

MSG No. 225.117  $Fm\bar{3}m1'$  [ Type II, cubic ]

Table 1: Wyckoff site: 4a, site symmetry:  $m\bar{3}m1'$

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, 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]
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, 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]
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, 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]
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, 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: 4b, site symmetry:  $m\bar{3}m1'$

No.	position	mapping
1	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 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]
2	$[\frac{1}{2}, 0, 0]$	[49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 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]
3	$[0, \frac{1}{2}, 0]$	[97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 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]
4	$[0, 0, \frac{1}{2}]$	[145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168, 169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192, 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 3: Wyckoff site: 8c, site symmetry:  $-43m1'$ 

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

Table 4: Wyckoff site: 24d, site symmetry:  $m.mm1'$ 

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

Table 5: Wyckoff site: 24e, site symmetry:  $4m.m1'$ 

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

Table 6: Wyckoff site: 32f, site symmetry:  $.3m1'$ 

No.	position	mapping
1	$[x, x, x]$	$[1, 17, 18, 36, 38, 40, 193, 209, 210, 228, 230, 232]$
2	$[x, -x, x]$	$[2, 7, 15, 33, 43, 48, 194, 199, 207, 225, 235, 240]$
3	$[x, x, -x]$	$[3, 4, 11, 34, 44, 45, 195, 196, 203, 226, 236, 237]$
4	$[-x, x, x]$	$[5, 6, 13, 32, 46, 47, 197, 198, 205, 224, 238, 239]$
5	$[x, -x, -x]$	$[8, 22, 23, 29, 30, 37, 200, 214, 215, 221, 222, 229]$
6	$[-x, x, -x]$	$[9, 19, 24, 26, 31, 39, 201, 211, 216, 218, 223, 231]$
7	$[-x, -x, x]$	$[10, 20, 21, 27, 28, 35, 202, 212, 213, 219, 220, 227]$
8	$[-x, -x, -x]$	$[12, 14, 16, 25, 41, 42, 204, 206, 208, 217, 233, 234]$
9	$[x, x + \frac{1}{2}, x + \frac{1}{2}]$	$[49, 65, 66, 84, 86, 88, 241, 257, 258, 276, 278, 280]$
10	$[x, \frac{1}{2} - x, x + \frac{1}{2}]$	$[50, 55, 63, 81, 91, 96, 242, 247, 255, 273, 283, 288]$
11	$[x, x + \frac{1}{2}, \frac{1}{2} - x]$	$[51, 52, 59, 82, 92, 93, 243, 244, 251, 274, 284, 285]$
12	$[-x, x + \frac{1}{2}, x + \frac{1}{2}]$	$[53, 54, 61, 80, 94, 95, 245, 246, 253, 272, 286, 287]$
13	$[x, \frac{1}{2} - x, \frac{1}{2} - x]$	$[56, 70, 71, 77, 78, 85, 248, 262, 263, 269, 270, 277]$
14	$[-x, x + \frac{1}{2}, \frac{1}{2} - x]$	$[57, 67, 72, 74, 79, 87, 249, 259, 264, 266, 271, 279]$

continued ...

Table 6

No.	position	mapping
15	$[-x, \frac{1}{2} - x, x + \frac{1}{2}]$	[58, 68, 69, 75, 76, 83, 250, 260, 261, 267, 268, 275]
16	$[-x, \frac{1}{2} - x, \frac{1}{2} - x]$	[60, 62, 64, 73, 89, 90, 252, 254, 256, 265, 281, 282]
17	$[x + \frac{1}{2}, x, x + \frac{1}{2}]$	[97, 113, 114, 132, 134, 136, 289, 305, 306, 324, 326, 328]
18	$[x + \frac{1}{2}, -x, x + \frac{1}{2}]$	[98, 103, 111, 129, 139, 144, 290, 295, 303, 321, 331, 336]
19	$[x + \frac{1}{2}, x, \frac{1}{2} - x]$	[99, 100, 107, 130, 140, 141, 291, 292, 299, 322, 332, 333]
20	$[\frac{1}{2} - x, x, x + \frac{1}{2}]$	[101, 102, 109, 128, 142, 143, 293, 294, 301, 320, 334, 335]
21	$[x + \frac{1}{2}, -x, \frac{1}{2} - x]$	[104, 118, 119, 125, 126, 133, 296, 310, 311, 317, 318, 325]
22	$[\frac{1}{2} - x, x, \frac{1}{2} - x]$	[105, 115, 120, 122, 127, 135, 297, 307, 312, 314, 319, 327]
23	$[\frac{1}{2} - x, -x, x + \frac{1}{2}]$	[106, 116, 117, 123, 124, 131, 298, 308, 309, 315, 316, 323]
24	$[\frac{1}{2} - x, -x, \frac{1}{2} - x]$	[108, 110, 112, 121, 137, 138, 300, 302, 304, 313, 329, 330]
25	$[x + \frac{1}{2}, x + \frac{1}{2}, x]$	[145, 161, 162, 180, 182, 184, 337, 353, 354, 372, 374, 376]
26	$[x + \frac{1}{2}, \frac{1}{2} - x, x]$	[146, 151, 159, 177, 187, 192, 338, 343, 351, 369, 379, 384]
27	$[x + \frac{1}{2}, x + \frac{1}{2}, -x]$	[147, 148, 155, 178, 188, 189, 339, 340, 347, 370, 380, 381]
28	$[\frac{1}{2} - x, x + \frac{1}{2}, x]$	[149, 150, 157, 176, 190, 191, 341, 342, 349, 368, 382, 383]
29	$[x + \frac{1}{2}, \frac{1}{2} - x, -x]$	[152, 166, 167, 173, 174, 181, 344, 358, 359, 365, 366, 373]
30	$[\frac{1}{2} - x, x + \frac{1}{2}, -x]$	[153, 163, 168, 170, 175, 183, 345, 355, 360, 362, 367, 375]
31	$[\frac{1}{2} - x, \frac{1}{2} - x, x]$	[154, 164, 165, 171, 172, 179, 346, 356, 357, 363, 364, 371]
32	$[\frac{1}{2} - x, \frac{1}{2} - x, -x]$	[156, 158, 160, 169, 185, 186, 348, 350, 352, 361, 377, 378]

