-y, y + \frac{1}{2}, \frac{1}{4}]$	[67, 87, 245, 287]
44	$[-y, \frac{1}{4}, y + \frac{1}{2}]$	[68, 83, 198, 238]
45	$[-y, \frac{1}{2} - y, \frac{3}{4}]$	[69, 76, 256, 282]
46	$[y, \frac{1}{4}, \frac{1}{2} - y]$	[70, 78, 203, 236]
47	$[y, \frac{1}{2} - y, \frac{1}{4}]$	[71, 77, 255, 283]
48	$[-y, \frac{3}{4}, \frac{1}{2} - y]$	[72, 79, 204, 233]
49	$[\frac{3}{4}, y, y + \frac{1}{2}]$	[97, 134, 205, 224]
50	$[\frac{3}{4}, -y, y + \frac{1}{2}]$	[98, 129, 202, 219]
51	$[\frac{3}{4}, y, \frac{1}{2} - y]$	[99, 130, 201, 218]
52	$[y + \frac{1}{2}, y, \frac{1}{4}]$	[100, 141, 306, 328]
53	$[\frac{1}{2} - y, y, \frac{3}{4}]$	[101, 143, 307, 327]
54	$[\frac{1}{2} - y, \frac{1}{4}, y + \frac{1}{2}]$	[102, 142, 356, 371]
55	$[y + \frac{1}{2}, \frac{3}{4}, y + \frac{1}{2}]$	[103, 144, 353, 372]
56	$[\frac{3}{4}, -y, \frac{1}{2} - y]$	[104, 133, 206, 217]
57	$[\frac{1}{4}, y, \frac{1}{2} - y]$	[105, 122, 195, 226]
58	$[\frac{1}{4}, -y, y + \frac{1}{2}]$	[106, 123, 194, 225]
59	$[y + \frac{1}{2}, \frac{1}{4}, \frac{1}{2} - y]$	[107, 140, 358, 366]
60	$[\frac{1}{2} - y, \frac{3}{4}, \frac{1}{2} - y]$	[108, 137, 360, 367]
61	$[\frac{1}{4}, y, y + \frac{1}{2}]$	[109, 128, 193, 230]
62	$[\frac{1}{4}, -y, \frac{1}{2} - y]$	[110, 121, 200, 229]
63	$[y + \frac{1}{2}, -y, \frac{3}{4}]$	[111, 139, 311, 317]
64	$[\frac{1}{2} - y, -y, \frac{1}{4}]$	[112, 138, 309, 316]
65	$[y + \frac{1}{2}, \frac{1}{4}, y + \frac{1}{2}]$	[113, 132, 343, 384]
66	$[y + \frac{1}{2}, y, \frac{3}{4}]$	[114, 136, 292, 333]
67	$[\frac{1}{2} - y, y, \frac{1}{4}]$	[115, 135, 293, 335]

continued ...

Table 10

No.	position	mapping
68	$[\frac{1}{2} - y, \frac{3}{4}, y + \frac{1}{2}]$	[116, 131, 342, 382]
69	$[\frac{1}{2} - y, -y, \frac{3}{4}]$	[117, 124, 304, 330]
70	$[y + \frac{1}{2}, \frac{3}{4}, \frac{1}{2} - y]$	[118, 126, 347, 380]
71	$[y + \frac{1}{2}, -y, \frac{1}{4}]$	[119, 125, 303, 331]
72	$[\frac{1}{2} - y, \frac{1}{4}, \frac{1}{2} - y]$	[120, 127, 348, 377]
73	$[\frac{3}{4}, y + \frac{1}{2}, y]$	[145, 182, 253, 272]
74	$[\frac{3}{4}, \frac{1}{2} - y, y]$	[146, 177, 250, 267]
75	$[\frac{3}{4}, y + \frac{1}{2}, -y]$	[147, 178, 249, 266]
76	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$	[148, 189, 354, 376]
77	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{4}]$	[149, 191, 355, 375]
78	$[\frac{1}{2} - y, \frac{3}{4}, y]$	[150, 190, 308, 323]
79	$[y + \frac{1}{2}, \frac{1}{4}, y]$	[151, 192, 305, 324]
80	$[\frac{3}{4}, \frac{1}{2} - y, -y]$	[152, 181, 254, 265]
81	$[\frac{1}{4}, y + \frac{1}{2}, -y]$	[153, 170, 243, 274]
82	$[\frac{1}{4}, \frac{1}{2} - y, y]$	[154, 171, 242, 273]
83	$[y + \frac{1}{2}, \frac{3}{4}, -y]$	[155, 188, 310, 318]
84	$[\frac{1}{2} - y, \frac{1}{4}, -y]$	[156, 185, 312, 319]
85	$[\frac{1}{4}, y + \frac{1}{2}, y]$	[157, 176, 241, 278]
86	$[\frac{1}{4}, \frac{1}{2} - y, -y]$	[158, 169, 248, 277]
87	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{4}]$	[159, 187, 359, 365]
88	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{3}{4}]$	[160, 186, 357, 364]
89	$[y + \frac{1}{2}, \frac{3}{4}, y]$	[161, 180, 295, 336]
90	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{4}]$	[162, 184, 340, 381]
91	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{3}{4}]$	[163, 183, 341, 383]
92	$[\frac{1}{2} - y, \frac{1}{4}, y]$	[164, 179, 294, 334]
93	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{4}]$	[165, 172, 352, 378]
94	$[y + \frac{1}{2}, \frac{1}{4}, -y]$	[166, 174, 299, 332]
95	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{3}{4}]$	[167, 173, 351, 379]
96	$[\frac{1}{2} - y, \frac{3}{4}, -y]$	[168, 175, 300, 329]

Table 11: Wyckoff site: 192k, site symmetry: m . .

No.	position	mapping
1	$[0, y, z]$	[1, 32]
2	$[0, -z, y]$	[2, 27]
3	$[0, z, -y]$	[3, 26]
4	$[z, y, 0]$	[4, 40]
5	$[-z, y, 0]$	[5, 39]
6	$[-y, 0, z]$	[6, 35]
7	$[y, 0, z]$	[7, 36]
8	$[0, -y, -z]$	[8, 25]
9	$[0, y, -z]$	[9, 34]
10	$[0, -y, z]$	[10, 33]
11	$[y, 0, -z]$	[11, 30]

continued ...

