

MSG No. 227.129  $Fd\bar{3}m1'$  [ Type II, cubic ]

Table 1: Wyckoff site: 8a, site symmetry:  $-43m1'$

No.	position	mapping
1	$[\frac{1}{8}, \frac{1}{8}, \frac{1}{8}]$	[1, 8, 9, 10, 17, 18, 19, 20, 21, 22, 23, 24, 26, 27, 28, 29, 30, 31, 35, 36, 37, 38, 39, 40, 193, 200, 201, 202, 209, 210, 211, 212, 213, 214, 215, 216, 218, 219, 220, 221, 222, 223, 227, 228, 229, 230, 231, 232]
2	$[\frac{3}{8}, \frac{7}{8}, \frac{3}{8}]$	[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	$[\frac{3}{8}, \frac{3}{8}, \frac{7}{8}]$	[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	$[\frac{7}{8}, \frac{3}{8}, \frac{3}{8}]$	[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	$[\frac{7}{8}, \frac{7}{8}, \frac{7}{8}]$	[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]
6	$[\frac{1}{8}, \frac{5}{8}, \frac{5}{8}]$	[49, 56, 57, 58, 65, 66, 67, 68, 69, 70, 71, 72, 74, 75, 76, 77, 78, 79, 83, 84, 85, 86, 87, 88, 241, 248, 249, 250, 257, 258, 259, 260, 261, 262, 263, 264, 266, 267, 268, 269, 270, 271, 275, 276, 277, 278, 279, 280]
7	$[\frac{5}{8}, \frac{1}{8}, \frac{5}{8}]$	[97, 104, 105, 106, 113, 114, 115, 116, 117, 118, 119, 120, 122, 123, 124, 125, 126, 127, 131, 132, 133, 134, 135, 136, 289, 296, 297, 298, 305, 306, 307, 308, 309, 310, 311, 312, 314, 315, 316, 317, 318, 319, 323, 324, 325, 326, 327, 328]
8	$[\frac{5}{8}, \frac{5}{8}, \frac{1}{8}]$	[145, 152, 153, 154, 161, 162, 163, 164, 165, 166, 167, 168, 170, 171, 172, 173, 174, 175, 179, 180, 181, 182, 183, 184, 337, 344, 345, 346, 353, 354, 355, 356, 357, 358, 359, 360, 362, 363, 364, 365, 366, 367, 371, 372, 373, 374, 375, 376]

Table 2: Wyckoff site: 8b, site symmetry:  $-43m1'$

No.	position	mapping
1	$[\frac{3}{8}, \frac{3}{8}, \frac{3}{8}]$	[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	$[\frac{5}{8}, \frac{5}{8}, \frac{5}{8}]$	[2, 3, 4, 5, 6, 7, 11, 12, 13, 14, 15, 16, 25, 32, 33, 34, 41, 42, 43, 44, 45, 46, 47, 48, 194, 195, 196, 197, 198, 199, 203, 204, 205, 206, 207, 208, 217, 224, 225, 226, 233, 234, 235, 236, 237, 238, 239, 240]
3	$[\frac{3}{8}, \frac{7}{8}, \frac{7}{8}]$	[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]
4	$[\frac{7}{8}, \frac{3}{8}, \frac{7}{8}]$	[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]
5	$[\frac{7}{8}, \frac{7}{8}, \frac{3}{8}]$	[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]
6	$[\frac{5}{8}, \frac{1}{8}, \frac{1}{8}]$	[50, 51, 52, 53, 54, 55, 59, 60, 61, 62, 63, 64, 73, 80, 81, 82, 89, 90, 91, 92, 93, 94, 95, 96, 242, 243, 244, 245, 246, 247, 251, 252, 253, 254, 255, 256, 265, 272, 273, 274, 281, 282, 283, 284, 285, 286, 287, 288]
7	$[\frac{1}{8}, \frac{5}{8}, \frac{1}{8}]$	[98, 99, 100, 101, 102, 103, 107, 108, 109, 110, 111, 112, 121, 128, 129, 130, 137, 138, 139, 140, 141, 142, 143, 144, 290, 291, 292, 293, 294, 295, 299, 300, 301, 302, 303, 304, 313, 320, 321, 322, 329, 330, 331, 332, 333, 334, 335, 336]
8	$[\frac{1}{8}, \frac{1}{8}, \frac{5}{8}]$	[146, 147, 148, 149, 150, 151, 155, 156, 157, 158, 159, 160, 169, 176, 177, 178, 185, 186, 187, 188, 189, 190, 191, 192, 338, 339, 340, 341, 342, 343, 347, 348, 349, 350, 351, 352, 361, 368, 369, 370, 377, 378, 379, 380, 381, 382, 383, 384]

Table 3: Wyckoff site: 16c, site symmetry:  $..-3m1'$ 

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

Table 4: Wyckoff site: 16d, site symmetry:  $..-3m1'$ 

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

Table 5: Wyckoff site: 32e, site symmetry:  $..3m1'$ 

No.	position	mapping
1	$[x, x, x]$	[1, 17, 18, 36, 38, 40, 193, 209, 210, 228, 230, 232]

continued ...

