

MSG No. 226.127 $F_5m\bar{3}c$ [Type IV, cubic]

Table 1: Wyckoff site: 8a, site symmetry: $m\bar{3}m'$

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

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, 12, 14, 16, 17, 18, 53, 54, 56, 61, 70, 71, 98, 103, 105, 111, 115, 120, 147, 148, 154, 155, 164, 165, 219, 220, 226, 227, 236, 237, 266, 271, 273, 279, 283, 288, 317, 318, 320, 325, 334, 335, 361, 372, 374, 376, 377, 378]
2	$[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}]$	[2, 7, 9, 15, 19, 24, 51, 52, 58, 59, 68, 69, 97, 108, 110, 112, 113, 114, 149, 150, 152, 157, 166, 167, 221, 222, 224, 229, 238, 239, 265, 276, 278, 280, 281, 282, 315, 316, 322, 323, 332, 333, 362, 367, 369, 375, 379, 384]
3	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}]$	[3, 4, 10, 11, 20, 21, 50, 55, 57, 63, 67, 72, 101, 102, 104, 109, 118, 119, 145, 156, 158, 160, 161, 162, 217, 228, 230, 232, 233, 234, 269, 270, 272, 277, 286, 287, 314, 319, 321, 327, 331, 336, 363, 364, 370, 371, 380, 381]
4	$[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}]$	[5, 6, 8, 13, 22, 23, 49, 60, 62, 64, 65, 66, 99, 100, 106, 107, 116, 117, 146, 151, 153, 159, 163, 168, 218, 223, 225, 231, 235, 240, 267, 268, 274, 275, 284, 285, 313, 324, 326, 328, 329, 330, 365, 366, 368, 373, 382, 383]
5	$[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}]$	[25, 36, 38, 40, 41, 42, 77, 78, 80, 85, 94, 95, 122, 127, 129, 135, 139, 144, 171, 172, 178, 179, 188, 189, 195, 196, 202, 203, 212, 213, 242, 247, 249, 255, 259, 264, 293, 294, 296, 301, 310, 311, 337, 348, 350, 352, 353, 354]
6	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}]$	[26, 31, 33, 39, 43, 48, 75, 76, 82, 83, 92, 93, 121, 132, 134, 136, 137, 138, 173, 174, 176, 181, 190, 191, 197, 198, 200, 205, 214, 215, 241, 252, 254, 256, 257, 258, 291, 292, 298, 299, 308, 309, 338, 343, 345, 351, 355, 360]
7	$[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}]$	[27, 28, 34, 35, 44, 45, 74, 79, 81, 87, 91, 96, 125, 126, 128, 133, 142, 143, 169, 180, 182, 184, 185, 186, 193, 204, 206, 208, 209, 210, 245, 246, 248, 253, 262, 263, 290, 295, 297, 303, 307, 312, 339, 340, 346, 347, 356, 357]
8	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}]$	[29, 30, 32, 37, 46, 47, 73, 84, 86, 88, 89, 90, 123, 124, 130, 131, 140, 141, 170, 175, 177, 183, 187, 192, 194, 199, 201, 207, 211, 216, 243, 244, 250, 251, 260, 261, 289, 300, 302, 304, 305, 306, 341, 342, 344, 349, 358, 359]

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

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

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

No.	position	mapping
1	$[\frac{1}{4}, 0, 0]$	[1, 8, 33, 34, 61, 62, 74, 75, 297, 298, 313, 320, 338, 339, 373, 374]
2	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}]$	[2, 3, 37, 38, 57, 58, 73, 80, 301, 302, 314, 315, 337, 344, 369, 370]
3	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[4, 16, 29, 39, 162, 165, 187, 191, 197, 207, 220, 232, 355, 359, 378, 381]
4	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[5, 15, 28, 40, 163, 167, 186, 189, 196, 208, 221, 231, 354, 357, 379, 383]
5	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{2}]$	[6, 11, 31, 36, 116, 118, 137, 144, 247, 252, 270, 275, 353, 360, 380, 382]
6	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2}]$	[7, 12, 30, 35, 113, 120, 140, 142, 246, 251, 271, 276, 356, 358, 377, 384]
7	$[\frac{3}{4}, 0, 0]$	[9, 10, 25, 32, 50, 51, 85, 86, 289, 296, 321, 322, 349, 350, 362, 363]
8	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}]$	[13, 14, 26, 27, 49, 56, 81, 82, 290, 291, 325, 326, 345, 346, 361, 368]
9	$[0, \frac{1}{4}, 0]$	[17, 24, 44, 46, 103, 108, 126, 131, 260, 262, 281, 288, 342, 347, 367, 372]
10	$[0, 0, \frac{1}{4}]$	[18, 21, 43, 47, 148, 160, 173, 183, 211, 215, 234, 237, 341, 351, 364, 376]
11	$[0, 0, \frac{3}{4}]$	[19, 23, 42, 45, 149, 159, 172, 184, 210, 213, 235, 239, 340, 352, 365, 375]
12	$[0, \frac{3}{4}, 0]$	[20, 22, 41, 48, 102, 107, 127, 132, 257, 264, 284, 286, 343, 348, 366, 371]
13	$[\frac{1}{2}, 0, \frac{3}{4}]$	[52, 64, 77, 87, 114, 117, 139, 143, 245, 255, 268, 280, 307, 311, 330, 333]
14	$[\frac{1}{2}, 0, \frac{1}{4}]$	[53, 63, 76, 88, 115, 119, 138, 141, 244, 256, 269, 279, 306, 309, 331, 335]
15	$[\frac{1}{2}, \frac{1}{4}, 0]$	[54, 59, 79, 84, 164, 166, 185, 192, 199, 204, 222, 227, 305, 312, 332, 334]

continued ...

Table 4

No.	position	mapping
16	$[\frac{1}{2}, \frac{3}{4}, 0]$	[55, 60, 78, 83, 161, 168, 188, 190, 198, 203, 223, 228, 308, 310, 329, 336]
17	$[0, \frac{3}{4}, \frac{1}{2}]$	[65, 72, 92, 94, 151, 156, 174, 179, 212, 214, 233, 240, 294, 299, 319, 324]
18	$[0, \frac{1}{2}, \frac{3}{4}]$	[66, 69, 91, 95, 100, 112, 125, 135, 259, 263, 282, 285, 293, 303, 316, 328]
19	$[0, \frac{1}{2}, \frac{1}{4}]$	[67, 71, 90, 93, 101, 111, 124, 136, 258, 261, 283, 287, 292, 304, 317, 327]
20	$[0, \frac{1}{4}, \frac{1}{2}]$	[68, 70, 89, 96, 150, 155, 175, 180, 209, 216, 236, 238, 295, 300, 318, 323]
21	$[\frac{3}{4}, 0, \frac{1}{2}]$	[97, 104, 129, 130, 157, 158, 170, 171, 201, 202, 217, 224, 242, 243, 277, 278]
22	$[\frac{1}{4}, \frac{1}{2}, 0]$	[98, 99, 133, 134, 153, 154, 169, 176, 205, 206, 218, 219, 241, 248, 273, 274]
23	$[\frac{1}{4}, 0, \frac{1}{2}]$	[105, 106, 121, 128, 146, 147, 181, 182, 193, 200, 225, 226, 253, 254, 266, 267]
24	$[\frac{3}{4}, \frac{1}{2}, 0]$	[109, 110, 122, 123, 145, 152, 177, 178, 194, 195, 229, 230, 249, 250, 265, 272]

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

No.	position	mapping
1	$[x, 0, 0]$	[1, 8, 33, 34, 338, 339, 373, 374]
2	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[2, 3, 37, 38, 337, 344, 369, 370]
3	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	[4, 16, 29, 39, 355, 359, 378, 381]
4	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	[5, 15, 28, 40, 354, 357, 379, 383]
5	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[6, 11, 31, 36, 353, 360, 380, 382]
6	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[7, 12, 30, 35, 356, 358, 377, 384]
7	$[-x, 0, 0]$	[9, 10, 25, 32, 349, 350, 362, 363]
8	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[13, 14, 26, 27, 345, 346, 361, 368]
9	$[0, x, 0]$	[17, 24, 44, 46, 342, 347, 367, 372]
10	$[0, 0, x]$	[18, 21, 43, 47, 341, 351, 364, 376]
11	$[0, 0, -x]$	[19, 23, 42, 45, 340, 352, 365, 375]
12	$[0, -x, 0]$	[20, 22, 41, 48, 343, 348, 366, 371]
13	$[x, \frac{1}{2}, \frac{1}{2}]$	[49, 56, 81, 82, 290, 291, 325, 326]
14	$[x + \frac{1}{2}, 0, 0]$	[50, 51, 85, 86, 289, 296, 321, 322]
15	$[\frac{1}{2}, 0, -x]$	[52, 64, 77, 87, 307, 311, 330, 333]
16	$[\frac{1}{2}, 0, x]$	[53, 63, 76, 88, 306, 309, 331, 335]
17	$[\frac{1}{2}, x, 0]$	[54, 59, 79, 84, 305, 312, 332, 334]
18	$[\frac{1}{2}, -x, 0]$	[55, 60, 78, 83, 308, 310, 329, 336]
19	$[-x, \frac{1}{2}, \frac{1}{2}]$	[57, 58, 73, 80, 301, 302, 314, 315]
20	$[\frac{1}{2} - x, 0, 0]$	[61, 62, 74, 75, 297, 298, 313, 320]
21	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[65, 72, 92, 94, 294, 299, 319, 324]
22	$[0, \frac{1}{2}, x + \frac{1}{2}]$	[66, 69, 91, 95, 293, 303, 316, 328]
23	$[0, \frac{1}{2}, \frac{1}{2} - x]$	[67, 71, 90, 93, 292, 304, 317, 327]
24	$[0, \frac{1}{2} - x, \frac{1}{2}]$	[68, 70, 89, 96, 295, 300, 318, 323]
25	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	[97, 104, 129, 130, 242, 243, 277, 278]
26	$[x, \frac{1}{2}, 0]$	[98, 99, 133, 134, 241, 248, 273, 274]
27	$[0, \frac{1}{2}, -x]$	[100, 112, 125, 135, 259, 263, 282, 285]
28	$[0, \frac{1}{2}, x]$	[101, 111, 124, 136, 258, 261, 283, 287]
29	$[0, x + \frac{1}{2}, 0]$	[102, 107, 127, 132, 257, 264, 284, 286]
30	$[0, \frac{1}{2} - x, 0]$	[103, 108, 126, 131, 260, 262, 281, 288]
31	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[105, 106, 121, 128, 253, 254, 266, 267]

continued ...