Table 11

No.	position	mapping
12	$[-y, 0, -z]$	[12,31]
13	$[0, z, y]$	[13,38]
14	$[0, -z, -y]$	[14,37]
15	$[z, -y, 0]$	[15,29]
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]

continued ...

Table 11

No.	position	mapping
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]
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]
97	$[0, y, z + \frac{1}{2}]$	[193, 224]
98	$[0, -z, y + \frac{1}{2}]$	[194, 219]
99	$[0, z, \frac{1}{2} - y]$	[195, 218]
100	$[z, y, \frac{1}{2}]$	[196, 232]
101	$[-z, y, \frac{1}{2}]$	[197, 231]
102	$[-y, 0, z + \frac{1}{2}]$	[198, 227]
103	$[y, 0, z + \frac{1}{2}]$	[199, 228]
104	$[0, -y, \frac{1}{2} - z]$	[200, 217]
105	$[0, y, \frac{1}{2} - z]$	[201, 226]

continued ...

Table 11

No.	position	mapping
106	$[0, -y, z + \frac{1}{2}]$	[202, 225]
107	$[y, 0, \frac{1}{2} - z]$	[203, 222]
108	$[-y, 0, \frac{1}{2} - z]$	[204, 223]
109	$[0, z, y + \frac{1}{2}]$	[205, 230]
110	$[0, -z, \frac{1}{2} - y]$	[206, 229]
111	$[z, -y, \frac{1}{2}]$	[207, 221]
112	$[-z, -y, \frac{1}{2}]$	[208, 220]
113	$[z, 0, y + \frac{1}{2}]$	[209, 240]
114	$[y, z, \frac{1}{2}]$	[210, 237]
115	$[-y, z, \frac{1}{2}]$	[211, 239]
116	$[-z, 0, y + \frac{1}{2}]$	[212, 238]
117	$[-y, -z, \frac{1}{2}]$	[213, 234]
118	$[z, 0, \frac{1}{2} - y]$	[214, 236]
119	$[y, -z, \frac{1}{2}]$	[215, 235]
120	$[-z, 0, \frac{1}{2} - y]$	[216, 233]
121	$[0, y + \frac{1}{2}, z]$	[241, 272]
122	$[0, \frac{1}{2} - z, y]$	[242, 267]
123	$[0, z + \frac{1}{2}, -y]$	[243, 266]
124	$[z, y + \frac{1}{2}, 0]$	[244, 280]
125	$[-z, y + \frac{1}{2}, 0]$	[245, 279]
126	$[-y, \frac{1}{2}, z]$	[246, 275]
127	$[y, \frac{1}{2}, z]$	[247, 276]
128	$[0, \frac{1}{2} - y, -z]$	[248, 265]
129	$[0, y + \frac{1}{2}, -z]$	[249, 274]
130	$[0, \frac{1}{2} - y, z]$	[250, 273]
131	$[y, \frac{1}{2}, -z]$	[251, 270]
132	$[-y, \frac{1}{2}, -z]$	[252, 271]
133	$[0, z + \frac{1}{2}, y]$	[253, 278]
134	$[0, \frac{1}{2} - z, -y]$	[254, 277]
135	$[z, \frac{1}{2} - y, 0]$	[255, 269]
136	$[-z, \frac{1}{2} - y, 0]$	[256, 268]
137	$[z, \frac{1}{2}, y]$	[257, 288]
138	$[y, z + \frac{1}{2}, 0]$	[258, 285]
139	$[-y, z + \frac{1}{2}, 0]$	[259, 287]
140	$[-z, \frac{1}{2}, y]$	[260, 286]
141	$[-y, \frac{1}{2} - z, 0]$	[261, 282]
142	$[z, \frac{1}{2}, -y]$	[262, 284]
143	$[y, \frac{1}{2} - z, 0]$	[263, 283]
144	$[-z, \frac{1}{2}, -y]$	[264, 281]
145	$[\frac{1}{2}, y, z]$	[289, 320]
146	$[\frac{1}{2}, -z, y]$	[290, 315]
147	$[\frac{1}{2}, z, -y]$	[291, 314]
148	$[z + \frac{1}{2}, y, 0]$	[292, 328]
149	$[\frac{1}{2} - z, y, 0]$	[293, 327]
150	$[\frac{1}{2} - y, 0, z]$	[294, 323]
151	$[y + \frac{1}{2}, 0, z]$	[295, 324]
152	$[\frac{1}{2}, -y, -z]$	[296, 313]

continued ...

Table 11

No.	position	mapping
153	$[\frac{1}{2}, y, -z]$	[297, 322]
154	$[\frac{1}{2}, -y, z]$	[298, 321]
155	$[y + \frac{1}{2}, 0, -z]$	[299, 318]
156	$[\frac{1}{2} - y, 0, -z]$	[300, 319]
157	$[\frac{1}{2}, z, y]$	[301, 326]
158	$[\frac{1}{2}, -z, -y]$	[302, 325]
159	$[z + \frac{1}{2}, -y, 0]$	[303, 317]
160	$[\frac{1}{2} - z, -y, 0]$	[304, 316]
161	$[z + \frac{1}{2}, 0, y]$	[305, 336]
162	$[y + \frac{1}{2}, z, 0]$	[306, 333]
163	$[\frac{1}{2} - y, z, 0]$	[307, 335]
164	$[\frac{1}{2} - z, 0, y]$	[308, 334]
165	$[\frac{1}{2} - y, -z, 0]$	[309, 330]
166	$[z + \frac{1}{2}, 0, -y]$	[310, 332]
167	$[y + \frac{1}{2}, -z, 0]$	[311, 331]
168	$[\frac{1}{2} - z, 0, -y]$	[312, 329]
169	$[\frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[337, 368]
170	$[\frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[338, 363]
171	$[\frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[339, 362]
172	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[340, 376]
173	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2}]$	[341, 375]
174	$[\frac{1}{2} - y, \frac{1}{2}, z + \frac{1}{2}]$	[342, 371]
175	$[y + \frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[343, 372]
176	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[344, 361]
177	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[345, 370]
178	$[\frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[346, 369]
179	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[347, 366]
180	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - z]$	[348, 367]
181	$[\frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[349, 374]
182	$[\frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[350, 373]
183	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[351, 365]
184	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2}]$	[352, 364]
185	$[z + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}]$	[353, 384]
186	$[y + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2}]$	[354, 381]
187	$[\frac{1}{2} - y, z + \frac{1}{2}, \frac{1}{2}]$	[355, 383]
188	$[\frac{1}{2} - z, \frac{1}{2}, y + \frac{1}{2}]$	[356, 382]
189	$[\frac{1}{2} - y, \frac{1}{2} - z, \frac{1}{2}]$	[357, 378]
190	$[z + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - y]$	[358, 380]
191	$[y + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2}]$	[359, 379]
192	$[\frac{1}{2} - z, \frac{1}{2}, \frac{1}{2} - y]$	[360, 377]

Table 12: Wyckoff site: 1921, site symmetry: m' . .