Table 5

No.	position	mapping
2	$[x + \frac{1}{4}, -x, x + \frac{1}{4}]$	[2, 7, 15, 33, 43, 48, 194, 199, 207, 225, 235, 240]
3	$[x + \frac{1}{4}, x + \frac{1}{4}, -x]$	[3, 4, 11, 34, 44, 45, 195, 196, 203, 226, 236, 237]
4	$[-x, x + \frac{1}{4}, x + \frac{1}{4}]$	[5, 6, 13, 32, 46, 47, 197, 198, 205, 224, 238, 239]
5	$[x, \frac{1}{4} - x, \frac{1}{4} - x]$	[8, 22, 23, 29, 30, 37, 200, 214, 215, 221, 222, 229]
6	$[\frac{1}{4} - x, x, \frac{1}{4} - x]$	[9, 19, 24, 26, 31, 39, 201, 211, 216, 218, 223, 231]
7	$[\frac{1}{4} - x, \frac{1}{4} - x, x]$	[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	$[x + \frac{1}{4}, \frac{1}{2} - x, x + \frac{3}{4}]$	[50, 55, 63, 81, 91, 96, 242, 247, 255, 273, 283, 288]
11	$[x + \frac{1}{4}, x + \frac{3}{4}, \frac{1}{2} - x]$	[51, 52, 59, 82, 92, 93, 243, 244, 251, 274, 284, 285]
12	$[-x, x + \frac{3}{4}, x + \frac{3}{4}]$	[53, 54, 61, 80, 94, 95, 245, 246, 253, 272, 286, 287]
13	$[x, \frac{3}{4} - x, \frac{3}{4} - x]$	[56, 70, 71, 77, 78, 85, 248, 262, 263, 269, 270, 277]
14	$[\frac{1}{4} - x, x + \frac{1}{2}, \frac{3}{4} - x]$	[57, 67, 72, 74, 79, 87, 249, 259, 264, 266, 271, 279]
15	$[\frac{1}{4} - x, \frac{3}{4} - x, x + \frac{1}{2}]$	[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	$[x + \frac{3}{4}, -x, x + \frac{3}{4}]$	[98, 103, 111, 129, 139, 144, 290, 295, 303, 321, 331, 336]
19	$[x + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{2} - x]$	[99, 100, 107, 130, 140, 141, 291, 292, 299, 322, 332, 333]
20	$[\frac{1}{2} - x, x + \frac{1}{4}, x + \frac{3}{4}]$	[101, 102, 109, 128, 142, 143, 293, 294, 301, 320, 334, 335]
21	$[x + \frac{1}{2}, \frac{1}{4} - x, \frac{3}{4} - x]$	[104, 118, 119, 125, 126, 133, 296, 310, 311, 317, 318, 325]
22	$[\frac{3}{4} - x, x, \frac{3}{4} - x]$	[105, 115, 120, 122, 127, 135, 297, 307, 312, 314, 319, 327]
23	$[\frac{3}{4} - x, \frac{1}{4} - x, x + \frac{1}{2}]$	[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	$[x + \frac{3}{4}, \frac{1}{2} - x, x + \frac{1}{4}]$	[146, 151, 159, 177, 187, 192, 338, 343, 351, 369, 379, 384]
27	$[x + \frac{3}{4}, x + \frac{3}{4}, -x]$	[147, 148, 155, 178, 188, 189, 339, 340, 347, 370, 380, 381]
28	$[\frac{1}{2} - x, x + \frac{3}{4}, x + \frac{1}{4}]$	[149, 150, 157, 176, 190, 191, 341, 342, 349, 368, 382, 383]
29	$[x + \frac{1}{2}, \frac{3}{4} - x, \frac{1}{4} - x]$	[152, 166, 167, 173, 174, 181, 344, 358, 359, 365, 366, 373]
30	$[\frac{3}{4} - x, x + \frac{1}{2}, \frac{1}{4} - x]$	[153, 163, 168, 170, 175, 183, 345, 355, 360, 362, 367, 375]
31	$[\frac{3}{4} - x, \frac{3}{4} - x, x]$	[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 6: Wyckoff site: 48f, site symmetry:  $2.mm1'$ 

No.	position	mapping
1	$[x, \frac{1}{8}, \frac{1}{8}]$	[1, 8, 37, 38, 193, 200, 229, 230]
2	$[x + \frac{1}{4}, \frac{7}{8}, \frac{3}{8}]$	[2, 33, 51, 82, 194, 225, 243, 274]
3	$[x + \frac{1}{4}, \frac{3}{8}, \frac{7}{8}]$	[3, 34, 50, 81, 195, 226, 242, 273]
4	$[\frac{3}{8}, \frac{3}{8}, -x]$	[4, 45, 160, 186, 196, 237, 352, 378]
5	$[\frac{7}{8}, \frac{3}{8}, x + \frac{1}{4}]$	[5, 47, 159, 187, 197, 239, 351, 379]
6	$[\frac{7}{8}, x + \frac{1}{4}, \frac{3}{8}]$	[6, 46, 107, 140, 198, 238, 299, 332]
7	$[\frac{3}{8}, -x, \frac{3}{8}]$	[7, 48, 108, 137, 199, 240, 300, 329]
8	$[\frac{1}{4} - x, \frac{1}{8}, \frac{1}{8}]$	[9, 10, 26, 27, 201, 202, 218, 219]
9	$[\frac{3}{8}, x + \frac{1}{4}, \frac{7}{8}]$	[11, 44, 102, 142, 203, 236, 294, 334]

*continued ...*

Table 6

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

Table 7: Wyckoff site: 96g, site symmetry:  $..m1'$ 

No.	position	mapping
1	$[x, x, z]$	[1, 36, 193, 228]