Table 7: Wyckoff site: 48g, site symmetry:  $2.mm1'$ 

No.	position	mapping
1	$[x, \frac{1}{4}, \frac{1}{4}]$	[1, 38, 56, 85, 193, 230, 248, 277]
2	$[x, \frac{3}{4}, \frac{1}{4}]$	[2, 33, 51, 82, 194, 225, 243, 274]
3	$[x, \frac{1}{4}, \frac{3}{4}]$	[3, 34, 50, 81, 195, 226, 242, 273]
4	$[\frac{1}{4}, \frac{1}{4}, -x]$	[4, 45, 160, 186, 196, 237, 352, 378]
5	$[\frac{3}{4}, \frac{1}{4}, x]$	[5, 47, 159, 187, 197, 239, 351, 379]
6	$[\frac{3}{4}, x, \frac{1}{4}]$	[6, 46, 107, 140, 198, 238, 299, 332]
7	$[\frac{1}{4}, -x, \frac{1}{4}]$	[7, 48, 108, 137, 199, 240, 300, 329]
8	$[x, \frac{3}{4}, \frac{3}{4}]$	[8, 37, 49, 86, 200, 229, 241, 278]
9	$[-x, \frac{1}{4}, \frac{3}{4}]$	[9, 26, 58, 75, 201, 218, 250, 267]
10	$[-x, \frac{3}{4}, \frac{1}{4}]$	[10, 27, 57, 74, 202, 219, 249, 266]
11	$[\frac{1}{4}, x, \frac{3}{4}]$	[11, 44, 102, 142, 203, 236, 294, 334]
12	$[\frac{3}{4}, -x, \frac{3}{4}]$	[12, 41, 103, 144, 204, 233, 295, 336]
13	$[-x, \frac{1}{4}, \frac{1}{4}]$	[13, 32, 62, 73, 205, 224, 254, 265]
14	$[-x, \frac{3}{4}, \frac{3}{4}]$	[14, 25, 61, 80, 206, 217, 253, 272]
15	$[\frac{1}{4}, \frac{3}{4}, x]$	[15, 43, 149, 191, 207, 235, 341, 383]
16	$[\frac{3}{4}, \frac{3}{4}, -x]$	[16, 42, 148, 189, 208, 234, 340, 381]
17	$[\frac{1}{4}, x, \frac{1}{4}]$	[17, 36, 120, 127, 209, 228, 312, 319]
18	$[\frac{1}{4}, \frac{1}{4}, x]$	[18, 40, 165, 172, 210, 232, 357, 364]
19	$[\frac{3}{4}, \frac{1}{4}, -x]$	[19, 39, 167, 173, 211, 231, 359, 365]
20	$[\frac{3}{4}, -x, \frac{1}{4}]$	[20, 35, 118, 126, 212, 227, 310, 318]
21	$[\frac{3}{4}, \frac{3}{4}, x]$	[21, 28, 162, 184, 213, 220, 354, 376]
22	$[\frac{1}{4}, -x, \frac{3}{4}]$	[22, 30, 116, 131, 214, 222, 308, 323]

continued ...

Table 7

No.	position	mapping
23	$[\frac{1}{4}, \frac{3}{4}, -x]$	[23, 29, 163, 183, 215, 221, 355, 375]
24	$[\frac{3}{4}, x, \frac{3}{4}]$	[24, 31, 113, 132, 216, 223, 305, 324]
25	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[52, 93, 112, 138, 244, 285, 304, 330]
26	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[53, 95, 111, 139, 245, 287, 303, 331]
27	$[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[54, 94, 155, 188, 246, 286, 347, 380]
28	$[\frac{1}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[55, 96, 156, 185, 247, 288, 348, 377]
29	$[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[59, 92, 150, 190, 251, 284, 342, 382]
30	$[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[60, 89, 151, 192, 252, 281, 343, 384]
31	$[\frac{1}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[63, 91, 101, 143, 255, 283, 293, 335]
32	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[64, 90, 100, 141, 256, 282, 292, 333]
33	$[\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[65, 84, 168, 175, 257, 276, 360, 367]
34	$[\frac{1}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[66, 88, 117, 124, 258, 280, 309, 316]
35	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[67, 87, 119, 125, 259, 279, 311, 317]
36	$[\frac{3}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[68, 83, 166, 174, 260, 275, 358, 366]
37	$[\frac{3}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[69, 76, 114, 136, 261, 268, 306, 328]
38	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[70, 78, 164, 179, 262, 270, 356, 371]
39	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[71, 77, 115, 135, 263, 269, 307, 327]
40	$[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[72, 79, 161, 180, 264, 271, 353, 372]
41	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[97, 134, 152, 181, 289, 326, 344, 373]
42	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[98, 129, 147, 178, 290, 321, 339, 370]
43	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[99, 130, 146, 177, 291, 322, 338, 369]
44	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[104, 133, 145, 182, 296, 325, 337, 374]
45	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[105, 122, 154, 171, 297, 314, 346, 363]
46	$[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$	[106, 123, 153, 170, 298, 315, 345, 362]
47	$[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$	[109, 128, 158, 169, 301, 320, 350, 361]
48	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]$	[110, 121, 157, 176, 302, 313, 349, 368]

Table 8: Wyckoff site: 48h, site symmetry:  $m.2m1'$ 

No.	position	mapping
1	$[0, y, y]$	[1, 13, 32, 38, 193, 205, 224, 230]
2	$[0, -y, y]$	[2, 10, 27, 33, 194, 202, 219, 225]
3	$[0, y, -y]$	[3, 9, 26, 34, 195, 201, 218, 226]
4	$[y, y, 0]$	[4, 18, 40, 45, 196, 210, 232, 237]
5	$[-y, y, 0]$	[5, 19, 39, 47, 197, 211, 231, 239]
6	$[-y, 0, y]$	[6, 20, 35, 46, 198, 212, 227, 238]
7	$[y, 0, y]$	[7, 17, 36, 48, 199, 209, 228, 240]
8	$[0, -y, -y]$	[8, 14, 25, 37, 200, 206, 217, 229]
9	$[y, 0, -y]$	[11, 22, 30, 44, 203, 214, 222, 236]
10	$[-y, 0, -y]$	[12, 24, 31, 41, 204, 216, 223, 233]
11	$[y, -y, 0]$	[15, 23, 29, 43, 207, 215, 221, 235]
12	$[-y, -y, 0]$	[16, 21, 28, 42, 208, 213, 220, 234]
13	$[0, y + \frac{1}{2}, y + \frac{1}{2}]$	[49, 61, 80, 86, 241, 253, 272, 278]
14	$[0, \frac{1}{2} - y, y + \frac{1}{2}]$	[50, 58, 75, 81, 242, 250, 267, 273]