No.	position	mapping
1	$[\frac{1}{4}, y, z]$	[1, 320]
2	$[\frac{1}{4}, -z, y]$	[2, 315]
3	$[\frac{1}{4}, z, -y]$	[3, 314]
4	$[z, y, \frac{3}{4}]$	[4, 232]
5	$[-z, y, \frac{1}{4}]$	[5, 231]
6	$[-y, \frac{1}{4}, z]$	[6, 275]
7	$[y, \frac{3}{4}, z]$	[7, 276]
8	$[\frac{1}{4}, -y, -z]$	[8, 313]
9	$[\frac{3}{4}, y, -z]$	[9, 322]
10	$[\frac{3}{4}, -y, z]$	[10, 321]
11	$[y, \frac{1}{4}, -z]$	[11, 270]
12	$[-y, \frac{3}{4}, -z]$	[12, 271]
13	$[\frac{3}{4}, z, y]$	[13, 326]
14	$[\frac{3}{4}, -z, -y]$	[14, 325]
15	$[z, -y, \frac{1}{4}]$	[15, 221]
16	$[-z, -y, \frac{3}{4}]$	[16, 220]
17	$[z, \frac{1}{4}, y]$	[17, 288]
18	$[y, z, \frac{1}{4}]$	[18, 237]
19	$[-y, z, \frac{3}{4}]$	[19, 239]
20	$[-z, \frac{3}{4}, y]$	[20, 286]
21	$[-y, -z, \frac{1}{4}]$	[21, 234]
22	$[z, \frac{3}{4}, -y]$	[22, 284]
23	$[y, -z, \frac{3}{4}]$	[23, 235]
24	$[-z, \frac{1}{4}, -y]$	[24, 281]
25	$[\frac{3}{4}, -y, -z]$	[25, 296]
26	$[\frac{3}{4}, z, -y]$	[26, 291]
27	$[\frac{3}{4}, -z, y]$	[27, 290]
28	$[-z, -y, \frac{1}{4}]$	[28, 208]
29	$[z, -y, \frac{3}{4}]$	[29, 207]
30	$[y, \frac{3}{4}, -z]$	[30, 251]
31	$[-y, \frac{1}{4}, -z]$	[31, 252]
32	$[\frac{3}{4}, y, z]$	[32, 289]
33	$[\frac{1}{4}, -y, z]$	[33, 298]
34	$[\frac{1}{4}, y, -z]$	[34, 297]
35	$[-y, \frac{3}{4}, z]$	[35, 246]
36	$[y, \frac{1}{4}, z]$	[36, 247]
37	$[\frac{1}{4}, -z, -y]$	[37, 302]
38	$[\frac{1}{4}, z, y]$	[38, 301]
39	$[-z, y, \frac{3}{4}]$	[39, 197]
40	$[z, y, \frac{1}{4}]$	[40, 196]
41	$[-z, \frac{3}{4}, -y]$	[41, 264]
42	$[-y, -z, \frac{3}{4}]$	[42, 213]
43	$[y, -z, \frac{1}{4}]$	[43, 215]
44	$[z, \frac{1}{4}, -y]$	[44, 262]
45	$[y, z, \frac{3}{4}]$	[45, 210]
46	$[-z, \frac{1}{4}, y]$	[46, 260]

continued ...

Table 12

No.	position	mapping
47	$[-y, z, \frac{1}{4}]$	[47,211]
48	$[z, \frac{3}{4}, y]$	[48,257]
49	$[\frac{1}{4}, y + \frac{1}{2}, z + \frac{1}{2}]$	[49,368]
50	$[\frac{1}{4}, \frac{1}{2} - z, y + \frac{1}{2}]$	[50,363]
51	$[\frac{1}{4}, z + \frac{1}{2}, \frac{1}{2} - y]$	[51,362]
52	$[z, y + \frac{1}{2}, \frac{1}{4}]$	[52,280]
53	$[-z, y + \frac{1}{2}, \frac{3}{4}]$	[53,279]
54	$[-y, \frac{3}{4}, z + \frac{1}{2}]$	[54,227]
55	$[y, \frac{1}{4}, z + \frac{1}{2}]$	[55,228]
56	$[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{2} - z]$	[56,361]
57	$[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{2} - z]$	[57,370]
58	$[\frac{3}{4}, \frac{1}{2} - y, z + \frac{1}{2}]$	[58,369]
59	$[y, \frac{3}{4}, \frac{1}{2} - z]$	[59,222]
60	$[-y, \frac{1}{4}, \frac{1}{2} - z]$	[60,223]
61	$[\frac{3}{4}, z + \frac{1}{2}, y + \frac{1}{2}]$	[61,374]
62	$[\frac{3}{4}, \frac{1}{2} - z, \frac{1}{2} - y]$	[62,373]
63	$[z, \frac{1}{2} - y, \frac{3}{4}]$	[63,269]
64	$[-z, \frac{1}{2} - y, \frac{1}{4}]$	[64,268]
65	$[z, \frac{3}{4}, y + \frac{1}{2}]$	[65,240]
66	$[y, z + \frac{1}{2}, \frac{3}{4}]$	[66,285]
67	$[-y, z + \frac{1}{2}, \frac{1}{4}]$	[67,287]
68	$[-z, \frac{1}{4}, y + \frac{1}{2}]$	[68,238]
69	$[-y, \frac{1}{2} - z, \frac{3}{4}]$	[69,282]
70	$[z, \frac{1}{4}, \frac{1}{2} - y]$	[70,236]
71	$[y, \frac{1}{2} - z, \frac{1}{4}]$	[71,283]
72	$[-z, \frac{3}{4}, \frac{1}{2} - y]$	[72,233]
73	$[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{2} - z]$	[73,344]
74	$[\frac{3}{4}, z + \frac{1}{2}, \frac{1}{2} - y]$	[74,339]
75	$[\frac{3}{4}, \frac{1}{2} - z, y + \frac{1}{2}]$	[75,338]
76	$[-z, \frac{1}{2} - y, \frac{3}{4}]$	[76,256]
77	$[z, \frac{1}{2} - y, \frac{1}{4}]$	[77,255]
78	$[y, \frac{1}{4}, \frac{1}{2} - z]$	[78,203]
79	$[-y, \frac{3}{4}, \frac{1}{2} - z]$	[79,204]
80	$[\frac{3}{4}, y + \frac{1}{2}, z + \frac{1}{2}]$	[80,337]
81	$[\frac{1}{4}, \frac{1}{2} - y, z + \frac{1}{2}]$	[81,346]
82	$[\frac{1}{4}, y + \frac{1}{2}, \frac{1}{2} - z]$	[82,345]
83	$[-y, \frac{1}{4}, z + \frac{1}{2}]$	[83,198]
84	$[y, \frac{3}{4}, z + \frac{1}{2}]$	[84,199]
85	$[\frac{1}{4}, \frac{1}{2} - z, \frac{1}{2} - y]$	[85,350]
86	$[\frac{1}{4}, z + \frac{1}{2}, y + \frac{1}{2}]$	[86,349]
87	$[-z, y + \frac{1}{2}, \frac{1}{4}]$	[87,245]
88	$[z, y + \frac{1}{2}, \frac{3}{4}]$	[88,244]
89	$[-z, \frac{1}{4}, \frac{1}{2} - y]$	[89,216]
90	$[-y, \frac{1}{2} - z, \frac{1}{4}]$	[90,261]
91	$[y, \frac{1}{2} - z, \frac{3}{4}]$	[91,263]
92	$[z, \frac{3}{4}, \frac{1}{2} - y]$	[92,214]
93	$[y, z + \frac{1}{2}, \frac{1}{4}]$	[93,258]