Table 5

No.	position	mapping
32	$[-x, \frac{1}{2}, 0]$	[109, 110, 122, 123, 249, 250, 265, 272]
33	$[\frac{1}{2}, x, \frac{1}{2}]$	[113, 120, 140, 142, 246, 251, 271, 276]
34	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[114, 117, 139, 143, 245, 255, 268, 280]
35	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[115, 119, 138, 141, 244, 256, 269, 279]
36	$[\frac{1}{2}, -x, \frac{1}{2}]$	[116, 118, 137, 144, 247, 252, 270, 275]
37	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[145, 152, 177, 178, 194, 195, 229, 230]
38	$[x, 0, \frac{1}{2}]$	[146, 147, 181, 182, 193, 200, 225, 226]
39	$[0, 0, \frac{1}{2} - x]$	[148, 160, 173, 183, 211, 215, 234, 237]
40	$[0, 0, x + \frac{1}{2}]$	[149, 159, 172, 184, 210, 213, 235, 239]
41	$[0, x, \frac{1}{2}]$	[150, 155, 175, 180, 209, 216, 236, 238]
42	$[0, -x, \frac{1}{2}]$	[151, 156, 174, 179, 212, 214, 233, 240]
43	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[153, 154, 169, 176, 205, 206, 218, 219]
44	$[-x, 0, \frac{1}{2}]$	[157, 158, 170, 171, 201, 202, 217, 224]
45	$[\frac{1}{2}, x + \frac{1}{2}, 0]$	[161, 168, 188, 190, 198, 203, 223, 228]
46	$[\frac{1}{2}, \frac{1}{2}, x]$	[162, 165, 187, 191, 197, 207, 220, 232]
47	$[\frac{1}{2}, \frac{1}{2}, -x]$	[163, 167, 186, 189, 196, 208, 221, 231]
48	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	[164, 166, 185, 192, 199, 204, 222, 227]

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

No.	position	mapping
1	$[x, \frac{1}{4}, \frac{1}{4}]$	[1, 56, 98, 147, 226, 273, 325, 374]
2	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[2, 51, 97, 152, 229, 278, 322, 369]
3	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[3, 50, 104, 145, 230, 277, 321, 370]
4	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[4, 67, 119, 160, 234, 269, 327, 381]
5	$[\frac{1}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[5, 66, 117, 159, 235, 268, 328, 383]
6	$[\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[6, 65, 107, 168, 223, 284, 324, 382]
7	$[\frac{3}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[7, 68, 108, 166, 222, 281, 323, 384]
8	$[x, \frac{3}{4}, \frac{3}{4}]$	[8, 49, 99, 146, 225, 274, 326, 373]
9	$[-x, \frac{1}{4}, \frac{3}{4}]$	[9, 58, 110, 157, 224, 265, 315, 362]
10	$[-x, \frac{3}{4}, \frac{1}{4}]$	[10, 57, 109, 158, 217, 272, 314, 363]
11	$[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[11, 72, 102, 161, 228, 286, 319, 380]
12	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[12, 70, 103, 164, 227, 288, 318, 377]
13	$[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$	[13, 62, 106, 153, 218, 267, 313, 368]
14	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[14, 61, 105, 154, 219, 266, 320, 361]
15	$[\frac{3}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[15, 69, 114, 149, 239, 280, 316, 379]
16	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[16, 71, 115, 148, 237, 279, 317, 378]
17	$[\frac{1}{4}, x, \frac{1}{4}]$	[17, 54, 120, 155, 236, 271, 334, 372]
18	$[\frac{1}{4}, \frac{1}{4}, x]$	[18, 53, 111, 165, 220, 283, 335, 376]
19	$[\frac{3}{4}, \frac{1}{4}, -x]$	[19, 52, 112, 167, 221, 282, 333, 375]
20	$[\frac{3}{4}, -x, \frac{1}{4}]$	[20, 55, 118, 156, 233, 270, 336, 371]
21	$[\frac{3}{4}, \frac{3}{4}, x]$	[21, 63, 101, 162, 232, 287, 331, 364]
22	$[\frac{1}{4}, -x, \frac{3}{4}]$	[22, 60, 116, 151, 240, 275, 329, 366]
23	$[\frac{1}{4}, \frac{3}{4}, -x]$	[23, 64, 100, 163, 231, 285, 330, 365]

continued ...

Table 6

No.	position	mapping
24	$[\frac{3}{4}, x, \frac{3}{4}]$	[24, 59, 113, 150, 238, 276, 332, 367]
25	$[-x, \frac{3}{4}, \frac{3}{4}]$	[25, 80, 122, 171, 202, 249, 301, 350]
26	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]$	[26, 75, 121, 176, 205, 254, 298, 345]
27	$[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$	[27, 74, 128, 169, 206, 253, 297, 346]
28	$[\frac{1}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[28, 91, 143, 184, 210, 245, 303, 357]
29	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[29, 90, 141, 183, 211, 244, 304, 359]
30	$[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[30, 89, 131, 192, 199, 260, 300, 358]
31	$[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[31, 92, 132, 190, 198, 257, 299, 360]
32	$[-x, \frac{1}{4}, \frac{1}{4}]$	[32, 73, 123, 170, 201, 250, 302, 349]
33	$[x, \frac{3}{4}, \frac{1}{4}]$	[33, 82, 134, 181, 200, 241, 291, 338]
34	$[x, \frac{1}{4}, \frac{3}{4}]$	[34, 81, 133, 182, 193, 248, 290, 339]
35	$[\frac{1}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[35, 96, 126, 185, 204, 262, 295, 356]
36	$[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[36, 94, 127, 188, 203, 264, 294, 353]
37	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[37, 86, 130, 177, 194, 243, 289, 344]
38	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[38, 85, 129, 178, 195, 242, 296, 337]
39	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[39, 93, 138, 173, 215, 256, 292, 355]
40	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[40, 95, 139, 172, 213, 255, 293, 354]
41	$[\frac{3}{4}, -x, \frac{3}{4}]$	[41, 78, 144, 179, 212, 247, 310, 348]
42	$[\frac{3}{4}, \frac{3}{4}, -x]$	[42, 77, 135, 189, 196, 259, 311, 352]
43	$[\frac{1}{4}, \frac{3}{4}, x]$	[43, 76, 136, 191, 197, 258, 309, 351]
44	$[\frac{1}{4}, x, \frac{3}{4}]$	[44, 79, 142, 180, 209, 246, 312, 347]
45	$[\frac{1}{4}, \frac{1}{4}, -x]$	[45, 87, 125, 186, 208, 263, 307, 340]
46	$[\frac{3}{4}, x, \frac{1}{4}]$	[46, 84, 140, 175, 216, 251, 305, 342]
47	$[\frac{3}{4}, \frac{1}{4}, x]$	[47, 88, 124, 187, 207, 261, 306, 341]
48	$[\frac{1}{4}, -x, \frac{1}{4}]$	[48, 83, 137, 174, 214, 252, 308, 343]

Table 7: Wyckoff site: $64g$, site symmetry: $.3m'$

No.	position	mapping
1	$[x, x, x]$	[1, 17, 18, 372, 374, 376]
2	$[x + \frac{1}{2}, \frac{1}{2} - x, x + \frac{1}{2}]$	[2, 7, 15, 369, 379, 384]
3	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - x]$	[3, 4, 11, 370, 380, 381]
4	$[\frac{1}{2} - x, x + \frac{1}{2}, x + \frac{1}{2}]$	[5, 6, 13, 368, 382, 383]
5	$[x, -x, -x]$	[8, 22, 23, 365, 366, 373]
6	$[-x, x, -x]$	[9, 19, 24, 362, 367, 375]
7	$[-x, -x, x]$	[10, 20, 21, 363, 364, 371]
8	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x]$	[12, 14, 16, 361, 377, 378]
9	$[-x, -x, -x]$	[25, 41, 42, 348, 350, 352]
10	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - x]$	[26, 31, 39, 345, 355, 360]
11	$[\frac{1}{2} - x, \frac{1}{2} - x, x + \frac{1}{2}]$	[27, 28, 35, 346, 356, 357]
12	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x]$	[29, 30, 37, 344, 358, 359]
13	$[-x, x, x]$	[32, 46, 47, 341, 342, 349]
14	$[x, -x, x]$	[33, 43, 48, 338, 343, 351]
15	$[x, x, -x]$	[34, 44, 45, 339, 340, 347]

continued ...

Table 7

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

continued ...

Table 7

No.	position	mapping
63	$[x + \frac{1}{2}, x + \frac{1}{2}, -x]$	[178, 188, 189, 195, 196, 203]
64	$[x, x, x + \frac{1}{2}]$	[180, 182, 184, 193, 209, 210]

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

No.	position	mapping
1	$[x, \frac{1}{4}, 0]$	[1, 34, 248, 273]
2	$[x + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[2, 38, 195, 229]
3	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[3, 37, 194, 230]
4	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{2} - x]$	[4, 39, 256, 269]
5	$[\frac{1}{2}, \frac{3}{4}, x + \frac{1}{2}]$	[5, 40, 255, 268]
6	$[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{2}]$	[6, 31, 299, 324]
7	$[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{2}]$	[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	$[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{2}]$	[11, 36, 294, 319]
12	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{2}]$	[12, 35, 295, 318]
13	$[\frac{1}{2} - x, \frac{1}{2}, \frac{3}{4}]$	[13, 27, 206, 218]
14	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{4}]$	[14, 26, 205, 219]
15	$[\frac{1}{2}, \frac{1}{4}, x + \frac{1}{2}]$	[15, 28, 245, 280]
16	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2} - x]$	[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	$[x + \frac{1}{2}, 0, \frac{1}{4}]$	[50, 86, 243, 277]
27	$[x + \frac{1}{2}, 0, \frac{3}{4}]$	[51, 85, 242, 278]
28	$[\frac{1}{2}, \frac{1}{4}, -x]$	[52, 87, 208, 221]
29	$[\frac{1}{2}, \frac{1}{4}, x]$	[53, 88, 207, 220]
30	$[\frac{1}{4}, x, 0]$	[54, 79, 347, 372]
31	$[\frac{3}{4}, -x, 0]$	[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	$[\frac{3}{4}, x, 0]$	[59, 84, 342, 367]
36	$[\frac{1}{4}, -x, 0]$	[60, 83, 343, 366]
37	$[\frac{1}{2} - x, 0, \frac{1}{4}]$	[61, 75, 254, 266]
38	$[\frac{1}{2} - x, 0, \frac{3}{4}]$	[62, 74, 253, 267]

continued ...