*continued ...*

Table 7

No.	position	mapping
2	$[x + \frac{1}{4}, -z, x + \frac{1}{4}]$	[2, 43, 194, 235]
3	$[x + \frac{1}{4}, z + \frac{1}{4}, -x]$	[3, 45, 195, 237]
4	$[z + \frac{1}{4}, x + \frac{1}{4}, -x]$	[4, 44, 196, 236]
5	$[-z, x + \frac{1}{4}, x + \frac{1}{4}]$	[5, 46, 197, 238]
6	$[-x, x + \frac{1}{4}, z + \frac{1}{4}]$	[6, 32, 198, 224]
7	$[x + \frac{1}{4}, -x, z + \frac{1}{4}]$	[7, 33, 199, 225]
8	$[x, \frac{1}{4} - x, \frac{1}{4} - z]$	[8, 30, 200, 222]
9	$[\frac{1}{4} - x, x, \frac{1}{4} - z]$	[9, 31, 201, 223]
10	$[\frac{1}{4} - x, \frac{1}{4} - x, z]$	[10, 35, 202, 227]
11	$[x + \frac{1}{4}, x + \frac{1}{4}, -z]$	[11, 34, 203, 226]
12	$[-x, -x, -z]$	[12, 25, 204, 217]
13	$[-x, z + \frac{1}{4}, x + \frac{1}{4}]$	[13, 47, 205, 239]
14	$[-x, -z, -x]$	[14, 42, 206, 234]
15	$[z + \frac{1}{4}, -x, x + \frac{1}{4}]$	[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	$[\frac{1}{4} - x, z, \frac{1}{4} - x]$	[19, 26, 211, 218]
20	$[\frac{1}{4} - z, \frac{1}{4} - x, x]$	[20, 28, 212, 220]
21	$[\frac{1}{4} - x, \frac{1}{4} - z, x]$	[21, 27, 213, 219]
22	$[z, \frac{1}{4} - x, \frac{1}{4} - x]$	[22, 29, 214, 221]
23	$[x, \frac{1}{4} - z, \frac{1}{4} - x]$	[23, 37, 215, 229]
24	$[\frac{1}{4} - z, x, \frac{1}{4} - x]$	[24, 39, 216, 231]
25	$[x, x + \frac{1}{2}, z + \frac{1}{2}]$	[49, 84, 241, 276]
26	$[x + \frac{1}{4}, \frac{1}{2} - z, x + \frac{3}{4}]$	[50, 91, 242, 283]
27	$[x + \frac{1}{4}, z + \frac{3}{4}, \frac{1}{2} - x]$	[51, 93, 243, 285]
28	$[z + \frac{1}{4}, x + \frac{3}{4}, \frac{1}{2} - x]$	[52, 92, 244, 284]
29	$[-z, x + \frac{3}{4}, x + \frac{3}{4}]$	[53, 94, 245, 286]
30	$[-x, x + \frac{3}{4}, z + \frac{3}{4}]$	[54, 80, 246, 272]
31	$[x + \frac{1}{4}, \frac{1}{2} - x, z + \frac{3}{4}]$	[55, 81, 247, 273]
32	$[x, \frac{3}{4} - x, \frac{3}{4} - z]$	[56, 78, 248, 270]
33	$[\frac{1}{4} - x, x + \frac{1}{2}, \frac{3}{4} - z]$	[57, 79, 249, 271]
34	$[\frac{1}{4} - x, \frac{3}{4} - x, z + \frac{1}{2}]$	[58, 83, 250, 275]
35	$[x + \frac{1}{4}, x + \frac{3}{4}, \frac{1}{2} - z]$	[59, 82, 251, 274]
36	$[-x, \frac{1}{2} - x, \frac{1}{2} - z]$	[60, 73, 252, 265]
37	$[-x, z + \frac{3}{4}, x + \frac{3}{4}]$	[61, 95, 253, 287]
38	$[-x, \frac{1}{2} - z, \frac{1}{2} - x]$	[62, 90, 254, 282]
39	$[z + \frac{1}{4}, \frac{1}{2} - x, x + \frac{3}{4}]$	[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	$[\frac{1}{4} - x, z + \frac{1}{2}, \frac{3}{4} - x]$	[67, 74, 259, 266]
44	$[\frac{1}{4} - z, \frac{3}{4} - x, x + \frac{1}{2}]$	[68, 76, 260, 268]
45	$[\frac{1}{4} - x, \frac{3}{4} - z, x + \frac{1}{2}]$	[69, 75, 261, 267]
46	$[z, \frac{3}{4} - x, \frac{3}{4} - x]$	[70, 77, 262, 269]
47	$[x, \frac{3}{4} - z, \frac{3}{4} - x]$	[71, 85, 263, 277]
48	$[\frac{1}{4} - z, x + \frac{1}{2}, \frac{3}{4} - x]$	[72, 87, 264, 279]

continued ...

Table 7

No.	position	mapping
49	$[x + \frac{1}{2}, x, z + \frac{1}{2}]$	[97, 132, 289, 324]
50	$[x + \frac{3}{4}, -z, x + \frac{3}{4}]$	[98, 139, 290, 331]
51	$[x + \frac{3}{4}, z + \frac{1}{4}, \frac{1}{2} - x]$	[99, 141, 291, 333]
52	$[z + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{2} - x]$	[100, 140, 292, 332]
53	$[\frac{1}{2} - z, x + \frac{1}{4}, x + \frac{3}{4}]$	[101, 142, 293, 334]
54	$[\frac{1}{2} - x, x + \frac{1}{4}, z + \frac{3}{4}]$	[102, 128, 294, 320]
55	$[x + \frac{3}{4}, -x, z + \frac{3}{4}]$	[103, 129, 295, 321]
56	$[x + \frac{1}{2}, \frac{1}{4} - x, \frac{3}{4} - z]$	[104, 126, 296, 318]
57	$[\frac{3}{4} - x, x, \frac{3}{4} - z]$	[105, 127, 297, 319]
58	$[\frac{3}{4} - x, \frac{1}{4} - x, z + \frac{1}{2}]$	[106, 131, 298, 323]
59	$[x + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{2} - z]$	[107, 130, 299, 322]
60	$[\frac{1}{2} - x, -x, \frac{1}{2} - z]$	[108, 121, 300, 313]
61	$[\frac{1}{2} - x, z + \frac{1}{4}, x + \frac{3}{4}]$	[109, 143, 301, 335]
62	$[\frac{1}{2} - x, -z, \frac{1}{2} - x]$	[110, 138, 302, 330]
63	$[z + \frac{3}{4}, -x, x + \frac{3}{4}]$	[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	$[\frac{3}{4} - x, z, \frac{3}{4} - x]$	[115, 122, 307, 314]
68	$[\frac{3}{4} - z, \frac{1}{4} - x, x + \frac{1}{2}]$	[116, 124, 308, 316]
69	$[\frac{3}{4} - x, \frac{1}{4} - z, x + \frac{1}{2}]$	[117, 123, 309, 315]
70	$[z + \frac{1}{2}, \frac{1}{4} - x, \frac{3}{4} - x]$	[118, 125, 310, 317]
71	$[x + \frac{1}{2}, \frac{1}{4} - z, \frac{3}{4} - x]$	[119, 133, 311, 325]
72	$[\frac{3}{4} - z, x, \frac{3}{4} - x]$	[120, 135, 312, 327]
73	$[x + \frac{1}{2}, x + \frac{1}{2}, z]$	[145, 180, 337, 372]
74	$[x + \frac{3}{4}, \frac{1}{2} - z, x + \frac{1}{4}]$	[146, 187, 338, 379]
75	$[x + \frac{3}{4}, z + \frac{3}{4}, -x]$	[147, 189, 339, 381]
76	$[z + \frac{3}{4}, x + \frac{3}{4}, -x]$	[148, 188, 340, 380]
77	$[\frac{1}{2} - z, x + \frac{3}{4}, x + \frac{1}{4}]$	[149, 190, 341, 382]
78	$[\frac{1}{2} - x, x + \frac{3}{4}, z + \frac{1}{4}]$	[150, 176, 342, 368]
79	$[x + \frac{3}{4}, \frac{1}{2} - x, z + \frac{1}{4}]$	[151, 177, 343, 369]
80	$[x + \frac{1}{2}, \frac{3}{4} - x, \frac{1}{4} - z]$	[152, 174, 344, 366]
81	$[\frac{3}{4} - x, x + \frac{1}{2}, \frac{1}{4} - z]$	[153, 175, 345, 367]
82	$[\frac{3}{4} - x, \frac{3}{4} - x, z]$	[154, 179, 346, 371]
83	$[x + \frac{3}{4}, x + \frac{3}{4}, -z]$	[155, 178, 347, 370]
84	$[\frac{1}{2} - x, \frac{1}{2} - x, -z]$	[156, 169, 348, 361]
85	$[\frac{1}{2} - x, z + \frac{3}{4}, x + \frac{1}{4}]$	[157, 191, 349, 383]
86	$[\frac{1}{2} - x, \frac{1}{2} - z, -x]$	[158, 186, 350, 378]
87	$[z + \frac{3}{4}, \frac{1}{2} - x, x + \frac{1}{4}]$	[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	$[\frac{3}{4} - x, z + \frac{1}{2}, \frac{1}{4} - x]$	[163, 170, 355, 362]
92	$[\frac{3}{4} - z, \frac{3}{4} - x, x]$	[164, 172, 356, 364]
93	$[\frac{3}{4} - x, \frac{3}{4} - z, x]$	[165, 171, 357, 363]
94	$[z + \frac{1}{2}, \frac{3}{4} - x, \frac{1}{4} - x]$	[166, 173, 358, 365]
95	$[x + \frac{1}{2}, \frac{3}{4} - z, \frac{1}{4} - x]$	[167, 181, 359, 373]