continued ...

Table 12

No.	position	mapping
94	$[-z, \frac{3}{4}, y + \frac{1}{2}]$	[94,212]
95	$[-y, z + \frac{1}{2}, \frac{3}{4}]$	[95,259]
96	$[z, \frac{1}{4}, y + \frac{1}{2}]$	[96,209]
97	$[\frac{3}{4}, y, z + \frac{1}{2}]$	[97,224]
98	$[\frac{3}{4}, -z, y + \frac{1}{2}]$	[98,219]
99	$[\frac{3}{4}, z, \frac{1}{2} - y]$	[99,218]
100	$[z + \frac{1}{2}, y, \frac{1}{4}]$	[100,328]
101	$[\frac{1}{2} - z, y, \frac{3}{4}]$	[101,327]
102	$[\frac{1}{2} - y, \frac{1}{4}, z + \frac{1}{2}]$	[102,371]
103	$[y + \frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}]$	[103,372]
104	$[\frac{3}{4}, -y, \frac{1}{2} - z]$	[104,217]
105	$[\frac{1}{4}, y, \frac{1}{2} - z]$	[105,226]
106	$[\frac{1}{4}, -y, z + \frac{1}{2}]$	[106,225]
107	$[y + \frac{1}{2}, \frac{1}{4}, \frac{1}{2} - z]$	[107,366]
108	$[\frac{1}{2} - y, \frac{3}{4}, \frac{1}{2} - z]$	[108,367]
109	$[\frac{1}{4}, z, y + \frac{1}{2}]$	[109,230]
110	$[\frac{1}{4}, -z, \frac{1}{2} - y]$	[110,229]
111	$[z + \frac{1}{2}, -y, \frac{3}{4}]$	[111,317]
112	$[\frac{1}{2} - z, -y, \frac{1}{4}]$	[112,316]
113	$[z + \frac{1}{2}, \frac{1}{4}, y + \frac{1}{2}]$	[113,384]
114	$[y + \frac{1}{2}, z, \frac{3}{4}]$	[114,333]
115	$[\frac{1}{2} - y, z, \frac{1}{4}]$	[115,335]
116	$[\frac{1}{2} - z, \frac{3}{4}, y + \frac{1}{2}]$	[116,382]
117	$[\frac{1}{2} - y, -z, \frac{3}{4}]$	[117,330]
118	$[z + \frac{1}{2}, \frac{3}{4}, \frac{1}{2} - y]$	[118,380]
119	$[y + \frac{1}{2}, -z, \frac{1}{4}]$	[119,331]
120	$[\frac{1}{2} - z, \frac{1}{4}, \frac{1}{2} - y]$	[120,377]
121	$[\frac{1}{4}, -y, \frac{1}{2} - z]$	[121,200]
122	$[\frac{1}{4}, z, \frac{1}{2} - y]$	[122,195]
123	$[\frac{1}{4}, -z, y + \frac{1}{2}]$	[123,194]
124	$[\frac{1}{2} - z, -y, \frac{3}{4}]$	[124,304]
125	$[z + \frac{1}{2}, -y, \frac{1}{4}]$	[125,303]
126	$[y + \frac{1}{2}, \frac{3}{4}, \frac{1}{2} - z]$	[126,347]
127	$[\frac{1}{2} - y, \frac{1}{4}, \frac{1}{2} - z]$	[127,348]
128	$[\frac{1}{4}, y, z + \frac{1}{2}]$	[128,193]
129	$[\frac{3}{4}, -y, z + \frac{1}{2}]$	[129,202]
130	$[\frac{3}{4}, y, \frac{1}{2} - z]$	[130,201]
131	$[\frac{1}{2} - y, \frac{3}{4}, z + \frac{1}{2}]$	[131,342]
132	$[y + \frac{1}{2}, \frac{1}{4}, z + \frac{1}{2}]$	[132,343]
133	$[\frac{3}{4}, -z, \frac{1}{2} - y]$	[133,206]
134	$[\frac{3}{4}, z, y + \frac{1}{2}]$	[134,205]
135	$[\frac{1}{2} - z, y, \frac{1}{4}]$	[135,293]
136	$[z + \frac{1}{2}, y, \frac{3}{4}]$	[136,292]
137	$[\frac{1}{2} - z, \frac{3}{4}, \frac{1}{2} - y]$	[137,360]
138	$[\frac{1}{2} - y, -z, \frac{1}{4}]$	[138,309]
139	$[y + \frac{1}{2}, -z, \frac{3}{4}]$	[139,311]
140	$[z + \frac{1}{2}, \frac{1}{4}, \frac{1}{2} - y]$	[140,358]

continued ...