*continued ...*

Table 8

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

Table 9: Wyckoff site: 48i, site symmetry:  $m.2m1'$ 

No.	position	mapping
1	$[\frac{1}{2}, y, y]$	[1, 13, 32, 38, 193, 205, 224, 230]
2	$[\frac{1}{2}, -y, y]$	[2, 10, 27, 33, 194, 202, 219, 225]
3	$[\frac{1}{2}, y, -y]$	[3, 9, 26, 34, 195, 201, 218, 226]
4	$[y, y, \frac{1}{2}]$	[4, 18, 40, 45, 196, 210, 232, 237]
5	$[-y, y, \frac{1}{2}]$	[5, 19, 39, 47, 197, 211, 231, 239]
6	$[-y, \frac{1}{2}, y]$	[6, 20, 35, 46, 198, 212, 227, 238]

*continued ...*

Table 9

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

Table 10: Wyckoff site:  $96j$ , site symmetry:  $m..1'$ 

No.	position	mapping
1	$[0, y, z]$	$[1, 32, 193, 224]$
2	$[0, -z, y]$	$[2, 27, 194, 219]$
3	$[0, z, -y]$	$[3, 26, 195, 218]$
4	$[z, y, 0]$	$[4, 40, 196, 232]$
5	$[-z, y, 0]$	$[5, 39, 197, 231]$
6	$[-y, 0, z]$	$[6, 35, 198, 227]$
7	$[y, 0, z]$	$[7, 36, 199, 228]$
8	$[0, -y, -z]$	$[8, 25, 200, 217]$
9	$[0, y, -z]$	$[9, 34, 201, 226]$
10	$[0, -y, z]$	$[10, 33, 202, 225]$
11	$[y, 0, -z]$	$[11, 30, 203, 222]$
12	$[-y, 0, -z]$	$[12, 31, 204, 223]$
13	$[0, z, y]$	$[13, 38, 205, 230]$
14	$[0, -z, -y]$	$[14, 37, 206, 229]$
15	$[z, -y, 0]$	$[15, 29, 207, 221]$
16	$[-z, -y, 0]$	$[16, 28, 208, 220]$
17	$[z, 0, y]$	$[17, 48, 209, 240]$
18	$[y, z, 0]$	$[18, 45, 210, 237]$
19	$[-y, z, 0]$	$[19, 47, 211, 239]$
20	$[-z, 0, y]$	$[20, 46, 212, 238]$
21	$[-y, -z, 0]$	$[21, 42, 213, 234]$
22	$[z, 0, -y]$	$[22, 44, 214, 236]$
23	$[y, -z, 0]$	$[23, 43, 215, 235]$
24	$[-z, 0, -y]$	$[24, 41, 216, 233]$
25	$[0, y + \frac{1}{2}, z + \frac{1}{2}]$	$[49, 80, 241, 272]$
26	$[0, \frac{1}{2} - z, y + \frac{1}{2}]$	$[50, 75, 242, 267]$
27	$[0, z + \frac{1}{2}, \frac{1}{2} - y]$	$[51, 74, 243, 266]$
28	$[z, y + \frac{1}{2}, \frac{1}{2}]$	$[52, 88, 244, 280]$
29	$[-z, y + \frac{1}{2}, \frac{1}{2}]$	$[53, 87, 245, 279]$
30	$[-y, \frac{1}{2}, z + \frac{1}{2}]$	$[54, 83, 246, 275]$
31	$[y, \frac{1}{2}, z + \frac{1}{2}]$	$[55, 84, 247, 276]$
32	$[0, \frac{1}{2} - y, \frac{1}{2} - z]$	$[56, 73, 248, 265]$
33	$[0, y + \frac{1}{2}, \frac{1}{2} - z]$	$[57, 82, 249, 274]$
34	$[0, \frac{1}{2} - y, z + \frac{1}{2}]$	$[58, 81, 250, 273]$
35	$[y, \frac{1}{2}, \frac{1}{2} - z]$	$[59, 78, 251, 270]$
36	$[-y, \frac{1}{2}, \frac{1}{2} - z]$	$[60, 79, 252, 271]$
37	$[0, z + \frac{1}{2}, y + \frac{1}{2}]$	$[61, 86, 253, 278]$
38	$[0, \frac{1}{2} - z, \frac{1}{2} - y]$	$[62, 85, 254, 277]$
39	$[z, \frac{1}{2} - y, \frac{1}{2}]$	$[63, 77, 255, 269]$
40	$[-z, \frac{1}{2} - y, \frac{1}{2}]$	$[64, 76, 256, 268]$
41	$[z, \frac{1}{2}, y + \frac{1}{2}]$	$[65, 96, 257, 288]$
42	$[y, z + \frac{1}{2}, \frac{1}{2}]$	$[66, 93, 258, 285]$
43	$[-y, z + \frac{1}{2}, \frac{1}{2}]$	$[67, 95, 259, 287]$
44	$[-z, \frac{1}{2}, y + \frac{1}{2}]$	$[68, 94, 260, 286]$
45	$[-y, \frac{1}{2} - z, \frac{1}{2}]$	$[69, 90, 261, 282]$
46	$[z, \frac{1}{2}, \frac{1}{2} - y]$	$[70, 92, 262, 284]$