Table 8

No.	position	mapping
39	$[\frac{1}{2}, \frac{3}{4}, x]$	[63, 76, 197, 232]
40	$[\frac{1}{2}, \frac{3}{4}, -x]$	[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	$[x, \frac{1}{2}, \frac{1}{4}]$	[98, 134, 291, 325]
51	$[x, \frac{1}{2}, \frac{3}{4}]$	[99, 133, 290, 326]
52	$[0, \frac{3}{4}, -x]$	[100, 135, 352, 365]
53	$[0, \frac{3}{4}, x]$	[101, 136, 351, 364]
54	$[\frac{3}{4}, x + \frac{1}{2}, 0]$	[102, 127, 203, 228]
55	$[\frac{1}{4}, \frac{1}{2} - x, 0]$	[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	$[\frac{1}{4}, x + \frac{1}{2}, 0]$	[107, 132, 198, 223]
60	$[\frac{3}{4}, \frac{1}{2} - x, 0]$	[108, 131, 199, 222]
61	$[-x, \frac{1}{2}, \frac{1}{4}]$	[109, 123, 302, 314]
62	$[-x, \frac{1}{2}, \frac{3}{4}]$	[110, 122, 301, 315]
63	$[0, \frac{1}{4}, x]$	[111, 124, 341, 376]
64	$[0, \frac{1}{4}, -x]$	[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	$[x, 0, \frac{3}{4}]$	[146, 182, 339, 373]
75	$[x, 0, \frac{1}{4}]$	[147, 181, 338, 374]
76	$[0, \frac{1}{4}, \frac{1}{2} - x]$	[148, 183, 304, 317]
77	$[0, \frac{1}{4}, x + \frac{1}{2}]$	[149, 184, 303, 316]
78	$[\frac{3}{4}, x, \frac{1}{2}]$	[150, 175, 251, 276]
79	$[\frac{1}{4}, -x, \frac{1}{2}]$	[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	$[\frac{1}{4}, x, \frac{1}{2}]$	[155, 180, 246, 271]
84	$[\frac{3}{4}, -x, \frac{1}{2}]$	[156, 179, 247, 270]
85	$[-x, 0, \frac{3}{4}]$	[157, 171, 350, 362]

continued ...

Table 8

No.	position	mapping
86	$[-x, 0, \frac{1}{4}]$	[158, 170, 349, 363]
87	$[0, \frac{3}{4}, x + \frac{1}{2}]$	[159, 172, 293, 328]
88	$[0, \frac{3}{4}, \frac{1}{2} - x]$	[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: $m.2'm'$

No.	position	mapping
1	$[0, y, y]$	[1, 32, 349, 374]
2	$[\frac{1}{2}, \frac{1}{2} - y, y + \frac{1}{2}]$	[2, 27, 346, 369]
3	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - y]$	[3, 26, 345, 370]
4	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[4, 40, 354, 381]
5	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{2}]$	[5, 39, 355, 383]
6	$[\frac{1}{2} - y, \frac{1}{2}, y + \frac{1}{2}]$	[6, 35, 356, 382]
7	$[y + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}]$	[7, 36, 353, 384]
8	$[0, -y, -y]$	[8, 25, 350, 373]
9	$[0, y, -y]$	[9, 34, 339, 362]
10	$[0, -y, y]$	[10, 33, 338, 363]
11	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - y]$	[11, 30, 358, 380]
12	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - y]$	[12, 31, 360, 377]
13	$[\frac{1}{2}, y + \frac{1}{2}, y + \frac{1}{2}]$	[13, 38, 337, 368]
14	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - y]$	[14, 37, 344, 361]
15	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[15, 29, 359, 379]
16	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{2}]$	[16, 28, 357, 378]
17	$[y, 0, y]$	[17, 48, 343, 372]
18	$[y, y, 0]$	[18, 45, 340, 376]
19	$[-y, y, 0]$	[19, 47, 341, 375]
20	$[-y, 0, y]$	[20, 46, 342, 371]
21	$[-y, -y, 0]$	[21, 42, 352, 364]
22	$[y, 0, -y]$	[22, 44, 347, 366]
23	$[y, -y, 0]$	[23, 43, 351, 365]
24	$[-y, 0, -y]$	[24, 41, 348, 367]
25	$[0, y + \frac{1}{2}, y + \frac{1}{2}]$	[49, 80, 301, 326]
26	$[\frac{1}{2}, -y, y]$	[50, 75, 298, 321]
27	$[\frac{1}{2}, y, -y]$	[51, 74, 297, 322]
28	$[y + \frac{1}{2}, y, 0]$	[52, 88, 306, 333]
29	$[\frac{1}{2} - y, y, 0]$	[53, 87, 307, 335]

continued ...

Table 9

No.	position	mapping
30	$[\frac{1}{2} - y, 0, y]$	[54, 83, 308, 334]
31	$[y + \frac{1}{2}, 0, y]$	[55, 84, 305, 336]
32	$[0, \frac{1}{2} - y, \frac{1}{2} - y]$	[56, 73, 302, 325]
33	$[0, y + \frac{1}{2}, \frac{1}{2} - y]$	[57, 82, 291, 314]
34	$[0, \frac{1}{2} - y, y + \frac{1}{2}]$	[58, 81, 290, 315]
35	$[y + \frac{1}{2}, 0, -y]$	[59, 78, 310, 332]
36	$[\frac{1}{2} - y, 0, -y]$	[60, 79, 312, 329]
37	$[\frac{1}{2}, y, y]$	[61, 86, 289, 320]
38	$[\frac{1}{2}, -y, -y]$	[62, 85, 296, 313]
39	$[y + \frac{1}{2}, -y, 0]$	[63, 77, 311, 331]
40	$[\frac{1}{2} - y, -y, 0]$	[64, 76, 309, 330]
41	$[y, \frac{1}{2}, y + \frac{1}{2}]$	[65, 96, 295, 324]
42	$[y, y + \frac{1}{2}, \frac{1}{2}]$	[66, 93, 292, 328]
43	$[-y, y + \frac{1}{2}, \frac{1}{2}]$	[67, 95, 293, 327]
44	$[-y, \frac{1}{2}, y + \frac{1}{2}]$	[68, 94, 294, 323]
45	$[-y, \frac{1}{2} - y, \frac{1}{2}]$	[69, 90, 304, 316]
46	$[y, \frac{1}{2}, \frac{1}{2} - y]$	[70, 92, 299, 318]
47	$[y, \frac{1}{2} - y, \frac{1}{2}]$	[71, 91, 303, 317]
48	$[-y, \frac{1}{2}, \frac{1}{2} - y]$	[72, 89, 300, 319]
49	$[\frac{1}{2}, y, y + \frac{1}{2}]$	[97, 128, 253, 278]
50	$[0, \frac{1}{2} - y, y]$	[98, 123, 250, 273]
51	$[0, y + \frac{1}{2}, -y]$	[99, 122, 249, 274]
52	$[y, y + \frac{1}{2}, 0]$	[100, 136, 258, 285]
53	$[-y, y + \frac{1}{2}, 0]$	[101, 135, 259, 287]
54	$[-y, \frac{1}{2}, y]$	[102, 131, 260, 286]
55	$[y, \frac{1}{2}, y]$	[103, 132, 257, 288]
56	$[\frac{1}{2}, -y, \frac{1}{2} - y]$	[104, 121, 254, 277]
57	$[\frac{1}{2}, y, \frac{1}{2} - y]$	[105, 130, 243, 266]
58	$[\frac{1}{2}, -y, y + \frac{1}{2}]$	[106, 129, 242, 267]
59	$[y, \frac{1}{2}, -y]$	[107, 126, 262, 284]
60	$[-y, \frac{1}{2}, -y]$	[108, 127, 264, 281]
61	$[0, y + \frac{1}{2}, y]$	[109, 134, 241, 272]
62	$[0, \frac{1}{2} - y, -y]$	[110, 133, 248, 265]
63	$[y, \frac{1}{2} - y, 0]$	[111, 125, 263, 283]
64	$[-y, \frac{1}{2} - y, 0]$	[112, 124, 261, 282]
65	$[y + \frac{1}{2}, 0, y + \frac{1}{2}]$	[113, 144, 247, 276]
66	$[y + \frac{1}{2}, y, \frac{1}{2}]$	[114, 141, 244, 280]
67	$[\frac{1}{2} - y, y, \frac{1}{2}]$	[115, 143, 245, 279]
68	$[\frac{1}{2} - y, 0, y + \frac{1}{2}]$	[116, 142, 246, 275]
69	$[\frac{1}{2} - y, -y, \frac{1}{2}]$	[117, 138, 256, 268]
70	$[y + \frac{1}{2}, 0, \frac{1}{2} - y]$	[118, 140, 251, 270]
71	$[y + \frac{1}{2}, -y, \frac{1}{2}]$	[119, 139, 255, 269]
72	$[\frac{1}{2} - y, 0, \frac{1}{2} - y]$	[120, 137, 252, 271]
73	$[\frac{1}{2}, y + \frac{1}{2}, y]$	[145, 176, 205, 230]
74	$[0, -y, y + \frac{1}{2}]$	[146, 171, 202, 225]
75	$[0, y, \frac{1}{2} - y]$	[147, 170, 201, 226]
76	$[y, y, \frac{1}{2}]$	[148, 184, 210, 237]

continued ...

Table 9

No.	position	mapping
77	$[-y, y, \frac{1}{2}]$	[149, 183, 211, 239]
78	$[-y, 0, y + \frac{1}{2}]$	[150, 179, 212, 238]
79	$[y, 0, y + \frac{1}{2}]$	[151, 180, 209, 240]
80	$[\frac{1}{2}, \frac{1}{2} - y, -y]$	[152, 169, 206, 229]
81	$[\frac{1}{2}, y + \frac{1}{2}, -y]$	[153, 178, 195, 218]
82	$[\frac{1}{2}, \frac{1}{2} - y, y]$	[154, 177, 194, 219]
83	$[y, 0, \frac{1}{2} - y]$	[155, 174, 214, 236]
84	$[-y, 0, \frac{1}{2} - y]$	[156, 175, 216, 233]
85	$[0, y, y + \frac{1}{2}]$	[157, 182, 193, 224]
86	$[0, -y, \frac{1}{2} - y]$	[158, 181, 200, 217]
87	$[y, -y, \frac{1}{2}]$	[159, 173, 215, 235]
88	$[-y, -y, \frac{1}{2}]$	[160, 172, 213, 234]
89	$[y + \frac{1}{2}, \frac{1}{2}, y]$	[161, 192, 199, 228]
90	$[y + \frac{1}{2}, y + \frac{1}{2}, 0]$	[162, 189, 196, 232]
91	$[\frac{1}{2} - y, y + \frac{1}{2}, 0]$	[163, 191, 197, 231]
92	$[\frac{1}{2} - y, \frac{1}{2}, y]$	[164, 190, 198, 227]
93	$[\frac{1}{2} - y, \frac{1}{2} - y, 0]$	[165, 186, 208, 220]
94	$[y + \frac{1}{2}, \frac{1}{2}, -y]$	[166, 188, 203, 222]
95	$[y + \frac{1}{2}, \frac{1}{2} - y, 0]$	[167, 187, 207, 221]
96	$[\frac{1}{2} - y, \frac{1}{2}, -y]$	[168, 185, 204, 223]