Table 12

No.	position	mapping
141	$[y + \frac{1}{2}, z, \frac{1}{4}]$	[141,306]
142	$[\frac{1}{2} - z, \frac{1}{4}, y + \frac{1}{2}]$	[142,356]
143	$[\frac{1}{2} - y, z, \frac{3}{4}]$	[143,307]
144	$[z + \frac{1}{2}, \frac{3}{4}, y + \frac{1}{2}]$	[144,353]
145	$[\frac{3}{4}, y + \frac{1}{2}, z]$	[145,272]
146	$[\frac{3}{4}, \frac{1}{2} - z, y]$	[146,267]
147	$[\frac{3}{4}, z + \frac{1}{2}, -y]$	[147,266]
148	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$	[148,376]
149	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{4}]$	[149,375]
150	$[\frac{1}{2} - y, \frac{3}{4}, z]$	[150,323]
151	$[y + \frac{1}{2}, \frac{1}{4}, z]$	[151,324]
152	$[\frac{3}{4}, \frac{1}{2} - y, -z]$	[152,265]
153	$[\frac{1}{4}, y + \frac{1}{2}, -z]$	[153,274]
154	$[\frac{1}{4}, \frac{1}{2} - y, z]$	[154,273]
155	$[y + \frac{1}{2}, \frac{3}{4}, -z]$	[155,318]
156	$[\frac{1}{2} - y, \frac{1}{4}, -z]$	[156,319]
157	$[\frac{1}{4}, z + \frac{1}{2}, y]$	[157,278]
158	$[\frac{1}{4}, \frac{1}{2} - z, -y]$	[158,277]
159	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{4}]$	[159,365]
160	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{3}{4}]$	[160,364]
161	$[z + \frac{1}{2}, \frac{3}{4}, y]$	[161,336]
162	$[y + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{4}]$	[162,381]
163	$[\frac{1}{2} - y, z + \frac{1}{2}, \frac{3}{4}]$	[163,383]
164	$[\frac{1}{2} - z, \frac{1}{4}, y]$	[164,334]
165	$[\frac{1}{2} - y, \frac{1}{2} - z, \frac{1}{4}]$	[165,378]
166	$[z + \frac{1}{2}, \frac{1}{4}, -y]$	[166,332]
167	$[y + \frac{1}{2}, \frac{1}{2} - z, \frac{3}{4}]$	[167,379]
168	$[\frac{1}{2} - z, \frac{3}{4}, -y]$	[168,329]
169	$[\frac{1}{4}, \frac{1}{2} - y, -z]$	[169,248]
170	$[\frac{1}{4}, z + \frac{1}{2}, -y]$	[170,243]
171	$[\frac{1}{4}, \frac{1}{2} - z, y]$	[171,242]
172	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{4}]$	[172,352]
173	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{3}{4}]$	[173,351]
174	$[y + \frac{1}{2}, \frac{1}{4}, -z]$	[174,299]
175	$[\frac{1}{2} - y, \frac{3}{4}, -z]$	[175,300]
176	$[\frac{1}{4}, y + \frac{1}{2}, z]$	[176,241]
177	$[\frac{3}{4}, \frac{1}{2} - y, z]$	[177,250]
178	$[\frac{3}{4}, y + \frac{1}{2}, -z]$	[178,249]
179	$[\frac{1}{2} - y, \frac{1}{4}, z]$	[179,294]
180	$[y + \frac{1}{2}, \frac{3}{4}, z]$	[180,295]
181	$[\frac{3}{4}, \frac{1}{2} - z, -y]$	[181,254]
182	$[\frac{3}{4}, z + \frac{1}{2}, y]$	[182,253]
183	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{3}{4}]$	[183,341]
184	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{4}]$	[184,340]
185	$[\frac{1}{2} - z, \frac{1}{4}, -y]$	[185,312]
186	$[\frac{1}{2} - y, \frac{1}{2} - z, \frac{3}{4}]$	[186,357]
187	$[y + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{4}]$	[187,359]

continued ...

Table 12

No.	position	mapping
188	$[z + \frac{1}{2}, \frac{3}{4}, -y]$	[188,310]
189	$[y + \frac{1}{2}, z + \frac{1}{2}, \frac{3}{4}]$	[189,354]
190	$[\frac{1}{2} - z, \frac{3}{4}, y]$	[190,308]
191	$[\frac{1}{2} - y, z + \frac{1}{2}, \frac{1}{4}]$	[191,355]
192	$[z + \frac{1}{2}, \frac{1}{4}, y]$	[192,305]

Table 13: Wyckoff site: 192m, 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]
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]

continued ...

Table 13

No.	position	mapping
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]
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]

continued ...