continued ...

Table 7

No.	position	mapping
96	$[\frac{3}{4} - z, x + \frac{1}{2}, \frac{1}{4} - x]$	[168, 183, 360, 375]

Table 8: Wyckoff site: 96h, site symmetry:  $\cdot \cdot 21'$ 

No.	position	mapping
1	$[0, y, -y]$	[1, 14, 193, 206]
2	$[\frac{1}{4}, y, y + \frac{1}{4}]$	[2, 9, 194, 201]
3	$[\frac{1}{4}, \frac{1}{4} - y, -y]$	[3, 10, 195, 202]
4	$[\frac{1}{4} - y, y + \frac{1}{4}, 0]$	[4, 21, 196, 213]
5	$[y, y + \frac{1}{4}, \frac{1}{4}]$	[5, 23, 197, 215]
6	$[-y, \frac{1}{4}, \frac{1}{4} - y]$	[6, 22, 198, 214]
7	$[y + \frac{1}{4}, 0, \frac{1}{4} - y]$	[7, 24, 199, 216]
8	$[0, \frac{1}{4} - y, y + \frac{1}{4}]$	[8, 13, 200, 205]
9	$[y + \frac{1}{4}, \frac{1}{4}, y]$	[11, 20, 203, 212]
10	$[-y, 0, y]$	[12, 17, 204, 209]
11	$[\frac{1}{4} - y, -y, \frac{1}{4}]$	[15, 19, 207, 211]
12	$[y, -y, 0]$	[16, 18, 208, 210]
13	$[0, -y, y]$	[25, 38, 217, 230]
14	$[\frac{1}{4}, -y, \frac{1}{4} - y]$	[26, 33, 218, 225]
15	$[\frac{1}{4}, y + \frac{1}{4}, y]$	[27, 34, 219, 226]
16	$[y + \frac{1}{4}, \frac{1}{4} - y, 0]$	[28, 45, 220, 237]
17	$[-y, \frac{1}{4} - y, \frac{1}{4}]$	[29, 47, 221, 239]
18	$[y, \frac{1}{4}, y + \frac{1}{4}]$	[30, 46, 222, 238]
19	$[\frac{1}{4} - y, 0, y + \frac{1}{4}]$	[31, 48, 223, 240]
20	$[0, y + \frac{1}{4}, \frac{1}{4} - y]$	[32, 37, 224, 229]
21	$[\frac{1}{4} - y, \frac{1}{4}, -y]$	[35, 44, 227, 236]
22	$[y, 0, -y]$	[36, 41, 228, 233]
23	$[y + \frac{1}{4}, y, \frac{1}{4}]$	[39, 43, 231, 235]
24	$[-y, y, 0]$	[40, 42, 232, 234]
25	$[0, y + \frac{1}{2}, \frac{1}{2} - y]$	[49, 62, 241, 254]
26	$[\frac{1}{4}, y + \frac{1}{2}, y + \frac{3}{4}]$	[50, 57, 242, 249]
27	$[\frac{1}{4}, \frac{3}{4} - y, \frac{1}{2} - y]$	[51, 58, 243, 250]
28	$[\frac{1}{4} - y, y + \frac{3}{4}, \frac{1}{2}]$	[52, 69, 244, 261]
29	$[y, y + \frac{3}{4}, \frac{3}{4}]$	[53, 71, 245, 263]
30	$[-y, \frac{3}{4}, \frac{3}{4} - y]$	[54, 70, 246, 262]
31	$[y + \frac{1}{4}, \frac{1}{2}, \frac{3}{4} - y]$	[55, 72, 247, 264]
32	$[0, \frac{3}{4} - y, y + \frac{3}{4}]$	[56, 61, 248, 253]
33	$[y + \frac{1}{4}, \frac{3}{4}, y + \frac{1}{2}]$	[59, 68, 251, 260]
34	$[-y, \frac{1}{2}, y + \frac{1}{2}]$	[60, 65, 252, 257]
35	$[\frac{1}{4} - y, \frac{1}{2} - y, \frac{3}{4}]$	[63, 67, 255, 259]
36	$[y, \frac{1}{2} - y, \frac{1}{2}]$	[64, 66, 256, 258]
37	$[0, \frac{1}{2} - y, y + \frac{1}{2}]$	[73, 86, 265, 278]
38	$[\frac{1}{4}, \frac{1}{2} - y, \frac{3}{4} - y]$	[74, 81, 266, 273]
39	$[\frac{1}{4}, y + \frac{3}{4}, y + \frac{1}{2}]$	[75, 82, 267, 274]

continued ...