*continued ...*



Table 10

No.	position	mapping
47	$[y, \frac{1}{2} - z, \frac{1}{2}]$	[71, 91, 263, 283]
48	$[-z, \frac{1}{2}, \frac{1}{2} - y]$	[72, 89, 264, 281]
49	$[\frac{1}{2}, y, z + \frac{1}{2}]$	[97, 128, 289, 320]
50	$[\frac{1}{2}, -z, y + \frac{1}{2}]$	[98, 123, 290, 315]
51	$[\frac{1}{2}, z, \frac{1}{2} - y]$	[99, 122, 291, 314]
52	$[z + \frac{1}{2}, y, \frac{1}{2}]$	[100, 136, 292, 328]
53	$[\frac{1}{2} - z, y, \frac{1}{2}]$	[101, 135, 293, 327]
54	$[\frac{1}{2} - y, 0, z + \frac{1}{2}]$	[102, 131, 294, 323]
55	$[y + \frac{1}{2}, 0, z + \frac{1}{2}]$	[103, 132, 295, 324]
56	$[\frac{1}{2}, -y, \frac{1}{2} - z]$	[104, 121, 296, 313]
57	$[\frac{1}{2}, y, \frac{1}{2} - z]$	[105, 130, 297, 322]
58	$[\frac{1}{2}, -y, z + \frac{1}{2}]$	[106, 129, 298, 321]
59	$[y + \frac{1}{2}, 0, \frac{1}{2} - z]$	[107, 126, 299, 318]
60	$[\frac{1}{2} - y, 0, \frac{1}{2} - z]$	[108, 127, 300, 319]
61	$[\frac{1}{2}, z, y + \frac{1}{2}]$	[109, 134, 301, 326]
62	$[\frac{1}{2}, -z, \frac{1}{2} - y]$	[110, 133, 302, 325]
63	$[z + \frac{1}{2}, -y, \frac{1}{2}]$	[111, 125, 303, 317]
64	$[\frac{1}{2} - z, -y, \frac{1}{2}]$	[112, 124, 304, 316]
65	$[z + \frac{1}{2}, 0, y + \frac{1}{2}]$	[113, 144, 305, 336]
66	$[y + \frac{1}{2}, z, \frac{1}{2}]$	[114, 141, 306, 333]
67	$[\frac{1}{2} - y, z, \frac{1}{2}]$	[115, 143, 307, 335]
68	$[\frac{1}{2} - z, 0, y + \frac{1}{2}]$	[116, 142, 308, 334]
69	$[\frac{1}{2} - y, -z, \frac{1}{2}]$	[117, 138, 309, 330]
70	$[z + \frac{1}{2}, 0, \frac{1}{2} - y]$	[118, 140, 310, 332]
71	$[y + \frac{1}{2}, -z, \frac{1}{2}]$	[119, 139, 311, 331]
72	$[\frac{1}{2} - z, 0, \frac{1}{2} - y]$	[120, 137, 312, 329]
73	$[\frac{1}{2}, y + \frac{1}{2}, z]$	[145, 176, 337, 368]
74	$[\frac{1}{2}, \frac{1}{2} - z, y]$	[146, 171, 338, 363]
75	$[\frac{1}{2}, z + \frac{1}{2}, -y]$	[147, 170, 339, 362]
76	$[z + \frac{1}{2}, y + \frac{1}{2}, 0]$	[148, 184, 340, 376]
77	$[\frac{1}{2} - z, y + \frac{1}{2}, 0]$	[149, 183, 341, 375]
78	$[\frac{1}{2} - y, \frac{1}{2}, z]$	[150, 179, 342, 371]
79	$[y + \frac{1}{2}, \frac{1}{2}, z]$	[151, 180, 343, 372]
80	$[\frac{1}{2}, \frac{1}{2} - y, -z]$	[152, 169, 344, 361]
81	$[\frac{1}{2}, y + \frac{1}{2}, -z]$	[153, 178, 345, 370]
82	$[\frac{1}{2}, \frac{1}{2} - y, z]$	[154, 177, 346, 369]
83	$[y + \frac{1}{2}, \frac{1}{2}, -z]$	[155, 174, 347, 366]
84	$[\frac{1}{2} - y, \frac{1}{2}, -z]$	[156, 175, 348, 367]
85	$[\frac{1}{2}, z + \frac{1}{2}, y]$	[157, 182, 349, 374]
86	$[\frac{1}{2}, \frac{1}{2} - z, -y]$	[158, 181, 350, 373]
87	$[z + \frac{1}{2}, \frac{1}{2} - y, 0]$	[159, 173, 351, 365]
88	$[\frac{1}{2} - z, \frac{1}{2} - y, 0]$	[160, 172, 352, 364]
89	$[z + \frac{1}{2}, \frac{1}{2}, y]$	[161, 192, 353, 384]
90	$[y + \frac{1}{2}, z + \frac{1}{2}, 0]$	[162, 189, 354, 381]
91	$[\frac{1}{2} - y, z + \frac{1}{2}, 0]$	[163, 191, 355, 383]
92	$[\frac{1}{2} - z, \frac{1}{2}, y]$	[164, 190, 356, 382]
93	$[\frac{1}{2} - y, \frac{1}{2} - z, 0]$	[165, 186, 357, 378]

continued ...

Table 10

No.	position	mapping
94	$[z + \frac{1}{2}, \frac{1}{2}, -y]$	[166, 188, 358, 380]
95	$[y + \frac{1}{2}, \frac{1}{2} - z, 0]$	[167, 187, 359, 379]
96	$[\frac{1}{2} - z, \frac{1}{2}, -y]$	[168, 185, 360, 377]