Table 13

No.	position	mapping
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]
97	$[x, x, z + \frac{1}{2}]$	[193, 228]
98	$[x, -z, x + \frac{1}{2}]$	[194, 235]
99	$[x, z, \frac{1}{2} - x]$	[195, 237]
100	$[z, x, \frac{1}{2} - x]$	[196, 236]
101	$[-z, x, x + \frac{1}{2}]$	[197, 238]
102	$[-x, x, z + \frac{1}{2}]$	[198, 224]
103	$[x, -x, z + \frac{1}{2}]$	[199, 225]
104	$[x, -x, \frac{1}{2} - z]$	[200, 222]
105	$[-x, x, \frac{1}{2} - z]$	[201, 223]
106	$[-x, -x, z + \frac{1}{2}]$	[202, 227]
107	$[x, x, \frac{1}{2} - z]$	[203, 226]
108	$[-x, -x, \frac{1}{2} - z]$	[204, 217]
109	$[-x, z, x + \frac{1}{2}]$	[205, 239]
110	$[-x, -z, \frac{1}{2} - x]$	[206, 234]
111	$[z, -x, x + \frac{1}{2}]$	[207, 240]
112	$[-z, -x, \frac{1}{2} - x]$	[208, 233]
113	$[z, x, x + \frac{1}{2}]$	[209, 232]
114	$[x, z, x + \frac{1}{2}]$	[210, 230]
115	$[-x, z, \frac{1}{2} - x]$	[211, 218]
116	$[-z, -x, x + \frac{1}{2}]$	[212, 220]
117	$[-x, -z, x + \frac{1}{2}]$	[213, 219]
118	$[z, -x, \frac{1}{2} - x]$	[214, 221]
119	$[x, -z, \frac{1}{2} - x]$	[215, 229]
120	$[-z, x, \frac{1}{2} - x]$	[216, 231]
121	$[x, x + \frac{1}{2}, z]$	[241, 276]
122	$[x, \frac{1}{2} - z, x]$	[242, 283]
123	$[x, z + \frac{1}{2}, -x]$	[243, 285]
124	$[z, x + \frac{1}{2}, -x]$	[244, 284]
125	$[-z, x + \frac{1}{2}, x]$	[245, 286]
126	$[-x, x + \frac{1}{2}, z]$	[246, 272]
127	$[x, \frac{1}{2} - x, z]$	[247, 273]
128	$[x, \frac{1}{2} - x, -z]$	[248, 270]
129	$[-x, x + \frac{1}{2}, -z]$	[249, 271]

continued ...

Table 13

No.	position	mapping
130	$[-x, \frac{1}{2} - x, z]$	[250, 275]
131	$[x, x + \frac{1}{2}, -z]$	[251, 274]
132	$[-x, \frac{1}{2} - x, -z]$	[252, 265]
133	$[-x, z + \frac{1}{2}, x]$	[253, 287]
134	$[-x, \frac{1}{2} - z, -x]$	[254, 282]
135	$[z, \frac{1}{2} - x, x]$	[255, 288]
136	$[-z, \frac{1}{2} - x, -x]$	[256, 281]
137	$[z, x + \frac{1}{2}, x]$	[257, 280]
138	$[x, z + \frac{1}{2}, x]$	[258, 278]
139	$[-x, z + \frac{1}{2}, -x]$	[259, 266]
140	$[-z, \frac{1}{2} - x, x]$	[260, 268]
141	$[-x, \frac{1}{2} - z, x]$	[261, 267]
142	$[z, \frac{1}{2} - x, -x]$	[262, 269]
143	$[x, \frac{1}{2} - z, -x]$	[263, 277]
144	$[-z, x + \frac{1}{2}, -x]$	[264, 279]
145	$[x + \frac{1}{2}, x, z]$	[289, 324]
146	$[x + \frac{1}{2}, -z, x]$	[290, 331]
147	$[x + \frac{1}{2}, z, -x]$	[291, 333]
148	$[z + \frac{1}{2}, x, -x]$	[292, 332]
149	$[\frac{1}{2} - z, x, x]$	[293, 334]
150	$[\frac{1}{2} - x, x, z]$	[294, 320]
151	$[x + \frac{1}{2}, -x, z]$	[295, 321]
152	$[x + \frac{1}{2}, -x, -z]$	[296, 318]
153	$[\frac{1}{2} - x, x, -z]$	[297, 319]
154	$[\frac{1}{2} - x, -x, z]$	[298, 323]
155	$[x + \frac{1}{2}, x, -z]$	[299, 322]
156	$[\frac{1}{2} - x, -x, -z]$	[300, 313]
157	$[\frac{1}{2} - x, z, x]$	[301, 335]
158	$[\frac{1}{2} - x, -z, -x]$	[302, 330]
159	$[z + \frac{1}{2}, -x, x]$	[303, 336]
160	$[\frac{1}{2} - z, -x, -x]$	[304, 329]
161	$[z + \frac{1}{2}, x, x]$	[305, 328]
162	$[x + \frac{1}{2}, z, x]$	[306, 326]
163	$[\frac{1}{2} - x, z, -x]$	[307, 314]
164	$[\frac{1}{2} - z, -x, x]$	[308, 316]
165	$[\frac{1}{2} - x, -z, x]$	[309, 315]
166	$[z + \frac{1}{2}, -x, -x]$	[310, 317]
167	$[x + \frac{1}{2}, -z, -x]$	[311, 325]
168	$[\frac{1}{2} - z, x, -x]$	[312, 327]
169	$[x + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[337, 372]
170	$[x + \frac{1}{2}, \frac{1}{2} - z, x + \frac{1}{2}]$	[338, 379]
171	$[x + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - x]$	[339, 381]
172	$[z + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - x]$	[340, 380]
173	$[\frac{1}{2} - z, x + \frac{1}{2}, x + \frac{1}{2}]$	[341, 382]
174	$[\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}]$	[342, 368]
175	$[x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[343, 369]
176	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[344, 366]

continued ...

Table 13

No.	position	mapping
177	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - z]$	[345, 367]
178	$[\frac{1}{2} - x, \frac{1}{2} - x, z + \frac{1}{2}]$	[346, 371]
179	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[347, 370]
180	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - z]$	[348, 361]
181	$[\frac{1}{2} - x, z + \frac{1}{2}, x + \frac{1}{2}]$	[349, 383]
182	$[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - x]$	[350, 378]
183	$[z + \frac{1}{2}, \frac{1}{2} - x, x + \frac{1}{2}]$	[351, 384]
184	$[\frac{1}{2} - z, \frac{1}{2} - x, \frac{1}{2} - x]$	[352, 377]
185	$[z + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[353, 376]
186	$[x + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}]$	[354, 374]
187	$[\frac{1}{2} - x, z + \frac{1}{2}, \frac{1}{2} - x]$	[355, 362]
188	$[\frac{1}{2} - z, \frac{1}{2} - x, x + \frac{1}{2}]$	[356, 364]
189	$[\frac{1}{2} - x, \frac{1}{2} - z, x + \frac{1}{2}]$	[357, 363]
190	$[z + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x]$	[358, 365]
191	$[x + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - x]$	[359, 373]
192	$[\frac{1}{2} - z, x + \frac{1}{2}, \frac{1}{2} - x]$	[360, 375]

Table 14: Wyckoff site: 384n, 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]

continued ...

Table 14

No.	position	mapping
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]
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]

continued ...

Table 14

No.	position	mapping
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]
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]

continued ...

Table 14

No.	position	mapping
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]
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]

continued ...