Table 8

No.	position	mapping
40	$[y + \frac{1}{4}, \frac{3}{4} - y, \frac{1}{2}]$	[76, 93, 268, 285]
41	$[-y, \frac{3}{4} - y, \frac{3}{4}]$	[77, 95, 269, 287]
42	$[y, \frac{3}{4}, y + \frac{3}{4}]$	[78, 94, 270, 286]
43	$[\frac{1}{4} - y, \frac{1}{2}, y + \frac{3}{4}]$	[79, 96, 271, 288]
44	$[0, y + \frac{3}{4}, \frac{3}{4} - y]$	[80, 85, 272, 277]
45	$[\frac{1}{4} - y, \frac{3}{4}, \frac{1}{2} - y]$	[83, 92, 275, 284]
46	$[y, \frac{1}{2}, \frac{1}{2} - y]$	[84, 89, 276, 281]
47	$[y + \frac{1}{4}, y + \frac{1}{2}, \frac{3}{4}]$	[87, 91, 279, 283]
48	$[-y, y + \frac{1}{2}, \frac{1}{2}]$	[88, 90, 280, 282]
49	$[\frac{1}{2}, y, \frac{1}{2} - y]$	[97, 110, 289, 302]
50	$[\frac{3}{4}, y, y + \frac{3}{4}]$	[98, 105, 290, 297]
51	$[\frac{3}{4}, \frac{1}{4} - y, \frac{1}{2} - y]$	[99, 106, 291, 298]
52	$[\frac{3}{4} - y, y + \frac{1}{4}, \frac{1}{2}]$	[100, 117, 292, 309]
53	$[y + \frac{1}{2}, y + \frac{1}{4}, \frac{3}{4}]$	[101, 119, 293, 311]
54	$[\frac{1}{2} - y, \frac{1}{4}, \frac{3}{4} - y]$	[102, 118, 294, 310]
55	$[y + \frac{3}{4}, 0, \frac{3}{4} - y]$	[103, 120, 295, 312]
56	$[\frac{1}{2}, \frac{1}{4} - y, y + \frac{3}{4}]$	[104, 109, 296, 301]
57	$[y + \frac{3}{4}, \frac{1}{4}, y + \frac{1}{2}]$	[107, 116, 299, 308]
58	$[\frac{1}{2} - y, 0, y + \frac{1}{2}]$	[108, 113, 300, 305]
59	$[\frac{3}{4} - y, -y, \frac{3}{4}]$	[111, 115, 303, 307]
60	$[y + \frac{1}{2}, -y, \frac{1}{2}]$	[112, 114, 304, 306]
61	$[\frac{1}{2}, -y, y + \frac{1}{2}]$	[121, 134, 313, 326]
62	$[\frac{3}{4}, -y, \frac{3}{4} - y]$	[122, 129, 314, 321]
63	$[\frac{3}{4}, y + \frac{1}{4}, y + \frac{1}{2}]$	[123, 130, 315, 322]
64	$[y + \frac{3}{4}, \frac{1}{4} - y, \frac{1}{2}]$	[124, 141, 316, 333]
65	$[\frac{1}{2} - y, \frac{1}{4} - y, \frac{3}{4}]$	[125, 143, 317, 335]
66	$[y + \frac{1}{2}, \frac{1}{4}, y + \frac{3}{4}]$	[126, 142, 318, 334]
67	$[\frac{3}{4} - y, 0, y + \frac{3}{4}]$	[127, 144, 319, 336]
68	$[\frac{1}{2}, y + \frac{1}{4}, \frac{3}{4} - y]$	[128, 133, 320, 325]
69	$[\frac{3}{4} - y, \frac{1}{4}, \frac{1}{2} - y]$	[131, 140, 323, 332]
70	$[y + \frac{1}{2}, 0, \frac{1}{2} - y]$	[132, 137, 324, 329]
71	$[y + \frac{3}{4}, y, \frac{3}{4}]$	[135, 139, 327, 331]
72	$[\frac{1}{2} - y, y, \frac{1}{2}]$	[136, 138, 328, 330]
73	$[\frac{1}{2}, y + \frac{1}{2}, -y]$	[145, 158, 337, 350]
74	$[\frac{3}{4}, y + \frac{1}{2}, y + \frac{1}{4}]$	[146, 153, 338, 345]
75	$[\frac{3}{4}, \frac{3}{4} - y, -y]$	[147, 154, 339, 346]
76	$[\frac{3}{4} - y, y + \frac{3}{4}, 0]$	[148, 165, 340, 357]
77	$[y + \frac{1}{2}, y + \frac{3}{4}, \frac{1}{4}]$	[149, 167, 341, 359]
78	$[\frac{1}{2} - y, \frac{3}{4}, \frac{1}{4} - y]$	[150, 166, 342, 358]
79	$[y + \frac{3}{4}, \frac{1}{2}, \frac{1}{4} - y]$	[151, 168, 343, 360]
80	$[\frac{1}{2}, \frac{3}{4} - y, y + \frac{1}{4}]$	[152, 157, 344, 349]
81	$[y + \frac{3}{4}, \frac{3}{4}, y]$	[155, 164, 347, 356]
82	$[\frac{1}{2} - y, \frac{1}{2}, y]$	[156, 161, 348, 353]
83	$[\frac{3}{4} - y, \frac{1}{2} - y, \frac{1}{4}]$	[159, 163, 351, 355]
84	$[y + \frac{1}{2}, \frac{1}{2} - y, 0]$	[160, 162, 352, 354]
85	$[\frac{1}{2}, \frac{1}{2} - y, y]$	[169, 182, 361, 374]
86	$[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{4} - y]$	[170, 177, 362, 369]

continued ...