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

No.	position	mapping
1	$[\frac{1}{4}, y, y]$	[1, 61, 320, 374]
2	$[\frac{3}{4}, \frac{1}{2} - y, y + \frac{1}{2}]$	[2, 58, 315, 369]
3	$[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{2} - y]$	[3, 57, 314, 370]
4	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{4}]$	[4, 162, 232, 381]
5	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{3}{4}]$	[5, 163, 231, 383]
6	$[\frac{1}{2} - y, \frac{3}{4}, y + \frac{1}{2}]$	[6, 116, 275, 382]
7	$[y + \frac{1}{2}, \frac{1}{4}, y + \frac{1}{2}]$	[7, 113, 276, 384]
8	$[\frac{1}{4}, -y, -y]$	[8, 62, 313, 373]
9	$[\frac{3}{4}, y, -y]$	[9, 51, 322, 362]
10	$[\frac{3}{4}, -y, y]$	[10, 50, 321, 363]
11	$[y + \frac{1}{2}, \frac{3}{4}, \frac{1}{2} - y]$	[11, 118, 270, 380]
12	$[\frac{1}{2} - y, \frac{1}{4}, \frac{1}{2} - y]$	[12, 120, 271, 377]
13	$[\frac{1}{4}, y + \frac{1}{2}, y + \frac{1}{2}]$	[13, 49, 326, 368]
14	$[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{2} - y]$	[14, 56, 325, 361]
15	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{3}{4}]$	[15, 167, 221, 379]
16	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{4}]$	[16, 165, 220, 378]
17	$[y, \frac{1}{4}, y]$	[17, 103, 288, 372]
18	$[y, y, \frac{1}{4}]$	[18, 148, 237, 376]
19	$[-y, y, \frac{3}{4}]$	[19, 149, 239, 375]
20	$[-y, \frac{3}{4}, y]$	[20, 102, 286, 371]

continued ...

Table 10

No.	position	mapping
21	$[-y, -y, \frac{1}{4}]$	[21, 160, 234, 364]
22	$[y, \frac{3}{4}, -y]$	[22, 107, 284, 366]
23	$[y, -y, \frac{3}{4}]$	[23, 159, 235, 365]
24	$[-y, \frac{1}{4}, -y]$	[24, 108, 281, 367]
25	$[\frac{3}{4}, -y, -y]$	[25, 85, 296, 350]
26	$[\frac{1}{4}, y + \frac{1}{2}, \frac{1}{2} - y]$	[26, 82, 291, 345]
27	$[\frac{1}{4}, \frac{1}{2} - y, y + \frac{1}{2}]$	[27, 81, 290, 346]
28	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{3}{4}]$	[28, 186, 208, 357]
29	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{4}]$	[29, 187, 207, 359]
30	$[y + \frac{1}{2}, \frac{1}{4}, \frac{1}{2} - y]$	[30, 140, 251, 358]
31	$[\frac{1}{2} - y, \frac{3}{4}, \frac{1}{2} - y]$	[31, 137, 252, 360]
32	$[\frac{3}{4}, y, y]$	[32, 86, 289, 349]
33	$[\frac{1}{4}, -y, y]$	[33, 75, 298, 338]
34	$[\frac{1}{4}, y, -y]$	[34, 74, 297, 339]
35	$[\frac{1}{2} - y, \frac{1}{4}, y + \frac{1}{2}]$	[35, 142, 246, 356]
36	$[y + \frac{1}{2}, \frac{3}{4}, y + \frac{1}{2}]$	[36, 144, 247, 353]
37	$[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{2} - y]$	[37, 73, 302, 344]
38	$[\frac{3}{4}, y + \frac{1}{2}, y + \frac{1}{2}]$	[38, 80, 301, 337]
39	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{4}]$	[39, 191, 197, 355]
40	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$	[40, 189, 196, 354]
41	$[-y, \frac{3}{4}, -y]$	[41, 127, 264, 348]
42	$[-y, -y, \frac{3}{4}]$	[42, 172, 213, 352]
43	$[y, -y, \frac{1}{4}]$	[43, 173, 215, 351]
44	$[y, \frac{1}{4}, -y]$	[44, 126, 262, 347]
45	$[y, y, \frac{3}{4}]$	[45, 184, 210, 340]
46	$[-y, \frac{1}{4}, y]$	[46, 131, 260, 342]
47	$[-y, y, \frac{1}{4}]$	[47, 183, 211, 341]
48	$[y, \frac{3}{4}, y]$	[48, 132, 257, 343]
49	$[y + \frac{1}{2}, y, \frac{3}{4}]$	[52, 114, 280, 333]
50	$[\frac{1}{2} - y, y, \frac{1}{4}]$	[53, 115, 279, 335]
51	$[\frac{1}{2} - y, \frac{1}{4}, y]$	[54, 164, 227, 334]
52	$[y + \frac{1}{2}, \frac{3}{4}, y]$	[55, 161, 228, 336]
53	$[y + \frac{1}{2}, \frac{1}{4}, -y]$	[59, 166, 222, 332]
54	$[\frac{1}{2} - y, \frac{3}{4}, -y]$	[60, 168, 223, 329]
55	$[y + \frac{1}{2}, -y, \frac{1}{4}]$	[63, 119, 269, 331]
56	$[\frac{1}{2} - y, -y, \frac{3}{4}]$	[64, 117, 268, 330]
57	$[y, \frac{3}{4}, y + \frac{1}{2}]$	[65, 151, 240, 324]
58	$[y, y + \frac{1}{2}, \frac{3}{4}]$	[66, 100, 285, 328]
59	$[-y, y + \frac{1}{2}, \frac{1}{4}]$	[67, 101, 287, 327]
60	$[-y, \frac{1}{4}, y + \frac{1}{2}]$	[68, 150, 238, 323]
61	$[-y, \frac{1}{2} - y, \frac{3}{4}]$	[69, 112, 282, 316]
62	$[y, \frac{1}{4}, \frac{1}{2} - y]$	[70, 155, 236, 318]
63	$[y, \frac{1}{2} - y, \frac{1}{4}]$	[71, 111, 283, 317]
64	$[-y, \frac{3}{4}, \frac{1}{2} - y]$	[72, 156, 233, 319]
65	$[\frac{1}{2} - y, -y, \frac{1}{4}]$	[76, 138, 256, 309]
66	$[y + \frac{1}{2}, -y, \frac{3}{4}]$	[77, 139, 255, 311]
67	$[y + \frac{1}{2}, \frac{3}{4}, -y]$	[78, 188, 203, 310]

continued ...

Table 10

No.	position	mapping
68	$[\frac{1}{2} - y, \frac{1}{4}, -y]$	[79, 185, 204, 312]
69	$[\frac{1}{2} - y, \frac{3}{4}, y]$	[83, 190, 198, 308]
70	$[y + \frac{1}{2}, \frac{1}{4}, y]$	[84, 192, 199, 305]
71	$[\frac{1}{2} - y, y, \frac{3}{4}]$	[87, 143, 245, 307]
72	$[y + \frac{1}{2}, y, \frac{1}{4}]$	[88, 141, 244, 306]
73	$[-y, \frac{1}{4}, \frac{1}{2} - y]$	[89, 175, 216, 300]
74	$[-y, \frac{1}{2} - y, \frac{1}{4}]$	[90, 124, 261, 304]
75	$[y, \frac{1}{2} - y, \frac{3}{4}]$	[91, 125, 263, 303]
76	$[y, \frac{3}{4}, \frac{1}{2} - y]$	[92, 174, 214, 299]
77	$[y, y + \frac{1}{2}, \frac{1}{4}]$	[93, 136, 258, 292]
78	$[-y, \frac{3}{4}, y + \frac{1}{2}]$	[94, 179, 212, 294]
79	$[-y, y + \frac{1}{2}, \frac{3}{4}]$	[95, 135, 259, 293]
80	$[y, \frac{1}{4}, y + \frac{1}{2}]$	[96, 180, 209, 295]
81	$[\frac{3}{4}, y, y + \frac{1}{2}]$	[97, 157, 224, 278]
82	$[\frac{1}{4}, \frac{1}{2} - y, y]$	[98, 154, 219, 273]
83	$[\frac{1}{4}, y + \frac{1}{2}, -y]$	[99, 153, 218, 274]
84	$[\frac{3}{4}, -y, \frac{1}{2} - y]$	[104, 158, 217, 277]
85	$[\frac{1}{4}, y, \frac{1}{2} - y]$	[105, 147, 226, 266]
86	$[\frac{1}{4}, -y, y + \frac{1}{2}]$	[106, 146, 225, 267]
87	$[\frac{3}{4}, y + \frac{1}{2}, y]$	[109, 145, 230, 272]
88	$[\frac{3}{4}, \frac{1}{2} - y, -y]$	[110, 152, 229, 265]
89	$[\frac{1}{4}, -y, \frac{1}{2} - y]$	[121, 181, 200, 254]
90	$[\frac{3}{4}, y + \frac{1}{2}, -y]$	[122, 178, 195, 249]
91	$[\frac{3}{4}, \frac{1}{2} - y, y]$	[123, 177, 194, 250]
92	$[\frac{1}{4}, y, y + \frac{1}{2}]$	[128, 182, 193, 253]
93	$[\frac{3}{4}, -y, y + \frac{1}{2}]$	[129, 171, 202, 242]
94	$[\frac{3}{4}, y, \frac{1}{2} - y]$	[130, 170, 201, 243]
95	$[\frac{1}{4}, \frac{1}{2} - y, -y]$	[133, 169, 206, 248]
96	$[\frac{1}{4}, y + \frac{1}{2}, y]$	[134, 176, 205, 241]

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

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

continued ...