Table 14

No.	position	mapping
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]
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]
193	$[x, y, z + \frac{1}{2}]$	[193]
194	$[x, -z, y + \frac{1}{2}]$	[194]
195	$[x, z, \frac{1}{2} - y]$	[195]
196	$[z, y, \frac{1}{2} - x]$	[196]
197	$[-z, y, x + \frac{1}{2}]$	[197]
198	$[-y, x, z + \frac{1}{2}]$	[198]
199	$[y, -x, z + \frac{1}{2}]$	[199]
200	$[x, -y, \frac{1}{2} - z]$	[200]
201	$[-x, y, \frac{1}{2} - z]$	[201]
202	$[-x, -y, z + \frac{1}{2}]$	[202]
203	$[y, x, \frac{1}{2} - z]$	[203]
204	$[-y, -x, \frac{1}{2} - z]$	[204]
205	$[-x, z, y + \frac{1}{2}]$	[205]
206	$[-x, -z, \frac{1}{2} - y]$	[206]
207	$[z, -y, x + \frac{1}{2}]$	[207]
208	$[-z, -y, \frac{1}{2} - x]$	[208]
209	$[z, x, y + \frac{1}{2}]$	[209]
210	$[y, z, x + \frac{1}{2}]$	[210]
211	$[-y, z, \frac{1}{2} - x]$	[211]
212	$[-z, -x, y + \frac{1}{2}]$	[212]

continued ...

Table 14

No.	position	mapping
213	$[-y, -z, x + \frac{1}{2}]$	[213]
214	$[z, -x, \frac{1}{2} - y]$	[214]
215	$[y, -z, \frac{1}{2} - x]$	[215]
216	$[-z, x, \frac{1}{2} - y]$	[216]
217	$[-x, -y, \frac{1}{2} - z]$	[217]
218	$[-x, z, \frac{1}{2} - y]$	[218]
219	$[-x, -z, y + \frac{1}{2}]$	[219]
220	$[-z, -y, x + \frac{1}{2}]$	[220]
221	$[z, -y, \frac{1}{2} - x]$	[221]
222	$[y, -x, \frac{1}{2} - z]$	[222]
223	$[-y, x, \frac{1}{2} - z]$	[223]
224	$[-x, y, z + \frac{1}{2}]$	[224]
225	$[x, -y, z + \frac{1}{2}]$	[225]
226	$[x, y, \frac{1}{2} - z]$	[226]
227	$[-y, -x, z + \frac{1}{2}]$	[227]
228	$[y, x, z + \frac{1}{2}]$	[228]
229	$[x, -z, \frac{1}{2} - y]$	[229]
230	$[x, z, y + \frac{1}{2}]$	[230]
231	$[-z, y, \frac{1}{2} - x]$	[231]
232	$[z, y, x + \frac{1}{2}]$	[232]
233	$[-z, -x, \frac{1}{2} - y]$	[233]
234	$[-y, -z, \frac{1}{2} - x]$	[234]
235	$[y, -z, x + \frac{1}{2}]$	[235]
236	$[z, x, \frac{1}{2} - y]$	[236]
237	$[y, z, \frac{1}{2} - x]$	[237]
238	$[-z, x, y + \frac{1}{2}]$	[238]
239	$[-y, z, x + \frac{1}{2}]$	[239]
240	$[z, -x, y + \frac{1}{2}]$	[240]
241	$[x, y + \frac{1}{2}, z]$	[241]
242	$[x, \frac{1}{2} - z, y]$	[242]
243	$[x, z + \frac{1}{2}, -y]$	[243]
244	$[z, y + \frac{1}{2}, -x]$	[244]
245	$[-z, y + \frac{1}{2}, x]$	[245]
246	$[-y, x + \frac{1}{2}, z]$	[246]
247	$[y, \frac{1}{2} - x, z]$	[247]
248	$[x, \frac{1}{2} - y, -z]$	[248]
249	$[-x, y + \frac{1}{2}, -z]$	[249]
250	$[-x, \frac{1}{2} - y, z]$	[250]
251	$[y, x + \frac{1}{2}, -z]$	[251]
252	$[-y, \frac{1}{2} - x, -z]$	[252]
253	$[-x, z + \frac{1}{2}, y]$	[253]
254	$[-x, \frac{1}{2} - z, -y]$	[254]
255	$[z, \frac{1}{2} - y, x]$	[255]
256	$[-z, \frac{1}{2} - y, -x]$	[256]
257	$[z, x + \frac{1}{2}, y]$	[257]
258	$[y, z + \frac{1}{2}, x]$	[258]
259	$[-y, z + \frac{1}{2}, -x]$	[259]

continued ...

Table 14

No.	position	mapping
260	$[-z, \frac{1}{2} - x, y]$	[260]
261	$[-y, \frac{1}{2} - z, x]$	[261]
262	$[z, \frac{1}{2} - x, -y]$	[262]
263	$[y, \frac{1}{2} - z, -x]$	[263]
264	$[-z, x + \frac{1}{2}, -y]$	[264]
265	$[-x, \frac{1}{2} - y, -z]$	[265]
266	$[-x, z + \frac{1}{2}, -y]$	[266]
267	$[-x, \frac{1}{2} - z, y]$	[267]
268	$[-z, \frac{1}{2} - y, x]$	[268]
269	$[z, \frac{1}{2} - y, -x]$	[269]
270	$[y, \frac{1}{2} - x, -z]$	[270]
271	$[-y, x + \frac{1}{2}, -z]$	[271]
272	$[-x, y + \frac{1}{2}, z]$	[272]
273	$[x, \frac{1}{2} - y, z]$	[273]
274	$[x, y + \frac{1}{2}, -z]$	[274]
275	$[-y, \frac{1}{2} - x, z]$	[275]
276	$[y, x + \frac{1}{2}, z]$	[276]
277	$[x, \frac{1}{2} - z, -y]$	[277]
278	$[x, z + \frac{1}{2}, y]$	[278]
279	$[-z, y + \frac{1}{2}, -x]$	[279]
280	$[z, y + \frac{1}{2}, x]$	[280]
281	$[-z, \frac{1}{2} - x, -y]$	[281]
282	$[-y, \frac{1}{2} - z, -x]$	[282]
283	$[y, \frac{1}{2} - z, x]$	[283]
284	$[z, x + \frac{1}{2}, -y]$	[284]
285	$[y, z + \frac{1}{2}, -x]$	[285]
286	$[-z, x + \frac{1}{2}, y]$	[286]
287	$[-y, z + \frac{1}{2}, x]$	[287]
288	$[z, \frac{1}{2} - x, y]$	[288]
289	$[x + \frac{1}{2}, y, z]$	[289]
290	$[x + \frac{1}{2}, -z, y]$	[290]
291	$[x + \frac{1}{2}, z, -y]$	[291]
292	$[z + \frac{1}{2}, y, -x]$	[292]
293	$[\frac{1}{2} - z, y, x]$	[293]
294	$[\frac{1}{2} - y, x, z]$	[294]
295	$[y + \frac{1}{2}, -x, z]$	[295]
296	$[x + \frac{1}{2}, -y, -z]$	[296]
297	$[\frac{1}{2} - x, y, -z]$	[297]
298	$[\frac{1}{2} - x, -y, z]$	[298]
299	$[y + \frac{1}{2}, x, -z]$	[299]
300	$[\frac{1}{2} - y, -x, -z]$	[300]
301	$[\frac{1}{2} - x, z, y]$	[301]
302	$[\frac{1}{2} - x, -z, -y]$	[302]
303	$[z + \frac{1}{2}, -y, x]$	[303]
304	$[\frac{1}{2} - z, -y, -x]$	[304]
305	$[z + \frac{1}{2}, x, y]$	[305]
306	$[y + \frac{1}{2}, z, x]$	[306]