Table 8

No.	position	mapping
87	$[\frac{3}{4}, y + \frac{3}{4}, y]$	[171, 178, 363, 370]
88	$[y + \frac{3}{4}, \frac{3}{4} - y, 0]$	[172, 189, 364, 381]
89	$[\frac{1}{2} - y, \frac{3}{4} - y, \frac{1}{4}]$	[173, 191, 365, 383]
90	$[y + \frac{1}{2}, \frac{3}{4}, y + \frac{1}{4}]$	[174, 190, 366, 382]
91	$[\frac{3}{4} - y, \frac{1}{2}, y + \frac{1}{4}]$	[175, 192, 367, 384]
92	$[\frac{1}{2}, y + \frac{3}{4}, \frac{1}{4} - y]$	[176, 181, 368, 373]
93	$[\frac{3}{4} - y, \frac{3}{4}, -y]$	[179, 188, 371, 380]
94	$[y + \frac{1}{2}, \frac{1}{2}, -y]$	[180, 185, 372, 377]
95	$[y + \frac{3}{4}, y + \frac{1}{2}, \frac{1}{4}]$	[183, 187, 375, 379]
96	$[\frac{1}{2} - y, y + \frac{1}{2}, 0]$	[184, 186, 376, 378]

Table 9: Wyckoff site: 192i, site symmetry: 11'

No.	position	mapping
1	$[x, y, z]$	[1, 193]
2	$[x + \frac{1}{4}, -z, y + \frac{1}{4}]$	[2, 194]
3	$[x + \frac{1}{4}, z + \frac{1}{4}, -y]$	[3, 195]
4	$[z + \frac{1}{4}, y + \frac{1}{4}, -x]$	[4, 196]
5	$[-z, y + \frac{1}{4}, x + \frac{1}{4}]$	[5, 197]
6	$[-y, x + \frac{1}{4}, z + \frac{1}{4}]$	[6, 198]
7	$[y + \frac{1}{4}, -x, z + \frac{1}{4}]$	[7, 199]
8	$[x, \frac{1}{4} - y, \frac{1}{4} - z]$	[8, 200]
9	$[\frac{1}{4} - x, y, \frac{1}{4} - z]$	[9, 201]
10	$[\frac{1}{4} - x, \frac{1}{4} - y, z]$	[10, 202]
11	$[y + \frac{1}{4}, x + \frac{1}{4}, -z]$	[11, 203]
12	$[-y, -x, -z]$	[12, 204]
13	$[-x, z + \frac{1}{4}, y + \frac{1}{4}]$	[13, 205]
14	$[-x, -z, -y]$	[14, 206]
15	$[z + \frac{1}{4}, -y, x + \frac{1}{4}]$	[15, 207]
16	$[-z, -y, -x]$	[16, 208]
17	$[z, x, y]$	[17, 209]
18	$[y, z, x]$	[18, 210]
19	$[\frac{1}{4} - y, z, \frac{1}{4} - x]$	[19, 211]
20	$[\frac{1}{4} - z, \frac{1}{4} - x, y]$	[20, 212]
21	$[\frac{1}{4} - y, \frac{1}{4} - z, x]$	[21, 213]
22	$[z, \frac{1}{4} - x, \frac{1}{4} - y]$	[22, 214]
23	$[y, \frac{1}{4} - z, \frac{1}{4} - x]$	[23, 215]
24	$[\frac{1}{4} - z, x, \frac{1}{4} - y]$	[24, 216]
25	$[-x, -y, -z]$	[25, 217]
26	$[\frac{1}{4} - x, z, \frac{1}{4} - y]$	[26, 218]
27	$[\frac{1}{4} - x, \frac{1}{4} - z, y]$	[27, 219]
28	$[\frac{1}{4} - z, \frac{1}{4} - y, x]$	[28, 220]
29	$[z, \frac{1}{4} - y, \frac{1}{4} - x]$	[29, 221]
30	$[y, \frac{1}{4} - x, \frac{1}{4} - z]$	[30, 222]

continued ...

Table 9

No.	position	mapping
31	$[\frac{1}{4} - y, x, \frac{1}{4} - z]$	[31, 223]
32	$[-x, y + \frac{1}{4}, z + \frac{1}{4}]$	[32, 224]
33	$[x + \frac{1}{4}, -y, z + \frac{1}{4}]$	[33, 225]
34	$[x + \frac{1}{4}, y + \frac{1}{4}, -z]$	[34, 226]
35	$[\frac{1}{4} - y, \frac{1}{4} - x, z]$	[35, 227]
36	$[y, x, z]$	[36, 228]
37	$[x, \frac{1}{4} - z, \frac{1}{4} - y]$	[37, 229]
38	$[x, z, y]$	[38, 230]
39	$[\frac{1}{4} - z, y, \frac{1}{4} - x]$	[39, 231]
40	$[z, y, x]$	[40, 232]
41	$[-z, -x, -y]$	[41, 233]
42	$[-y, -z, -x]$	[42, 234]
43	$[y + \frac{1}{4}, -z, x + \frac{1}{4}]$	[43, 235]
44	$[z + \frac{1}{4}, x + \frac{1}{4}, -y]$	[44, 236]
45	$[y + \frac{1}{4}, z + \frac{1}{4}, -x]$	[45, 237]
46	$[-z, x + \frac{1}{4}, y + \frac{1}{4}]$	[46, 238]
47	$[-y, z + \frac{1}{4}, x + \frac{1}{4}]$	[47, 239]
48	$[z + \frac{1}{4}, -x, y + \frac{1}{4}]$	[48, 240]
49	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[49, 241]
50	$[x + \frac{1}{4}, \frac{1}{2} - z, y + \frac{3}{4}]$	[50, 242]
51	$[x + \frac{1}{4}, z + \frac{3}{4}, \frac{1}{2} - y]$	[51, 243]
52	$[z + \frac{1}{4}, y + \frac{3}{4}, \frac{1}{2} - x]$	[52, 244]
53	$[-z, y + \frac{3}{4}, x + \frac{3}{4}]$	[53, 245]
54	$[-y, x + \frac{3}{4}, z + \frac{3}{4}]$	[54, 246]
55	$[y + \frac{1}{4}, \frac{1}{2} - x, z + \frac{3}{4}]$	[55, 247]
56	$[x, \frac{3}{4} - y, \frac{3}{4} - z]$	[56, 248]
57	$[\frac{1}{4} - x, y + \frac{1}{2}, \frac{3}{4} - z]$	[57, 249]
58	$[\frac{1}{4} - x, \frac{3}{4} - y, z + \frac{1}{2}]$	[58, 250]
59	$[y + \frac{1}{4}, x + \frac{3}{4}, \frac{1}{2} - z]$	[59, 251]
60	$[-y, \frac{1}{2} - x, \frac{1}{2} - z]$	[60, 252]
61	$[-x, z + \frac{3}{4}, y + \frac{3}{4}]$	[61, 253]
62	$[-x, \frac{1}{2} - z, \frac{1}{2} - y]$	[62, 254]
63	$[z + \frac{1}{4}, \frac{1}{2} - y, x + \frac{3}{4}]$	[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	$[\frac{1}{4} - y, z + \frac{1}{2}, \frac{3}{4} - x]$	[67, 259]
68	$[\frac{1}{4} - z, \frac{3}{4} - x, y + \frac{1}{2}]$	[68, 260]
69	$[\frac{1}{4} - y, \frac{3}{4} - z, x + \frac{1}{2}]$	[69, 261]
70	$[z, \frac{3}{4} - x, \frac{3}{4} - y]$	[70, 262]
71	$[y, \frac{3}{4} - z, \frac{3}{4} - x]$	[71, 263]
72	$[\frac{1}{4} - z, x + \frac{1}{2}, \frac{3}{4} - y]$	[72, 264]
73	$[-x, \frac{1}{2} - y, \frac{1}{2} - z]$	[73, 265]
74	$[\frac{1}{4} - x, z + \frac{1}{2}, \frac{3}{4} - y]$	[74, 266]
75	$[\frac{1}{4} - x, \frac{3}{4} - z, y + \frac{1}{2}]$	[75, 267]
76	$[\frac{1}{4} - z, \frac{3}{4} - y, x + \frac{1}{2}]$	[76, 268]
77	$[z, \frac{3}{4} - y, \frac{3}{4} - x]$	[77, 269]