Table 11

No.	position	mapping
12	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - z]$	[12, 31]
13	$[\frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[13, 38]
14	$[\frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[14, 37]
15	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[15, 29]
16	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2}]$	[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	$[\frac{1}{2}, -z, y]$	[50, 75]
27	$[\frac{1}{2}, z, -y]$	[51, 74]
28	$[z + \frac{1}{2}, y, 0]$	[52, 88]
29	$[\frac{1}{2} - z, y, 0]$	[53, 87]
30	$[\frac{1}{2} - y, 0, z]$	[54, 83]
31	$[y + \frac{1}{2}, 0, z]$	[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	$[y + \frac{1}{2}, 0, -z]$	[59, 78]
36	$[\frac{1}{2} - y, 0, -z]$	[60, 79]
37	$[\frac{1}{2}, z, y]$	[61, 86]
38	$[\frac{1}{2}, -z, -y]$	[62, 85]
39	$[z + \frac{1}{2}, -y, 0]$	[63, 77]
40	$[\frac{1}{2} - z, -y, 0]$	[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	$[0, \frac{1}{2} - z, y]$	[98, 123]
51	$[0, z + \frac{1}{2}, -y]$	[99, 122]
52	$[z, y + \frac{1}{2}, 0]$	[100, 136]
53	$[-z, y + \frac{1}{2}, 0]$	[101, 135]
54	$[-y, \frac{1}{2}, z]$	[102, 131]
55	$[y, \frac{1}{2}, z]$	[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	$[y, \frac{1}{2}, -z]$	[107, 126]
60	$[-y, \frac{1}{2}, -z]$	[108, 127]
61	$[0, z + \frac{1}{2}, y]$	[109, 134]
62	$[0, \frac{1}{2} - z, -y]$	[110, 133]
63	$[z, \frac{1}{2} - y, 0]$	[111, 125]
64	$[-z, \frac{1}{2} - y, 0]$	[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	$[0, -z, y + \frac{1}{2}]$	[146, 171]
75	$[0, z, \frac{1}{2} - y]$	[147, 170]
76	$[z, y, \frac{1}{2}]$	[148, 184]
77	$[-z, y, \frac{1}{2}]$	[149, 183]
78	$[-y, 0, z + \frac{1}{2}]$	[150, 179]
79	$[y, 0, z + \frac{1}{2}]$	[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	$[y, 0, \frac{1}{2} - z]$	[155, 174]
84	$[-y, 0, \frac{1}{2} - z]$	[156, 175]
85	$[0, z, y + \frac{1}{2}]$	[157, 182]
86	$[0, -z, \frac{1}{2} - y]$	[158, 181]
87	$[z, -y, \frac{1}{2}]$	[159, 173]
88	$[-z, -y, \frac{1}{2}]$	[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	$[\frac{1}{2}, \frac{1}{2} - z, y]$	[194, 219]
99	$[\frac{1}{2}, z + \frac{1}{2}, -y]$	[195, 218]
100	$[z + \frac{1}{2}, y + \frac{1}{2}, 0]$	[196, 232]
101	$[\frac{1}{2} - z, y + \frac{1}{2}, 0]$	[197, 231]
102	$[\frac{1}{2} - y, \frac{1}{2}, z]$	[198, 227]
103	$[y + \frac{1}{2}, \frac{1}{2}, z]$	[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	$[y + \frac{1}{2}, \frac{1}{2}, -z]$	[203, 222]
108	$[\frac{1}{2} - y, \frac{1}{2}, -z]$	[204, 223]
109	$[\frac{1}{2}, z + \frac{1}{2}, y]$	[205, 230]
110	$[\frac{1}{2}, \frac{1}{2} - z, -y]$	[206, 229]
111	$[z + \frac{1}{2}, \frac{1}{2} - y, 0]$	[207, 221]
112	$[\frac{1}{2} - z, \frac{1}{2} - y, 0]$	[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	$[\frac{1}{2}, -z, y + \frac{1}{2}]$	[242, 267]
123	$[\frac{1}{2}, z, \frac{1}{2} - y]$	[243, 266]
124	$[z + \frac{1}{2}, y, \frac{1}{2}]$	[244, 280]
125	$[\frac{1}{2} - z, y, \frac{1}{2}]$	[245, 279]
126	$[\frac{1}{2} - y, 0, z + \frac{1}{2}]$	[246, 275]
127	$[y + \frac{1}{2}, 0, z + \frac{1}{2}]$	[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	$[y + \frac{1}{2}, 0, \frac{1}{2} - z]$	[251, 270]
132	$[\frac{1}{2} - y, 0, \frac{1}{2} - z]$	[252, 271]
133	$[\frac{1}{2}, z, y + \frac{1}{2}]$	[253, 278]
134	$[\frac{1}{2}, -z, \frac{1}{2} - y]$	[254, 277]
135	$[z + \frac{1}{2}, -y, \frac{1}{2}]$	[255, 269]
136	$[\frac{1}{2} - z, -y, \frac{1}{2}]$	[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	$[0, \frac{1}{2} - z, y + \frac{1}{2}]$	[290, 315]
147	$[0, z + \frac{1}{2}, \frac{1}{2} - y]$	[291, 314]
148	$[z, y + \frac{1}{2}, \frac{1}{2}]$	[292, 328]
149	$[-z, y + \frac{1}{2}, \frac{1}{2}]$	[293, 327]
150	$[-y, \frac{1}{2}, z + \frac{1}{2}]$	[294, 323]
151	$[y, \frac{1}{2}, z + \frac{1}{2}]$	[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	$[y, \frac{1}{2}, \frac{1}{2} - z]$	[299, 318]
156	$[-y, \frac{1}{2}, \frac{1}{2} - z]$	[300, 319]
157	$[0, z + \frac{1}{2}, y + \frac{1}{2}]$	[301, 326]
158	$[0, \frac{1}{2} - z, \frac{1}{2} - y]$	[302, 325]
159	$[z, \frac{1}{2} - y, \frac{1}{2}]$	[303, 317]
160	$[-z, \frac{1}{2} - y, \frac{1}{2}]$	[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	$[0, -z, y]$	[338, 363]
171	$[0, z, -y]$	[339, 362]
172	$[z, y, 0]$	[340, 376]
173	$[-z, y, 0]$	[341, 375]
174	$[-y, 0, z]$	[342, 371]
175	$[y, 0, z]$	[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	$[y, 0, -z]$	[347, 366]
180	$[-y, 0, -z]$	[348, 367]
181	$[0, z, y]$	[349, 374]
182	$[0, -z, -y]$	[350, 373]
183	$[z, -y, 0]$	[351, 365]
184	$[-z, -y, 0]$	[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	$[\frac{3}{4}, \frac{1}{2} - z, y + \frac{1}{2}]$	[2,315]
3	$[\frac{3}{4}, z + \frac{1}{2}, \frac{1}{2} - y]$	[3,314]
4	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{4}]$	[4,232]
5	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{3}{4}]$	[5,231]
6	$[\frac{1}{2} - y, \frac{3}{4}, z + \frac{1}{2}]$	[6,275]
7	$[y + \frac{1}{2}, \frac{1}{4}, z + \frac{1}{2}]$	[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	$[y + \frac{1}{2}, \frac{3}{4}, \frac{1}{2} - z]$	[11,270]
12	$[\frac{1}{2} - y, \frac{1}{4}, \frac{1}{2} - z]$	[12,271]
13	$[\frac{1}{4}, z + \frac{1}{2}, y + \frac{1}{2}]$	[13,326]
14	$[\frac{1}{4}, \frac{1}{2} - z, \frac{1}{2} - y]$	[14,325]
15	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{3}{4}]$	[15,221]
16	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{4}]$	[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	$[\frac{1}{4}, z + \frac{1}{2}, \frac{1}{2} - y]$	[26,291]
27	$[\frac{1}{4}, \frac{1}{2} - z, y + \frac{1}{2}]$	[27,290]
28	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{3}{4}]$	[28,208]
29	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{4}]$	[29,207]
30	$[y + \frac{1}{2}, \frac{1}{4}, \frac{1}{2} - z]$	[30,251]
31	$[\frac{1}{2} - y, \frac{3}{4}, \frac{1}{2} - z]$	[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	$[\frac{1}{2} - y, \frac{1}{4}, z + \frac{1}{2}]$	[35,246]
36	$[y + \frac{1}{2}, \frac{3}{4}, z + \frac{1}{2}]$	[36,247]
37	$[\frac{3}{4}, \frac{1}{2} - z, \frac{1}{2} - y]$	[37,302]
38	$[\frac{3}{4}, z + \frac{1}{2}, y + \frac{1}{2}]$	[38,301]
39	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{4}]$	[39,197]
40	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$	[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	$[\frac{3}{4}, -z, y]$	[50, 363]
51	$[\frac{3}{4}, z, -y]$	[51, 362]
52	$[z + \frac{1}{2}, y, \frac{3}{4}]$	[52, 280]
53	$[\frac{1}{2} - z, y, \frac{1}{4}]$	[53, 279]
54	$[\frac{1}{2} - y, \frac{1}{4}, z]$	[54, 227]
55	$[y + \frac{1}{2}, \frac{3}{4}, z]$	[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	$[y + \frac{1}{2}, \frac{1}{4}, -z]$	[59, 222]
60	$[\frac{1}{2} - y, \frac{3}{4}, -z]$	[60, 223]
61	$[\frac{1}{4}, z, y]$	[61, 374]
62	$[\frac{1}{4}, -z, -y]$	[62, 373]
63	$[z + \frac{1}{2}, -y, \frac{1}{4}]$	[63, 269]
64	$[\frac{1}{2} - z, -y, \frac{3}{4}]$	[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	$[\frac{1}{4}, z, -y]$	[74, 339]
75	$[\frac{1}{4}, -z, y]$	[75, 338]
76	$[\frac{1}{2} - z, -y, \frac{1}{4}]$	[76, 256]
77	$[z + \frac{1}{2}, -y, \frac{3}{4}]$	[77, 255]
78	$[y + \frac{1}{2}, \frac{3}{4}, -z]$	[78, 203]
79	$[\frac{1}{2} - y, \frac{1}{4}, -z]$	[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	$[\frac{1}{2} - y, \frac{3}{4}, z]$	[83, 198]
84	$[y + \frac{1}{2}, \frac{1}{4}, z]$	[84, 199]
85	$[\frac{3}{4}, -z, -y]$	[85, 350]
86	$[\frac{3}{4}, z, y]$	[86, 349]
87	$[\frac{1}{2} - z, y, \frac{3}{4}]$	[87, 245]
88	$[z + \frac{1}{2}, y, \frac{1}{4}]$	[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	$[\frac{1}{4}, \frac{1}{2} - z, y]$	[98, 219]
99	$[\frac{1}{4}, z + \frac{1}{2}, -y]$	[99, 218]
100	$[z, y + \frac{1}{2}, \frac{3}{4}]$	[100, 328]
101	$[-z, y + \frac{1}{2}, \frac{1}{4}]$	[101, 327]
102	$[-y, \frac{3}{4}, z]$	[102, 371]
103	$[y, \frac{1}{4}, z]$	[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	$[y, \frac{3}{4}, -z]$	[107, 366]
108	$[-y, \frac{1}{4}, -z]$	[108, 367]
109	$[\frac{3}{4}, z + \frac{1}{2}, y]$	[109, 230]
110	$[\frac{3}{4}, \frac{1}{2} - z, -y]$	[110, 229]
111	$[z, \frac{1}{2} - y, \frac{1}{4}]$	[111, 317]
112	$[-z, \frac{1}{2} - y, \frac{3}{4}]$	[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	$[\frac{3}{4}, z + \frac{1}{2}, -y]$	[122, 195]
123	$[\frac{3}{4}, \frac{1}{2} - z, y]$	[123, 194]
124	$[-z, \frac{1}{2} - y, \frac{1}{4}]$	[124, 304]
125	$[z, \frac{1}{2} - y, \frac{3}{4}]$	[125, 303]
126	$[y, \frac{1}{4}, -z]$	[126, 347]
127	$[-y, \frac{3}{4}, -z]$	[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	$[-y, \frac{1}{4}, z]$	[131, 342]
132	$[y, \frac{3}{4}, z]$	[132, 343]
133	$[\frac{1}{4}, \frac{1}{2} - z, -y]$	[133, 206]
134	$[\frac{1}{4}, z + \frac{1}{2}, y]$	[134, 205]
135	$[-z, y + \frac{1}{2}, \frac{3}{4}]$	[135, 293]
136	$[z, y + \frac{1}{2}, \frac{1}{4}]$	[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	$[\frac{1}{4}, -z, y + \frac{1}{2}]$	[146,267]
147	$[\frac{1}{4}, z, \frac{1}{2} - y]$	[147,266]
148	$[z, y, \frac{1}{4}]$	[148,376]
149	$[-z, y, \frac{3}{4}]$	[149,375]
150	$[-y, \frac{1}{4}, z + \frac{1}{2}]$	[150,323]
151	$[y, \frac{3}{4}, z + \frac{1}{2}]$	[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	$[y, \frac{1}{4}, \frac{1}{2} - z]$	[155,318]
156	$[-y, \frac{3}{4}, \frac{1}{2} - z]$	[156,319]
157	$[\frac{3}{4}, z, y + \frac{1}{2}]$	[157,278]
158	$[\frac{3}{4}, -z, \frac{1}{2} - y]$	[158,277]
159	$[z, -y, \frac{3}{4}]$	[159,365]
160	$[-z, -y, \frac{1}{4}]$	[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	$[\frac{3}{4}, z, \frac{1}{2} - y]$	[170,243]
171	$[\frac{3}{4}, -z, y + \frac{1}{2}]$	[171,242]
172	$[-z, -y, \frac{3}{4}]$	[172,352]
173	$[z, -y, \frac{1}{4}]$	[173,351]
174	$[y, \frac{3}{4}, \frac{1}{2} - z]$	[174,299]
175	$[-y, \frac{1}{4}, \frac{1}{2} - z]$	[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	$[-y, \frac{3}{4}, z + \frac{1}{2}]$	[179,294]
180	$[y, \frac{1}{4}, z + \frac{1}{2}]$	[180,295]
181	$[\frac{1}{4}, -z, \frac{1}{2} - y]$	[181,254]
182	$[\frac{1}{4}, z, y + \frac{1}{2}]$	[182,253]
183	$[-z, y, \frac{1}{4}]$	[183,341]
184	$[z, y, \frac{3}{4}]$	[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: $\dots m'$