continued ...

Table 14

No.	position	mapping
307	$[\frac{1}{2} - y, z, -x]$	[307]
308	$[\frac{1}{2} - z, -x, y]$	[308]
309	$[\frac{1}{2} - y, -z, x]$	[309]
310	$[z + \frac{1}{2}, -x, -y]$	[310]
311	$[y + \frac{1}{2}, -z, -x]$	[311]
312	$[\frac{1}{2} - z, x, -y]$	[312]
313	$[\frac{1}{2} - x, -y, -z]$	[313]
314	$[\frac{1}{2} - x, z, -y]$	[314]
315	$[\frac{1}{2} - x, -z, y]$	[315]
316	$[\frac{1}{2} - z, -y, x]$	[316]
317	$[z + \frac{1}{2}, -y, -x]$	[317]
318	$[y + \frac{1}{2}, -x, -z]$	[318]
319	$[\frac{1}{2} - y, x, -z]$	[319]
320	$[\frac{1}{2} - x, y, z]$	[320]
321	$[x + \frac{1}{2}, -y, z]$	[321]
322	$[x + \frac{1}{2}, y, -z]$	[322]
323	$[\frac{1}{2} - y, -x, z]$	[323]
324	$[y + \frac{1}{2}, x, z]$	[324]
325	$[x + \frac{1}{2}, -z, -y]$	[325]
326	$[x + \frac{1}{2}, z, y]$	[326]
327	$[\frac{1}{2} - z, y, -x]$	[327]
328	$[z + \frac{1}{2}, y, x]$	[328]
329	$[\frac{1}{2} - z, -x, -y]$	[329]
330	$[\frac{1}{2} - y, -z, -x]$	[330]
331	$[y + \frac{1}{2}, -z, x]$	[331]
332	$[z + \frac{1}{2}, x, -y]$	[332]
333	$[y + \frac{1}{2}, z, -x]$	[333]
334	$[\frac{1}{2} - z, x, y]$	[334]
335	$[\frac{1}{2} - y, z, x]$	[335]
336	$[z + \frac{1}{2}, -x, y]$	[336]
337	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[337]
338	$[x + \frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[338]
339	$[x + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[339]
340	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - x]$	[340]
341	$[\frac{1}{2} - z, y + \frac{1}{2}, x + \frac{1}{2}]$	[341]
342	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[342]
343	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[343]
344	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[344]
345	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[345]
346	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[346]
347	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[347]
348	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[348]
349	$[\frac{1}{2} - x, z + \frac{1}{2}, y + \frac{1}{2}]$	[349]
350	$[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y]$	[350]
351	$[z + \frac{1}{2}, \frac{1}{2} - y, x + \frac{1}{2}]$	[351]
352	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2} - x]$	[352]
353	$[z + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}]$	[353]

continued ...

Table 14

No.	position	mapping
354	$[y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}]$	[354]
355	$[\frac{1}{2} - y, z + \frac{1}{2}, \frac{1}{2} - x]$	[355]
356	$[\frac{1}{2} - z, \frac{1}{2} - x, y + \frac{1}{2}]$	[356]
357	$[\frac{1}{2} - y, \frac{1}{2} - z, x + \frac{1}{2}]$	[357]
358	$[z + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - y]$	[358]
359	$[y + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - x]$	[359]
360	$[\frac{1}{2} - z, x + \frac{1}{2}, \frac{1}{2} - y]$	[360]
361	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[361]
362	$[\frac{1}{2} - x, z + \frac{1}{2}, \frac{1}{2} - y]$	[362]
363	$[\frac{1}{2} - x, \frac{1}{2} - z, y + \frac{1}{2}]$	[363]
364	$[\frac{1}{2} - z, \frac{1}{2} - y, x + \frac{1}{2}]$	[364]
365	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - x]$	[365]
366	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[366]
367	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[367]
368	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[368]
369	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[369]
370	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[370]
371	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[371]
372	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[372]
373	$[x + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[373]
374	$[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[374]
375	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2} - x]$	[375]
376	$[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}]$	[376]
377	$[\frac{1}{2} - z, \frac{1}{2} - x, \frac{1}{2} - y]$	[377]
378	$[\frac{1}{2} - y, \frac{1}{2} - z, \frac{1}{2} - x]$	[378]
379	$[y + \frac{1}{2}, \frac{1}{2} - z, x + \frac{1}{2}]$	[379]
380	$[z + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - y]$	[380]
381	$[y + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - x]$	[381]
382	$[\frac{1}{2} - z, x + \frac{1}{2}, y + \frac{1}{2}]$	[382]
383	$[\frac{1}{2} - y, z + \frac{1}{2}, x + \frac{1}{2}]$	[383]
384	$[z + \frac{1}{2}, \frac{1}{2} - x, y + \frac{1}{2}]$	[384]