continued ...

Table 9

No.	position	mapping
78	$[y, \frac{3}{4} - x, \frac{3}{4} - z]$	[78, 270]
79	$[\frac{1}{4} - y, x + \frac{1}{2}, \frac{3}{4} - z]$	[79, 271]
80	$[-x, y + \frac{3}{4}, z + \frac{3}{4}]$	[80, 272]
81	$[x + \frac{1}{4}, \frac{1}{2} - y, z + \frac{3}{4}]$	[81, 273]
82	$[x + \frac{1}{4}, y + \frac{3}{4}, \frac{1}{2} - z]$	[82, 274]
83	$[\frac{1}{4} - y, \frac{3}{4} - x, z + \frac{1}{2}]$	[83, 275]
84	$[y, x + \frac{1}{2}, z + \frac{1}{2}]$	[84, 276]
85	$[x, \frac{3}{4} - z, \frac{3}{4} - y]$	[85, 277]
86	$[x, z + \frac{1}{2}, y + \frac{1}{2}]$	[86, 278]
87	$[\frac{1}{4} - z, y + \frac{1}{2}, \frac{3}{4} - x]$	[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	$[y + \frac{1}{4}, \frac{1}{2} - z, x + \frac{3}{4}]$	[91, 283]
92	$[z + \frac{1}{4}, x + \frac{3}{4}, \frac{1}{2} - y]$	[92, 284]
93	$[y + \frac{1}{4}, z + \frac{3}{4}, \frac{1}{2} - x]$	[93, 285]
94	$[-z, x + \frac{3}{4}, y + \frac{3}{4}]$	[94, 286]
95	$[-y, z + \frac{3}{4}, x + \frac{3}{4}]$	[95, 287]
96	$[z + \frac{1}{4}, \frac{1}{2} - x, y + \frac{3}{4}]$	[96, 288]
97	$[x + \frac{1}{2}, y, z + \frac{1}{2}]$	[97, 289]
98	$[x + \frac{3}{4}, -z, y + \frac{3}{4}]$	[98, 290]
99	$[x + \frac{3}{4}, z + \frac{1}{4}, \frac{1}{2} - y]$	[99, 291]
100	$[z + \frac{3}{4}, y + \frac{1}{4}, \frac{1}{2} - x]$	[100, 292]
101	$[\frac{1}{2} - z, y + \frac{1}{4}, x + \frac{3}{4}]$	[101, 293]
102	$[\frac{1}{2} - y, x + \frac{1}{4}, z + \frac{3}{4}]$	[102, 294]
103	$[y + \frac{3}{4}, -x, z + \frac{3}{4}]$	[103, 295]
104	$[x + \frac{1}{2}, \frac{1}{4} - y, \frac{3}{4} - z]$	[104, 296]
105	$[\frac{3}{4} - x, y, \frac{3}{4} - z]$	[105, 297]
106	$[\frac{3}{4} - x, \frac{1}{4} - y, z + \frac{1}{2}]$	[106, 298]
107	$[y + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{2} - z]$	[107, 299]
108	$[\frac{1}{2} - y, -x, \frac{1}{2} - z]$	[108, 300]
109	$[\frac{1}{2} - x, z + \frac{1}{4}, y + \frac{3}{4}]$	[109, 301]
110	$[\frac{1}{2} - x, -z, \frac{1}{2} - y]$	[110, 302]
111	$[z + \frac{3}{4}, -y, x + \frac{3}{4}]$	[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	$[\frac{3}{4} - y, z, \frac{3}{4} - x]$	[115, 307]
116	$[\frac{3}{4} - z, \frac{1}{4} - x, y + \frac{1}{2}]$	[116, 308]
117	$[\frac{3}{4} - y, \frac{1}{4} - z, x + \frac{1}{2}]$	[117, 309]
118	$[z + \frac{1}{2}, \frac{1}{4} - x, \frac{3}{4} - y]$	[118, 310]
119	$[y + \frac{1}{2}, \frac{1}{4} - z, \frac{3}{4} - x]$	[119, 311]
120	$[\frac{3}{4} - z, x, \frac{3}{4} - y]$	[120, 312]
121	$[\frac{1}{2} - x, -y, \frac{1}{2} - z]$	[121, 313]
122	$[\frac{3}{4} - x, z, \frac{3}{4} - y]$	[122, 314]
123	$[\frac{3}{4} - x, \frac{1}{4} - z, y + \frac{1}{2}]$	[123, 315]
124	$[\frac{3}{4} - z, \frac{1}{4} - y, x + \frac{1}{2}]$	[124, 316]

continued ...