Table 11: Wyckoff site: 96k, site symmetry:  $\dots m1'$ 

No.	position	mapping
1	$[x, x, z]$	[1, 36, 193, 228]
2	$[x, -z, x]$	[2, 43, 194, 235]
3	$[x, z, -x]$	[3, 45, 195, 237]
4	$[z, x, -x]$	[4, 44, 196, 236]
5	$[-z, x, x]$	[5, 46, 197, 238]
6	$[-x, x, z]$	[6, 32, 198, 224]
7	$[x, -x, z]$	[7, 33, 199, 225]
8	$[x, -x, -z]$	[8, 30, 200, 222]
9	$[-x, x, -z]$	[9, 31, 201, 223]
10	$[-x, -x, z]$	[10, 35, 202, 227]
11	$[x, x, -z]$	[11, 34, 203, 226]
12	$[-x, -x, -z]$	[12, 25, 204, 217]
13	$[-x, z, x]$	[13, 47, 205, 239]
14	$[-x, -z, -x]$	[14, 42, 206, 234]
15	$[z, -x, x]$	[15, 48, 207, 240]
16	$[-z, -x, -x]$	[16, 41, 208, 233]
17	$[z, x, x]$	[17, 40, 209, 232]
18	$[x, z, x]$	[18, 38, 210, 230]
19	$[-x, z, -x]$	[19, 26, 211, 218]
20	$[-z, -x, x]$	[20, 28, 212, 220]
21	$[-x, -z, x]$	[21, 27, 213, 219]
22	$[z, -x, -x]$	[22, 29, 214, 221]
23	$[x, -z, -x]$	[23, 37, 215, 229]
24	$[-z, x, -x]$	[24, 39, 216, 231]
25	$[x, x + \frac{1}{2}, z + \frac{1}{2}]$	[49, 84, 241, 276]
26	$[x, \frac{1}{2} - z, x + \frac{1}{2}]$	[50, 91, 242, 283]
27	$[x, z + \frac{1}{2}, \frac{1}{2} - x]$	[51, 93, 243, 285]
28	$[z, x + \frac{1}{2}, \frac{1}{2} - x]$	[52, 92, 244, 284]
29	$[-z, x + \frac{1}{2}, x + \frac{1}{2}]$	[53, 94, 245, 286]
30	$[-x, x + \frac{1}{2}, z + \frac{1}{2}]$	[54, 80, 246, 272]
31	$[x, \frac{1}{2} - x, z + \frac{1}{2}]$	[55, 81, 247, 273]
32	$[x, \frac{1}{2} - x, \frac{1}{2} - z]$	[56, 78, 248, 270]
33	$[-x, x + \frac{1}{2}, \frac{1}{2} - z]$	[57, 79, 249, 271]
34	$[-x, \frac{1}{2} - x, z + \frac{1}{2}]$	[58, 83, 250, 275]
35	$[x, x + \frac{1}{2}, \frac{1}{2} - z]$	[59, 82, 251, 274]
36	$[-x, \frac{1}{2} - x, \frac{1}{2} - z]$	[60, 73, 252, 265]
37	$[-x, z + \frac{1}{2}, x + \frac{1}{2}]$	[61, 95, 253, 287]

continued ...

Table 11

No.	position	mapping
38	$[-x, \frac{1}{2} - z, \frac{1}{2} - x]$	[62, 90, 254, 282]
39	$[z, \frac{1}{2} - x, x + \frac{1}{2}]$	[63, 96, 255, 288]
40	$[-z, \frac{1}{2} - x, \frac{1}{2} - x]$	[64, 89, 256, 281]
41	$[z, x + \frac{1}{2}, x + \frac{1}{2}]$	[65, 88, 257, 280]
42	$[x, z + \frac{1}{2}, x + \frac{1}{2}]$	[66, 86, 258, 278]
43	$[-x, z + \frac{1}{2}, \frac{1}{2} - x]$	[67, 74, 259, 266]
44	$[-z, \frac{1}{2} - x, x + \frac{1}{2}]$	[68, 76, 260, 268]
45	$[-x, \frac{1}{2} - z, x + \frac{1}{2}]$	[69, 75, 261, 267]
46	$[z, \frac{1}{2} - x, \frac{1}{2} - x]$	[70, 77, 262, 269]
47	$[x, \frac{1}{2} - z, \frac{1}{2} - x]$	[71, 85, 263, 277]
48	$[-z, x + \frac{1}{2}, \frac{1}{2} - x]$	[72, 87, 264, 279]
49	$[x + \frac{1}{2}, x, z + \frac{1}{2}]$	[97, 132, 289, 324]
50	$[x + \frac{1}{2}, -z, x + \frac{1}{2}]$	[98, 139, 290, 331]
51	$[x + \frac{1}{2}, z, \frac{1}{2} - x]$	[99, 141, 291, 333]
52	$[z + \frac{1}{2}, x, \frac{1}{2} - x]$	[100, 140, 292, 332]
53	$[\frac{1}{2} - z, x, x + \frac{1}{2}]$	[101, 142, 293, 334]
54	$[\frac{1}{2} - x, x, z + \frac{1}{2}]$	[102, 128, 294, 320]
55	$[x + \frac{1}{2}, -x, z + \frac{1}{2}]$	[103, 129, 295, 321]
56	$[x + \frac{1}{2}, -x, \frac{1}{2} - z]$	[104, 126, 296, 318]
57	$[\frac{1}{2} - x, x, \frac{1}{2} - z]$	[105, 127, 297, 319]
58	$[\frac{1}{2} - x, -x, z + \frac{1}{2}]$	[106, 131, 298, 323]
59	$[x + \frac{1}{2}, x, \frac{1}{2} - z]$	[107, 130, 299, 322]
60	$[\frac{1}{2} - x, -x, \frac{1}{2} - z]$	[108, 121, 300, 313]
61	$[\frac{1}{2} - x, z, x + \frac{1}{2}]$	[109, 143, 301, 335]
62	$[\frac{1}{2} - x, -z, \frac{1}{2} - x]$	[110, 138, 302, 330]
63	$[z + \frac{1}{2}, -x, x + \frac{1}{2}]$	[111, 144, 303, 336]
64	$[\frac{1}{2} - z, -x, \frac{1}{2} - x]$	[112, 137, 304, 329]
65	$[z + \frac{1}{2}, x, x + \frac{1}{2}]$	[113, 136, 305, 328]
66	$[x + \frac{1}{2}, z, x + \frac{1}{2}]$	[114, 134, 306, 326]
67	$[\frac{1}{2} - x, z, \frac{1}{2} - x]$	[115, 122, 307, 314]
68	$[\frac{1}{2} - z, -x, x + \frac{1}{2}]$	[116, 124, 308, 316]
69	$[\frac{1}{2} - x, -z, x + \frac{1}{2}]$	[117, 123, 309, 315]
70	$[z + \frac{1}{2}, -x, \frac{1}{2} - x]$	[118, 125, 310, 317]
71	$[x + \frac{1}{2}, -z, \frac{1}{2} - x]$	[119, 133, 311, 325]
72	$[\frac{1}{2} - z, x, \frac{1}{2} - x]$	[120, 135, 312, 327]
73	$[x + \frac{1}{2}, x + \frac{1}{2}, z]$	[145, 180, 337, 372]
74	$[x + \frac{1}{2}, \frac{1}{2} - z, x]$	[146, 187, 338, 379]
75	$[x + \frac{1}{2}, z + \frac{1}{2}, -x]$	[147, 189, 339, 381]
76	$[z + \frac{1}{2}, x + \frac{1}{2}, -x]$	[148, 188, 340, 380]
77	$[\frac{1}{2} - z, x + \frac{1}{2}, x]$	[149, 190, 341, 382]
78	$[\frac{1}{2} - x, x + \frac{1}{2}, z]$	[150, 176, 342, 368]
79	$[x + \frac{1}{2}, \frac{1}{2} - x, z]$	[151, 177, 343, 369]
80	$[x + \frac{1}{2}, \frac{1}{2} - x, -z]$	[152, 174, 344, 366]
81	$[\frac{1}{2} - x, x + \frac{1}{2}, -z]$	[153, 175, 345, 367]
82	$[\frac{1}{2} - x, \frac{1}{2} - x, z]$	[154, 179, 346, 371]
83	$[x + \frac{1}{2}, x + \frac{1}{2}, -z]$	[155, 178, 347, 370]
84	$[\frac{1}{2} - x, \frac{1}{2} - x, -z]$	[156, 169, 348, 361]