No.	position	mapping
1	$[x, x, z]$	[1,372]
2	$[x + \frac{1}{2}, \frac{1}{2} - z, x + \frac{1}{2}]$	[2,379]
3	$[x + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - x]$	[3,381]
4	$[z + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - x]$	[4,380]
5	$[\frac{1}{2} - z, x + \frac{1}{2}, x + \frac{1}{2}]$	[5,382]
6	$[\frac{1}{2} - x, x + \frac{1}{2}, z + \frac{1}{2}]$	[6,368]
7	$[x + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[7,369]
8	$[x, -x, -z]$	[8,366]
9	$[-x, x, -z]$	[9,367]
10	$[-x, -x, z]$	[10,371]
11	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[11,370]
12	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - z]$	[12,361]
13	$[\frac{1}{2} - x, z + \frac{1}{2}, x + \frac{1}{2}]$	[13,383]
14	$[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - x]$	[14,378]
15	$[z + \frac{1}{2}, \frac{1}{2} - x, x + \frac{1}{2}]$	[15,384]
16	$[\frac{1}{2} - z, \frac{1}{2} - x, \frac{1}{2} - x]$	[16,377]
17	$[z, x, x]$	[17,376]
18	$[x, z, x]$	[18,374]
19	$[-x, z, -x]$	[19,362]
20	$[-z, -x, x]$	[20,364]
21	$[-x, -z, x]$	[21,363]
22	$[z, -x, -x]$	[22,365]
23	$[x, -z, -x]$	[23,373]
24	$[-z, x, -x]$	[24,375]
25	$[-x, -x, -z]$	[25,348]
26	$[\frac{1}{2} - x, z + \frac{1}{2}, \frac{1}{2} - x]$	[26,355]
27	$[\frac{1}{2} - x, \frac{1}{2} - z, x + \frac{1}{2}]$	[27,357]
28	$[\frac{1}{2} - z, \frac{1}{2} - x, x + \frac{1}{2}]$	[28,356]
29	$[z + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x]$	[29,358]
30	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[30,344]
31	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - z]$	[31,345]
32	$[-x, x, z]$	[32,342]
33	$[x, -x, z]$	[33,343]
34	$[x, x, -z]$	[34,347]
35	$[\frac{1}{2} - x, \frac{1}{2} - x, z + \frac{1}{2}]$	[35,346]

continued ...

Table 13

No.	position	mapping
36	$[x + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[36, 337]
37	$[x + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - x]$	[37, 359]
38	$[x + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}]$	[38, 354]
39	$[\frac{1}{2} - z, x + \frac{1}{2}, \frac{1}{2} - x]$	[39, 360]
40	$[z + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[40, 353]
41	$[-z, -x, -x]$	[41, 352]
42	$[-x, -z, -x]$	[42, 350]
43	$[x, -z, x]$	[43, 338]
44	$[z, x, -x]$	[44, 340]
45	$[x, z, -x]$	[45, 339]
46	$[-z, x, x]$	[46, 341]
47	$[-x, z, x]$	[47, 349]
48	$[z, -x, x]$	[48, 351]
49	$[x, x + \frac{1}{2}, z + \frac{1}{2}]$	[49, 324]
50	$[x + \frac{1}{2}, -z, x]$	[50, 331]
51	$[x + \frac{1}{2}, z, -x]$	[51, 333]
52	$[z + \frac{1}{2}, x, -x]$	[52, 332]
53	$[\frac{1}{2} - z, x, x]$	[53, 334]
54	$[\frac{1}{2} - x, x, z]$	[54, 320]
55	$[x + \frac{1}{2}, -x, z]$	[55, 321]
56	$[x, \frac{1}{2} - x, \frac{1}{2} - z]$	[56, 318]
57	$[-x, x + \frac{1}{2}, \frac{1}{2} - z]$	[57, 319]
58	$[-x, \frac{1}{2} - x, z + \frac{1}{2}]$	[58, 323]
59	$[x + \frac{1}{2}, x, -z]$	[59, 322]
60	$[\frac{1}{2} - x, -x, -z]$	[60, 313]
61	$[\frac{1}{2} - x, z, x]$	[61, 335]
62	$[\frac{1}{2} - x, -z, -x]$	[62, 330]
63	$[z + \frac{1}{2}, -x, x]$	[63, 336]
64	$[\frac{1}{2} - z, -x, -x]$	[64, 329]
65	$[z, x + \frac{1}{2}, x + \frac{1}{2}]$	[65, 328]
66	$[x, z + \frac{1}{2}, x + \frac{1}{2}]$	[66, 326]
67	$[-x, z + \frac{1}{2}, \frac{1}{2} - x]$	[67, 314]
68	$[-z, \frac{1}{2} - x, x + \frac{1}{2}]$	[68, 316]
69	$[-x, \frac{1}{2} - z, x + \frac{1}{2}]$	[69, 315]
70	$[z, \frac{1}{2} - x, \frac{1}{2} - x]$	[70, 317]
71	$[x, \frac{1}{2} - z, \frac{1}{2} - x]$	[71, 325]
72	$[-z, x + \frac{1}{2}, \frac{1}{2} - x]$	[72, 327]
73	$[-x, \frac{1}{2} - x, \frac{1}{2} - z]$	[73, 300]
74	$[\frac{1}{2} - x, z, -x]$	[74, 307]
75	$[\frac{1}{2} - x, -z, x]$	[75, 309]
76	$[\frac{1}{2} - z, -x, x]$	[76, 308]
77	$[z + \frac{1}{2}, -x, -x]$	[77, 310]
78	$[x + \frac{1}{2}, -x, -z]$	[78, 296]
79	$[\frac{1}{2} - x, x, -z]$	[79, 297]
80	$[-x, x + \frac{1}{2}, z + \frac{1}{2}]$	[80, 294]
81	$[x, \frac{1}{2} - x, z + \frac{1}{2}]$	[81, 295]
82	$[x, x + \frac{1}{2}, \frac{1}{2} - z]$	[82, 299]

continued ...