Table 9

No.	position	mapping
125	$[z + \frac{1}{2}, \frac{1}{4} - y, \frac{3}{4} - x]$	[125, 317]
126	$[y + \frac{1}{2}, \frac{1}{4} - x, \frac{3}{4} - z]$	[126, 318]
127	$[\frac{3}{4} - y, x, \frac{3}{4} - z]$	[127, 319]
128	$[\frac{1}{2} - x, y + \frac{1}{4}, z + \frac{3}{4}]$	[128, 320]
129	$[x + \frac{3}{4}, -y, z + \frac{3}{4}]$	[129, 321]
130	$[x + \frac{3}{4}, y + \frac{1}{4}, \frac{1}{2} - z]$	[130, 322]
131	$[\frac{3}{4} - y, \frac{1}{4} - x, z + \frac{1}{2}]$	[131, 323]
132	$[y + \frac{1}{2}, x, z + \frac{1}{2}]$	[132, 324]
133	$[x + \frac{1}{2}, \frac{1}{4} - z, \frac{3}{4} - y]$	[133, 325]
134	$[x + \frac{1}{2}, z, y + \frac{1}{2}]$	[134, 326]
135	$[\frac{3}{4} - z, y, \frac{3}{4} - x]$	[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	$[y + \frac{3}{4}, -z, x + \frac{3}{4}]$	[139, 331]
140	$[z + \frac{3}{4}, x + \frac{1}{4}, \frac{1}{2} - y]$	[140, 332]
141	$[y + \frac{3}{4}, z + \frac{1}{4}, \frac{1}{2} - x]$	[141, 333]
142	$[\frac{1}{2} - z, x + \frac{1}{4}, y + \frac{3}{4}]$	[142, 334]
143	$[\frac{1}{2} - y, z + \frac{1}{4}, x + \frac{3}{4}]$	[143, 335]
144	$[z + \frac{3}{4}, -x, y + \frac{3}{4}]$	[144, 336]
145	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[145, 337]
146	$[x + \frac{3}{4}, \frac{1}{2} - z, y + \frac{1}{4}]$	[146, 338]
147	$[x + \frac{3}{4}, z + \frac{3}{4}, -y]$	[147, 339]
148	$[z + \frac{3}{4}, y + \frac{3}{4}, -x]$	[148, 340]
149	$[\frac{1}{2} - z, y + \frac{3}{4}, x + \frac{1}{4}]$	[149, 341]
150	$[\frac{1}{2} - y, x + \frac{3}{4}, z + \frac{1}{4}]$	[150, 342]
151	$[y + \frac{3}{4}, \frac{1}{2} - x, z + \frac{1}{4}]$	[151, 343]
152	$[x + \frac{1}{2}, \frac{3}{4} - y, \frac{1}{4} - z]$	[152, 344]
153	$[\frac{3}{4} - x, y + \frac{1}{2}, \frac{1}{4} - z]$	[153, 345]
154	$[\frac{3}{4} - x, \frac{3}{4} - y, z]$	[154, 346]
155	$[y + \frac{3}{4}, x + \frac{3}{4}, -z]$	[155, 347]
156	$[\frac{1}{2} - y, \frac{1}{2} - x, -z]$	[156, 348]
157	$[\frac{1}{2} - x, z + \frac{3}{4}, y + \frac{1}{4}]$	[157, 349]
158	$[\frac{1}{2} - x, \frac{1}{2} - z, -y]$	[158, 350]
159	$[z + \frac{3}{4}, \frac{1}{2} - y, x + \frac{1}{4}]$	[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	$[\frac{3}{4} - y, z + \frac{1}{2}, \frac{1}{4} - x]$	[163, 355]
164	$[\frac{3}{4} - z, \frac{3}{4} - x, y]$	[164, 356]
165	$[\frac{3}{4} - y, \frac{3}{4} - z, x]$	[165, 357]
166	$[z + \frac{1}{2}, \frac{3}{4} - x, \frac{1}{4} - y]$	[166, 358]
167	$[y + \frac{1}{2}, \frac{3}{4} - z, \frac{1}{4} - x]$	[167, 359]
168	$[\frac{3}{4} - z, x + \frac{1}{2}, \frac{1}{4} - y]$	[168, 360]
169	$[\frac{1}{2} - x, \frac{1}{2} - y, -z]$	[169, 361]
170	$[\frac{3}{4} - x, z + \frac{1}{2}, \frac{1}{4} - y]$	[170, 362]
171	$[\frac{3}{4} - x, \frac{3}{4} - z, y]$	[171, 363]

continued ...

Table 9

No.	position	mapping
172	$[\frac{3}{4} - z, \frac{3}{4} - y, x]$	[172, 364]
173	$[z + \frac{1}{2}, \frac{3}{4} - y, \frac{1}{4} - x]$	[173, 365]
174	$[y + \frac{1}{2}, \frac{3}{4} - x, \frac{1}{4} - z]$	[174, 366]
175	$[\frac{3}{4} - y, x + \frac{1}{2}, \frac{1}{4} - z]$	[175, 367]
176	$[\frac{1}{2} - x, y + \frac{3}{4}, z + \frac{1}{4}]$	[176, 368]
177	$[x + \frac{3}{4}, \frac{1}{2} - y, z + \frac{1}{4}]$	[177, 369]
178	$[x + \frac{3}{4}, y + \frac{3}{4}, -z]$	[178, 370]
179	$[\frac{3}{4} - y, \frac{3}{4} - x, z]$	[179, 371]
180	$[y + \frac{1}{2}, x + \frac{1}{2}, z]$	[180, 372]
181	$[x + \frac{1}{2}, \frac{3}{4} - z, \frac{1}{4} - y]$	[181, 373]
182	$[x + \frac{1}{2}, z + \frac{1}{2}, y]$	[182, 374]
183	$[\frac{3}{4} - z, y + \frac{1}{2}, \frac{1}{4} - x]$	[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	$[y + \frac{3}{4}, \frac{1}{2} - z, x + \frac{1}{4}]$	[187, 379]
188	$[z + \frac{3}{4}, x + \frac{3}{4}, -y]$	[188, 380]
189	$[y + \frac{3}{4}, z + \frac{3}{4}, -x]$	[189, 381]
190	$[\frac{1}{2} - z, x + \frac{3}{4}, y + \frac{1}{4}]$	[190, 382]
191	$[\frac{1}{2} - y, z + \frac{3}{4}, x + \frac{1}{4}]$	[191, 383]
192	$[z + \frac{3}{4}, \frac{1}{2} - x, y + \frac{1}{4}]$	[192, 384]