continued ...

Table 11

No.	position	mapping
85	$[\frac{1}{2} - x, z + \frac{1}{2}, x]$	[157, 191, 349, 383]
86	$[\frac{1}{2} - x, \frac{1}{2} - z, -x]$	[158, 186, 350, 378]
87	$[z + \frac{1}{2}, \frac{1}{2} - x, x]$	[159, 192, 351, 384]
88	$[\frac{1}{2} - z, \frac{1}{2} - x, -x]$	[160, 185, 352, 377]
89	$[z + \frac{1}{2}, x + \frac{1}{2}, x]$	[161, 184, 353, 376]
90	$[x + \frac{1}{2}, z + \frac{1}{2}, x]$	[162, 182, 354, 374]
91	$[\frac{1}{2} - x, z + \frac{1}{2}, -x]$	[163, 170, 355, 362]
92	$[\frac{1}{2} - z, \frac{1}{2} - x, x]$	[164, 172, 356, 364]
93	$[\frac{1}{2} - x, \frac{1}{2} - z, x]$	[165, 171, 357, 363]
94	$[z + \frac{1}{2}, \frac{1}{2} - x, -x]$	[166, 173, 358, 365]
95	$[x + \frac{1}{2}, \frac{1}{2} - z, -x]$	[167, 181, 359, 373]
96	$[\frac{1}{2} - z, x + \frac{1}{2}, -x]$	[168, 183, 360, 375]

Table 12: Wyckoff site: 1921, site symmetry:  $11'$ 

No.	position	mapping
1	$[x, y, z]$	[1, 193]
2	$[x, -z, y]$	[2, 194]
3	$[x, z, -y]$	[3, 195]
4	$[z, y, -x]$	[4, 196]
5	$[-z, y, x]$	[5, 197]
6	$[-y, x, z]$	[6, 198]
7	$[y, -x, z]$	[7, 199]
8	$[x, -y, -z]$	[8, 200]
9	$[-x, y, -z]$	[9, 201]
10	$[-x, -y, z]$	[10, 202]
11	$[y, x, -z]$	[11, 203]
12	$[-y, -x, -z]$	[12, 204]
13	$[-x, z, y]$	[13, 205]
14	$[-x, -z, -y]$	[14, 206]
15	$[z, -y, x]$	[15, 207]
16	$[-z, -y, -x]$	[16, 208]
17	$[z, x, y]$	[17, 209]
18	$[y, z, x]$	[18, 210]
19	$[-y, z, -x]$	[19, 211]
20	$[-z, -x, y]$	[20, 212]
21	$[-y, -z, x]$	[21, 213]
22	$[z, -x, -y]$	[22, 214]
23	$[y, -z, -x]$	[23, 215]
24	$[-z, x, -y]$	[24, 216]
25	$[-x, -y, -z]$	[25, 217]
26	$[-x, z, -y]$	[26, 218]
27	$[-x, -z, y]$	[27, 219]
28	$[-z, -y, x]$	[28, 220]

continued ...

Table 12

No.	position	mapping
29	$[z, -y, -x]$	[29, 221]
30	$[y, -x, -z]$	[30, 222]
31	$[-y, x, -z]$	[31, 223]
32	$[-x, y, z]$	[32, 224]
33	$[x, -y, z]$	[33, 225]
34	$[x, y, -z]$	[34, 226]
35	$[-y, -x, z]$	[35, 227]
36	$[y, x, z]$	[36, 228]
37	$[x, -z, -y]$	[37, 229]
38	$[x, z, y]$	[38, 230]
39	$[-z, y, -x]$	[39, 231]
40	$[z, y, x]$	[40, 232]
41	$[-z, -x, -y]$	[41, 233]
42	$[-y, -z, -x]$	[42, 234]
43	$[y, -z, x]$	[43, 235]
44	$[z, x, -y]$	[44, 236]
45	$[y, z, -x]$	[45, 237]
46	$[-z, x, y]$	[46, 238]
47	$[-y, z, x]$	[47, 239]
48	$[z, -x, y]$	[48, 240]
49	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[49, 241]
50	$[x, \frac{1}{2} - z, y + \frac{1}{2}]$	[50, 242]
51	$[x, z + \frac{1}{2}, \frac{1}{2} - y]$	[51, 243]
52	$[z, y + \frac{1}{2}, \frac{1}{2} - x]$	[52, 244]
53	$[-z, y + \frac{1}{2}, x + \frac{1}{2}]$	[53, 245]
54	$[-y, x + \frac{1}{2}, z + \frac{1}{2}]$	[54, 246]
55	$[y, \frac{1}{2} - x, z + \frac{1}{2}]$	[55, 247]
56	$[x, \frac{1}{2} - y, \frac{1}{2} - z]$	[56, 248]
57	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[57, 249]
58	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[58, 250]
59	$[y, x + \frac{1}{2}, \frac{1}{2} - z]$	[59, 251]
60	$[-y, \frac{1}{2} - x, \frac{1}{2} - z]$	[60, 252]
61	$[-x, z + \frac{1}{2}, y + \frac{1}{2}]$	[61, 253]
62	$[-x, \frac{1}{2} - z, \frac{1}{2} - y]$	[62, 254]
63	$[z, \frac{1}{2} - y, x + \frac{1}{2}]$	[63, 255]
64	$[-z, \frac{1}{2} - y, \frac{1}{2} - x]$	[64, 256]
65	$[z, x + \frac{1}{2}, y + \frac{1}{2}]$	[65, 257]
66	$[y, z + \frac{1}{2}, x + \frac{1}{2}]$	[66, 258]
67	$[-y, z + \frac{1}{2}, \frac{1}{2} - x]$	[67, 259]
68	$[-z, \frac{1}{2} - x, y + \frac{1}{2}]$	[68, 260]
69	$[-y, \frac{1}{2} - z, x + \frac{1}{2}]$	[69, 261]
70	$[z, \frac{1}{2} - x, \frac{1}{2} - y]$	[70, 262]
71	$[y, \frac{1}{2} - z, \frac{1}{2} - x]$	[71, 263]
72	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[72, 264]
73	$[-x, \frac{1}{2} - y, \frac{1}{2} - z]$	[73, 265]
74	$[-x, z + \frac{1}{2}, \frac{1}{2} - y]$	[74, 266]
75	$[-x, \frac{1}{2} - z, y + \frac{1}{2}]$	[75, 267]