Table 13

No.	position	mapping
83	$[\frac{1}{2} - x, -x, z]$	[83, 298]
84	$[x + \frac{1}{2}, x, z]$	[84, 289]
85	$[x + \frac{1}{2}, -z, -x]$	[85, 311]
86	$[x + \frac{1}{2}, z, x]$	[86, 306]
87	$[\frac{1}{2} - z, x, -x]$	[87, 312]
88	$[z + \frac{1}{2}, x, x]$	[88, 305]
89	$[-z, \frac{1}{2} - x, \frac{1}{2} - x]$	[89, 304]
90	$[-x, \frac{1}{2} - z, \frac{1}{2} - x]$	[90, 302]
91	$[x, \frac{1}{2} - z, x + \frac{1}{2}]$	[91, 290]
92	$[z, x + \frac{1}{2}, \frac{1}{2} - x]$	[92, 292]
93	$[x, z + \frac{1}{2}, \frac{1}{2} - x]$	[93, 291]
94	$[-z, x + \frac{1}{2}, x + \frac{1}{2}]$	[94, 293]
95	$[-x, z + \frac{1}{2}, x + \frac{1}{2}]$	[95, 301]
96	$[z, \frac{1}{2} - x, x + \frac{1}{2}]$	[96, 303]
97	$[x + \frac{1}{2}, x, z + \frac{1}{2}]$	[97, 276]
98	$[x, \frac{1}{2} - z, x]$	[98, 283]
99	$[x, z + \frac{1}{2}, -x]$	[99, 285]
100	$[z, x + \frac{1}{2}, -x]$	[100, 284]
101	$[-z, x + \frac{1}{2}, x]$	[101, 286]
102	$[-x, x + \frac{1}{2}, z]$	[102, 272]
103	$[x, \frac{1}{2} - x, z]$	[103, 273]
104	$[x + \frac{1}{2}, -x, \frac{1}{2} - z]$	[104, 270]
105	$[\frac{1}{2} - x, x, \frac{1}{2} - z]$	[105, 271]
106	$[\frac{1}{2} - x, -x, z + \frac{1}{2}]$	[106, 275]
107	$[x, x + \frac{1}{2}, -z]$	[107, 274]
108	$[-x, \frac{1}{2} - x, -z]$	[108, 265]
109	$[-x, z + \frac{1}{2}, x]$	[109, 287]
110	$[-x, \frac{1}{2} - z, -x]$	[110, 282]
111	$[z, \frac{1}{2} - x, x]$	[111, 288]
112	$[-z, \frac{1}{2} - x, -x]$	[112, 281]
113	$[z + \frac{1}{2}, x, x + \frac{1}{2}]$	[113, 280]
114	$[x + \frac{1}{2}, z, x + \frac{1}{2}]$	[114, 278]
115	$[\frac{1}{2} - x, z, \frac{1}{2} - x]$	[115, 266]
116	$[\frac{1}{2} - z, -x, x + \frac{1}{2}]$	[116, 268]
117	$[\frac{1}{2} - x, -z, x + \frac{1}{2}]$	[117, 267]
118	$[z + \frac{1}{2}, -x, \frac{1}{2} - x]$	[118, 269]
119	$[x + \frac{1}{2}, -z, \frac{1}{2} - x]$	[119, 277]
120	$[\frac{1}{2} - z, x, \frac{1}{2} - x]$	[120, 279]
121	$[\frac{1}{2} - x, -x, \frac{1}{2} - z]$	[121, 252]
122	$[-x, z + \frac{1}{2}, -x]$	[122, 259]
123	$[-x, \frac{1}{2} - z, x]$	[123, 261]
124	$[-z, \frac{1}{2} - x, x]$	[124, 260]
125	$[z, \frac{1}{2} - x, -x]$	[125, 262]
126	$[x, \frac{1}{2} - x, -z]$	[126, 248]
127	$[-x, x + \frac{1}{2}, -z]$	[127, 249]
128	$[\frac{1}{2} - x, x, z + \frac{1}{2}]$	[128, 246]
129	$[x + \frac{1}{2}, -x, z + \frac{1}{2}]$	[129, 247]

continued ...

Table 13

No.	position	mapping
130	$[x + \frac{1}{2}, x, \frac{1}{2} - z]$	[130, 251]
131	$[-x, \frac{1}{2} - x, z]$	[131, 250]
132	$[x, x + \frac{1}{2}, z]$	[132, 241]
133	$[x, \frac{1}{2} - z, -x]$	[133, 263]
134	$[x, z + \frac{1}{2}, x]$	[134, 258]
135	$[-z, x + \frac{1}{2}, -x]$	[135, 264]
136	$[z, x + \frac{1}{2}, x]$	[136, 257]
137	$[\frac{1}{2} - z, -x, \frac{1}{2} - x]$	[137, 256]
138	$[\frac{1}{2} - x, -z, \frac{1}{2} - x]$	[138, 254]
139	$[x + \frac{1}{2}, -z, x + \frac{1}{2}]$	[139, 242]
140	$[z + \frac{1}{2}, x, \frac{1}{2} - x]$	[140, 244]
141	$[x + \frac{1}{2}, z, \frac{1}{2} - x]$	[141, 243]
142	$[\frac{1}{2} - z, x, x + \frac{1}{2}]$	[142, 245]
143	$[\frac{1}{2} - x, z, x + \frac{1}{2}]$	[143, 253]
144	$[z + \frac{1}{2}, -x, x + \frac{1}{2}]$	[144, 255]
145	$[x + \frac{1}{2}, x + \frac{1}{2}, z]$	[145, 228]
146	$[x, -z, x + \frac{1}{2}]$	[146, 235]
147	$[x, z, \frac{1}{2} - x]$	[147, 237]
148	$[z, x, \frac{1}{2} - x]$	[148, 236]
149	$[-z, x, x + \frac{1}{2}]$	[149, 238]
150	$[-x, x, z + \frac{1}{2}]$	[150, 224]
151	$[x, -x, z + \frac{1}{2}]$	[151, 225]
152	$[x + \frac{1}{2}, \frac{1}{2} - x, -z]$	[152, 222]
153	$[\frac{1}{2} - x, x + \frac{1}{2}, -z]$	[153, 223]
154	$[\frac{1}{2} - x, \frac{1}{2} - x, z]$	[154, 227]
155	$[x, x, \frac{1}{2} - z]$	[155, 226]
156	$[-x, -x, \frac{1}{2} - z]$	[156, 217]
157	$[-x, z, x + \frac{1}{2}]$	[157, 239]
158	$[-x, -z, \frac{1}{2} - x]$	[158, 234]
159	$[z, -x, x + \frac{1}{2}]$	[159, 240]
160	$[-z, -x, \frac{1}{2} - x]$	[160, 233]
161	$[z + \frac{1}{2}, x + \frac{1}{2}, x]$	[161, 232]
162	$[x + \frac{1}{2}, z + \frac{1}{2}, x]$	[162, 230]
163	$[\frac{1}{2} - x, z + \frac{1}{2}, -x]$	[163, 218]
164	$[\frac{1}{2} - z, \frac{1}{2} - x, x]$	[164, 220]
165	$[\frac{1}{2} - x, \frac{1}{2} - z, x]$	[165, 219]
166	$[z + \frac{1}{2}, \frac{1}{2} - x, -x]$	[166, 221]
167	$[x + \frac{1}{2}, \frac{1}{2} - z, -x]$	[167, 229]
168	$[\frac{1}{2} - z, x + \frac{1}{2}, -x]$	[168, 231]
169	$[\frac{1}{2} - x, \frac{1}{2} - x, -z]$	[169, 204]
170	$[-x, z, \frac{1}{2} - x]$	[170, 211]
171	$[-x, -z, x + \frac{1}{2}]$	[171, 213]
172	$[-z, -x, x + \frac{1}{2}]$	[172, 212]
173	$[z, -x, \frac{1}{2} - x]$	[173, 214]
174	$[x, -x, \frac{1}{2} - z]$	[174, 200]
175	$[-x, x, \frac{1}{2} - z]$	[175, 201]
176	$[\frac{1}{2} - x, x + \frac{1}{2}, z]$	[176, 198]

continued ...

Table 13

No.	position	mapping
177	$[x + \frac{1}{2}, \frac{1}{2} - x, z]$	[177, 199]
178	$[x + \frac{1}{2}, x + \frac{1}{2}, -z]$	[178, 203]
179	$[-x, -x, z + \frac{1}{2}]$	[179, 202]
180	$[x, x, z + \frac{1}{2}]$	[180, 193]
181	$[x, -z, \frac{1}{2} - x]$	[181, 215]
182	$[x, z, x + \frac{1}{2}]$	[182, 210]
183	$[-z, x, \frac{1}{2} - x]$	[183, 216]
184	$[z, x, x + \frac{1}{2}]$	[184, 209]
185	$[\frac{1}{2} - z, \frac{1}{2} - x, -x]$	[185, 208]
186	$[\frac{1}{2} - x, \frac{1}{2} - z, -x]$	[186, 206]
187	$[x + \frac{1}{2}, \frac{1}{2} - z, x]$	[187, 194]
188	$[z + \frac{1}{2}, x + \frac{1}{2}, -x]$	[188, 196]
189	$[x + \frac{1}{2}, z + \frac{1}{2}, -x]$	[189, 195]
190	$[\frac{1}{2} - z, x + \frac{1}{2}, x]$	[190, 197]
191	$[\frac{1}{2} - x, z + \frac{1}{2}, x]$	[191, 205]
192	$[z + \frac{1}{2}, \frac{1}{2} - x, x]$	[192, 207]