continued ...

Table 12

No.	position	mapping
76	$[-z, \frac{1}{2} - y, x + \frac{1}{2}]$	[76, 268]
77	$[z, \frac{1}{2} - y, \frac{1}{2} - x]$	[77, 269]
78	$[y, \frac{1}{2} - x, \frac{1}{2} - z]$	[78, 270]
79	$[-y, x + \frac{1}{2}, \frac{1}{2} - z]$	[79, 271]
80	$[-x, y + \frac{1}{2}, z + \frac{1}{2}]$	[80, 272]
81	$[x, \frac{1}{2} - y, z + \frac{1}{2}]$	[81, 273]
82	$[x, y + \frac{1}{2}, \frac{1}{2} - z]$	[82, 274]
83	$[-y, \frac{1}{2} - x, z + \frac{1}{2}]$	[83, 275]
84	$[y, x + \frac{1}{2}, z + \frac{1}{2}]$	[84, 276]
85	$[x, \frac{1}{2} - z, \frac{1}{2} - y]$	[85, 277]
86	$[x, z + \frac{1}{2}, y + \frac{1}{2}]$	[86, 278]
87	$[-z, y + \frac{1}{2}, \frac{1}{2} - x]$	[87, 279]
88	$[z, y + \frac{1}{2}, x + \frac{1}{2}]$	[88, 280]
89	$[-z, \frac{1}{2} - x, \frac{1}{2} - y]$	[89, 281]
90	$[-y, \frac{1}{2} - z, \frac{1}{2} - x]$	[90, 282]
91	$[y, \frac{1}{2} - z, x + \frac{1}{2}]$	[91, 283]
92	$[z, x + \frac{1}{2}, \frac{1}{2} - y]$	[92, 284]
93	$[y, z + \frac{1}{2}, \frac{1}{2} - x]$	[93, 285]
94	$[-z, x + \frac{1}{2}, y + \frac{1}{2}]$	[94, 286]
95	$[-y, z + \frac{1}{2}, x + \frac{1}{2}]$	[95, 287]
96	$[z, \frac{1}{2} - x, y + \frac{1}{2}]$	[96, 288]
97	$[x + \frac{1}{2}, y, z + \frac{1}{2}]$	[97, 289]
98	$[x + \frac{1}{2}, -z, y + \frac{1}{2}]$	[98, 290]
99	$[x + \frac{1}{2}, z, \frac{1}{2} - y]$	[99, 291]
100	$[z + \frac{1}{2}, y, \frac{1}{2} - x]$	[100, 292]
101	$[\frac{1}{2} - z, y, x + \frac{1}{2}]$	[101, 293]
102	$[\frac{1}{2} - y, x, z + \frac{1}{2}]$	[102, 294]
103	$[y + \frac{1}{2}, -x, z + \frac{1}{2}]$	[103, 295]
104	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[104, 296]
105	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[105, 297]
106	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[106, 298]
107	$[y + \frac{1}{2}, x, \frac{1}{2} - z]$	[107, 299]
108	$[\frac{1}{2} - y, -x, \frac{1}{2} - z]$	[108, 300]
109	$[\frac{1}{2} - x, z, y + \frac{1}{2}]$	[109, 301]
110	$[\frac{1}{2} - x, -z, \frac{1}{2} - y]$	[110, 302]
111	$[z + \frac{1}{2}, -y, x + \frac{1}{2}]$	[111, 303]
112	$[\frac{1}{2} - z, -y, \frac{1}{2} - x]$	[112, 304]
113	$[z + \frac{1}{2}, x, y + \frac{1}{2}]$	[113, 305]
114	$[y + \frac{1}{2}, z, x + \frac{1}{2}]$	[114, 306]
115	$[\frac{1}{2} - y, z, \frac{1}{2} - x]$	[115, 307]
116	$[\frac{1}{2} - z, -x, y + \frac{1}{2}]$	[116, 308]
117	$[\frac{1}{2} - y, -z, x + \frac{1}{2}]$	[117, 309]
118	$[z + \frac{1}{2}, -x, \frac{1}{2} - y]$	[118, 310]
119	$[y + \frac{1}{2}, -z, \frac{1}{2} - x]$	[119, 311]
120	$[\frac{1}{2} - z, x, \frac{1}{2} - y]$	[120, 312]
121	$[\frac{1}{2} - x, -y, \frac{1}{2} - z]$	[121, 313]
122	$[\frac{1}{2} - x, z, \frac{1}{2} - y]$	[122, 314]

continued ...

Table 12

No.	position	mapping
123	$[\frac{1}{2} - x, -z, y + \frac{1}{2}]$	[123,315]
124	$[\frac{1}{2} - z, -y, x + \frac{1}{2}]$	[124,316]
125	$[z + \frac{1}{2}, -y, \frac{1}{2} - x]$	[125,317]
126	$[y + \frac{1}{2}, -x, \frac{1}{2} - z]$	[126,318]
127	$[\frac{1}{2} - y, x, \frac{1}{2} - z]$	[127,319]
128	$[\frac{1}{2} - x, y, z + \frac{1}{2}]$	[128,320]
129	$[x + \frac{1}{2}, -y, z + \frac{1}{2}]$	[129,321]
130	$[x + \frac{1}{2}, y, \frac{1}{2} - z]$	[130,322]
131	$[\frac{1}{2} - y, -x, z + \frac{1}{2}]$	[131,323]
132	$[y + \frac{1}{2}, x, z + \frac{1}{2}]$	[132,324]
133	$[x + \frac{1}{2}, -z, \frac{1}{2} - y]$	[133,325]
134	$[x + \frac{1}{2}, z, y + \frac{1}{2}]$	[134,326]
135	$[\frac{1}{2} - z, y, \frac{1}{2} - x]$	[135,327]
136	$[z + \frac{1}{2}, y, x + \frac{1}{2}]$	[136,328]
137	$[\frac{1}{2} - z, -x, \frac{1}{2} - y]$	[137,329]
138	$[\frac{1}{2} - y, -z, \frac{1}{2} - x]$	[138,330]
139	$[y + \frac{1}{2}, -z, x + \frac{1}{2}]$	[139,331]
140	$[z + \frac{1}{2}, x, \frac{1}{2} - y]$	[140,332]
141	$[y + \frac{1}{2}, z, \frac{1}{2} - x]$	[141,333]
142	$[\frac{1}{2} - z, x, y + \frac{1}{2}]$	[142,334]
143	$[\frac{1}{2} - y, z, x + \frac{1}{2}]$	[143,335]
144	$[z + \frac{1}{2}, -x, y + \frac{1}{2}]$	[144,336]
145	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[145,337]
146	$[x + \frac{1}{2}, \frac{1}{2} - z, y]$	[146,338]
147	$[x + \frac{1}{2}, z + \frac{1}{2}, -y]$	[147,339]
148	$[z + \frac{1}{2}, y + \frac{1}{2}, -x]$	[148,340]
149	$[\frac{1}{2} - z, y + \frac{1}{2}, x]$	[149,341]
150	$[\frac{1}{2} - y, x + \frac{1}{2}, z]$	[150,342]
151	$[y + \frac{1}{2}, \frac{1}{2} - x, z]$	[151,343]
152	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[152,344]
153	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[153,345]
154	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[154,346]
155	$[y + \frac{1}{2}, x + \frac{1}{2}, -z]$	[155,347]
156	$[\frac{1}{2} - y, \frac{1}{2} - x, -z]$	[156,348]
157	$[\frac{1}{2} - x, z + \frac{1}{2}, y]$	[157,349]
158	$[\frac{1}{2} - x, \frac{1}{2} - z, -y]$	[158,350]
159	$[z + \frac{1}{2}, \frac{1}{2} - y, x]$	[159,351]
160	$[\frac{1}{2} - z, \frac{1}{2} - y, -x]$	[160,352]
161	$[z + \frac{1}{2}, x + \frac{1}{2}, y]$	[161,353]
162	$[y + \frac{1}{2}, z + \frac{1}{2}, x]$	[162,354]
163	$[\frac{1}{2} - y, z + \frac{1}{2}, -x]$	[163,355]
164	$[\frac{1}{2} - z, \frac{1}{2} - x, y]$	[164,356]
165	$[\frac{1}{2} - y, \frac{1}{2} - z, x]$	[165,357]
166	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[166,358]
167	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[167,359]
168	$[\frac{1}{2} - z, x + \frac{1}{2}, -y]$	[168,360]
169	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[169,361]

continued ...

Table 12

No.	position	mapping
170	$[\frac{1}{2} - x, z + \frac{1}{2}, -y]$	[170,362]
171	$[\frac{1}{2} - x, \frac{1}{2} - z, y]$	[171,363]
172	$[\frac{1}{2} - z, \frac{1}{2} - y, x]$	[172,364]
173	$[z + \frac{1}{2}, \frac{1}{2} - y, -x]$	[173,365]
174	$[y + \frac{1}{2}, \frac{1}{2} - x, -z]$	[174,366]
175	$[\frac{1}{2} - y, x + \frac{1}{2}, -z]$	[175,367]
176	$[\frac{1}{2} - x, y + \frac{1}{2}, z]$	[176,368]
177	$[x + \frac{1}{2}, \frac{1}{2} - y, z]$	[177,369]
178	$[x + \frac{1}{2}, y + \frac{1}{2}, -z]$	[178,370]
179	$[\frac{1}{2} - y, \frac{1}{2} - x, z]$	[179,371]
180	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[180,372]
181	$[x + \frac{1}{2}, \frac{1}{2} - z, -y]$	[181,373]
182	$[x + \frac{1}{2}, z + \frac{1}{2}, y]$	[182,374]
183	$[\frac{1}{2} - z, y + \frac{1}{2}, -x]$	[183,375]
184	$[z + \frac{1}{2}, y + \frac{1}{2}, x]$	[184,376]
185	$[\frac{1}{2} - z, \frac{1}{2} - x, -y]$	[185,377]
186	$[\frac{1}{2} - y, \frac{1}{2} - z, -x]$	[186,378]
187	$[y + \frac{1}{2}, \frac{1}{2} - z, x]$	[187,379]
188	$[z + \frac{1}{2}, x + \frac{1}{2}, -y]$	[188,380]
189	$[y + \frac{1}{2}, z + \frac{1}{2}, -x]$	[189,381]
190	$[\frac{1}{2} - z, x + \frac{1}{2}, y]$	[190,382]
191	$[\frac{1}{2} - y, z + \frac{1}{2}, x]$	[191,383]
192	$[z + \frac{1}{2}, \frac{1}{2} - x, y]$	[192,384]