Table 14: Wyckoff site: 384n, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x + \frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[2]
3	$[x + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[3]
4	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - x]$	[4]
5	$[\frac{1}{2} - z, y + \frac{1}{2}, x + \frac{1}{2}]$	[5]
6	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[6]
7	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[7]
8	$[x, -y, -z]$	[8]
9	$[-x, y, -z]$	[9]
10	$[-x, -y, z]$	[10]
11	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[11]
12	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[12]
13	$[\frac{1}{2} - x, z + \frac{1}{2}, y + \frac{1}{2}]$	[13]
14	$[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y]$	[14]
15	$[z + \frac{1}{2}, \frac{1}{2} - y, x + \frac{1}{2}]$	[15]
16	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2} - x]$	[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	$[\frac{1}{2} - x, z + \frac{1}{2}, \frac{1}{2} - y]$	[26]
27	$[\frac{1}{2} - x, \frac{1}{2} - z, y + \frac{1}{2}]$	[27]
28	$[\frac{1}{2} - z, \frac{1}{2} - y, x + \frac{1}{2}]$	[28]
29	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - x]$	[29]
30	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[30]
31	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[31]
32	$[-x, y, z]$	[32]
33	$[x, -y, z]$	[33]
34	$[x, y, -z]$	[34]
35	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[35]
36	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[36]
37	$[x + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[37]
38	$[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[38]
39	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2} - x]$	[39]
40	$[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}]$	[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	$[x + \frac{1}{2}, -z, y]$	[50]
51	$[x + \frac{1}{2}, z, -y]$	[51]
52	$[z + \frac{1}{2}, y, -x]$	[52]
53	$[\frac{1}{2} - z, y, x]$	[53]
54	$[\frac{1}{2} - y, x, z]$	[54]
55	$[y + \frac{1}{2}, -x, z]$	[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	$[y + \frac{1}{2}, x, -z]$	[59]
60	$[\frac{1}{2} - y, -x, -z]$	[60]
61	$[\frac{1}{2} - x, z, y]$	[61]
62	$[\frac{1}{2} - x, -z, -y]$	[62]
63	$[z + \frac{1}{2}, -y, x]$	[63]
64	$[\frac{1}{2} - z, -y, -x]$	[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	$[\frac{1}{2} - x, z, -y]$	[74]
75	$[\frac{1}{2} - x, -z, y]$	[75]
76	$[\frac{1}{2} - z, -y, x]$	[76]
77	$[z + \frac{1}{2}, -y, -x]$	[77]
78	$[y + \frac{1}{2}, -x, -z]$	[78]
79	$[\frac{1}{2} - y, x, -z]$	[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	$[\frac{1}{2} - y, -x, z]$	[83]
84	$[y + \frac{1}{2}, x, z]$	[84]
85	$[x + \frac{1}{2}, -z, -y]$	[85]
86	$[x + \frac{1}{2}, z, y]$	[86]
87	$[\frac{1}{2} - z, y, -x]$	[87]
88	$[z + \frac{1}{2}, y, x]$	[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	$[x, \frac{1}{2} - z, y]$	[98]
99	$[x, z + \frac{1}{2}, -y]$	[99]
100	$[z, y + \frac{1}{2}, -x]$	[100]
101	$[-z, y + \frac{1}{2}, x]$	[101]
102	$[-y, x + \frac{1}{2}, z]$	[102]
103	$[y, \frac{1}{2} - x, z]$	[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	$[y, x + \frac{1}{2}, -z]$	[107]
108	$[-y, \frac{1}{2} - x, -z]$	[108]
109	$[-x, z + \frac{1}{2}, y]$	[109]
110	$[-x, \frac{1}{2} - z, -y]$	[110]
111	$[z, \frac{1}{2} - y, x]$	[111]
112	$[-z, \frac{1}{2} - y, -x]$	[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	$[-x, z + \frac{1}{2}, -y]$	[122]
123	$[-x, \frac{1}{2} - z, y]$	[123]
124	$[-z, \frac{1}{2} - y, x]$	[124]
125	$[z, \frac{1}{2} - y, -x]$	[125]
126	$[y, \frac{1}{2} - x, -z]$	[126]
127	$[-y, x + \frac{1}{2}, -z]$	[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	$[-y, \frac{1}{2} - x, z]$	[131]
132	$[y, x + \frac{1}{2}, z]$	[132]
133	$[x, \frac{1}{2} - z, -y]$	[133]
134	$[x, z + \frac{1}{2}, y]$	[134]
135	$[-z, y + \frac{1}{2}, -x]$	[135]
136	$[z, y + \frac{1}{2}, x]$	[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	$[x, -z, y + \frac{1}{2}]$	[146]
147	$[x, z, \frac{1}{2} - y]$	[147]
148	$[z, y, \frac{1}{2} - x]$	[148]
149	$[-z, y, x + \frac{1}{2}]$	[149]
150	$[-y, x, z + \frac{1}{2}]$	[150]
151	$[y, -x, z + \frac{1}{2}]$	[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	$[y, x, \frac{1}{2} - z]$	[155]
156	$[-y, -x, \frac{1}{2} - z]$	[156]
157	$[-x, z, y + \frac{1}{2}]$	[157]
158	$[-x, -z, \frac{1}{2} - y]$	[158]
159	$[z, -y, x + \frac{1}{2}]$	[159]
160	$[-z, -y, \frac{1}{2} - x]$	[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	$[-x, z, \frac{1}{2} - y]$	[170]
171	$[-x, -z, y + \frac{1}{2}]$	[171]
172	$[-z, -y, x + \frac{1}{2}]$	[172]
173	$[z, -y, \frac{1}{2} - x]$	[173]
174	$[y, -x, \frac{1}{2} - z]$	[174]
175	$[-y, x, \frac{1}{2} - z]$	[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	$[-y, -x, z + \frac{1}{2}]$	[179]
180	$[y, x, z + \frac{1}{2}]$	[180]
181	$[x, -z, \frac{1}{2} - y]$	[181]
182	$[x, z, y + \frac{1}{2}]$	[182]
183	$[-z, y, \frac{1}{2} - x]$	[183]
184	$[z, y, x + \frac{1}{2}]$	[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	$[x + \frac{1}{2}, \frac{1}{2} - z, y]$	[194]
195	$[x + \frac{1}{2}, z + \frac{1}{2}, -y]$	[195]
196	$[z + \frac{1}{2}, y + \frac{1}{2}, -x]$	[196]
197	$[\frac{1}{2} - z, y + \frac{1}{2}, x]$	[197]
198	$[\frac{1}{2} - y, x + \frac{1}{2}, z]$	[198]
199	$[y + \frac{1}{2}, \frac{1}{2} - x, z]$	[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	$[y + \frac{1}{2}, x + \frac{1}{2}, -z]$	[203]
204	$[\frac{1}{2} - y, \frac{1}{2} - x, -z]$	[204]
205	$[\frac{1}{2} - x, z + \frac{1}{2}, y]$	[205]
206	$[\frac{1}{2} - x, \frac{1}{2} - z, -y]$	[206]
207	$[z + \frac{1}{2}, \frac{1}{2} - y, x]$	[207]
208	$[\frac{1}{2} - z, \frac{1}{2} - y, -x]$	[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	$[\frac{1}{2} - x, z + \frac{1}{2}, -y]$	[218]
219	$[\frac{1}{2} - x, \frac{1}{2} - z, y]$	[219]
220	$[\frac{1}{2} - z, \frac{1}{2} - y, x]$	[220]
221	$[z + \frac{1}{2}, \frac{1}{2} - y, -x]$	[221]
222	$[y + \frac{1}{2}, \frac{1}{2} - x, -z]$	[222]
223	$[\frac{1}{2} - y, x + \frac{1}{2}, -z]$	[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	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[227]
228	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[228]
229	$[x + \frac{1}{2}, \frac{1}{2} - z, -y]$	[229]
230	$[x + \frac{1}{2}, z + \frac{1}{2}, y]$	[230]
231	$[\frac{1}{2} - z, y + \frac{1}{2}, -x]$	[231]
232	$[z + \frac{1}{2}, y + \frac{1}{2}, x]$	[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	$[x + \frac{1}{2}, -z, y + \frac{1}{2}]$	[242]
243	$[x + \frac{1}{2}, z, \frac{1}{2} - y]$	[243]
244	$[z + \frac{1}{2}, y, \frac{1}{2} - x]$	[244]
245	$[\frac{1}{2} - z, y, x + \frac{1}{2}]$	[245]
246	$[\frac{1}{2} - y, x, z + \frac{1}{2}]$	[246]
247	$[y + \frac{1}{2}, -x, z + \frac{1}{2}]$	[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	$[y + \frac{1}{2}, x, \frac{1}{2} - z]$	[251]
252	$[\frac{1}{2} - y, -x, \frac{1}{2} - z]$	[252]
253	$[\frac{1}{2} - x, z, y + \frac{1}{2}]$	[253]
254	$[\frac{1}{2} - x, -z, \frac{1}{2} - y]$	[254]
255	$[z + \frac{1}{2}, -y, x + \frac{1}{2}]$	[255]
256	$[\frac{1}{2} - z, -y, \frac{1}{2} - x]$	[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	$[\frac{1}{2} - x, z, \frac{1}{2} - y]$	[266]
267	$[\frac{1}{2} - x, -z, y + \frac{1}{2}]$	[267]
268	$[\frac{1}{2} - z, -y, x + \frac{1}{2}]$	[268]
269	$[z + \frac{1}{2}, -y, \frac{1}{2} - x]$	[269]
270	$[y + \frac{1}{2}, -x, \frac{1}{2} - z]$	[270]
271	$[\frac{1}{2} - y, x, \frac{1}{2} - z]$	[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	$[\frac{1}{2} - y, -x, z + \frac{1}{2}]$	[275]
276	$[y + \frac{1}{2}, x, z + \frac{1}{2}]$	[276]
277	$[x + \frac{1}{2}, -z, \frac{1}{2} - y]$	[277]
278	$[x + \frac{1}{2}, z, y + \frac{1}{2}]$	[278]
279	$[\frac{1}{2} - z, y, \frac{1}{2} - x]$	[279]
280	$[z + \frac{1}{2}, y, x + \frac{1}{2}]$	[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	$[x, \frac{1}{2} - z, y + \frac{1}{2}]$	[290]
291	$[x, z + \frac{1}{2}, \frac{1}{2} - y]$	[291]
292	$[z, y + \frac{1}{2}, \frac{1}{2} - x]$	[292]
293	$[-z, y + \frac{1}{2}, x + \frac{1}{2}]$	[293]
294	$[-y, x + \frac{1}{2}, z + \frac{1}{2}]$	[294]
295	$[y, \frac{1}{2} - x, z + \frac{1}{2}]$	[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	$[y, x + \frac{1}{2}, \frac{1}{2} - z]$	[299]
300	$[-y, \frac{1}{2} - x, \frac{1}{2} - z]$	[300]
301	$[-x, z + \frac{1}{2}, y + \frac{1}{2}]$	[301]
302	$[-x, \frac{1}{2} - z, \frac{1}{2} - y]$	[302]
303	$[z, \frac{1}{2} - y, x + \frac{1}{2}]$	[303]
304	$[-z, \frac{1}{2} - y, \frac{1}{2} - x]$	[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	$[-x, z + \frac{1}{2}, \frac{1}{2} - y]$	[314]
315	$[-x, \frac{1}{2} - z, y + \frac{1}{2}]$	[315]
316	$[-z, \frac{1}{2} - y, x + \frac{1}{2}]$	[316]
317	$[z, \frac{1}{2} - y, \frac{1}{2} - x]$	[317]
318	$[y, \frac{1}{2} - x, \frac{1}{2} - z]$	[318]
319	$[-y, x + \frac{1}{2}, \frac{1}{2} - z]$	[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	$[-y, \frac{1}{2} - x, z + \frac{1}{2}]$	[323]
324	$[y, x + \frac{1}{2}, z + \frac{1}{2}]$	[324]
325	$[x, \frac{1}{2} - z, \frac{1}{2} - y]$	[325]
326	$[x, z + \frac{1}{2}, y + \frac{1}{2}]$	[326]
327	$[-z, y + \frac{1}{2}, \frac{1}{2} - x]$	[327]
328	$[z, y + \frac{1}{2}, x + \frac{1}{2}]$	[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	$[x, -z, y]$	[338]
339	$[x, z, -y]$	[339]
340	$[z, y, -x]$	[340]
341	$[-z, y, x]$	[341]
342	$[-y, x, z]$	[342]
343	$[y, -x, z]$	[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	$[y, x, -z]$	[347]
348	$[-y, -x, -z]$	[348]
349	$[-x, z, y]$	[349]
350	$[-x, -z, -y]$	[350]
351	$[z, -y, x]$	[351]
352	$[-z, -y, -x]$	[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	$[-x, z, -y]$	[362]
363	$[-x, -z, y]$	[363]
364	$[-z, -y, x]$	[364]
365	$[z, -y, -x]$	[365]
366	$[y, -x, -z]$	[366]
367	$[-y, x, -z]$	[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	$[-y, -x, z]$	[371]
372	$[y, x, z]$	[372]
373	$[x, -z, -y]$	[373]
374	$[x, z, y]$	[374]
375	$[-z, y, -x]$	[375]
376	$[z, y, x]$	[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]