

MSG No. 209.51 F_5432 [Type IV, cubic]

Table 1: Wyckoff site: 8a, site symmetry: 432

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]
2	$[0, \frac{1}{2}, \frac{1}{2}]$	[25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48]
3	$[\frac{1}{2}, 0, \frac{1}{2}]$	[49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72]
4	$[\frac{1}{2}, \frac{1}{2}, 0]$	[73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96]
5	$[0, 0, \frac{1}{2}]$	[97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120]
6	$[0, \frac{1}{2}, 0]$	[121, 122, 123, 124, 125, 126, 127, 128, 129, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144]
7	$[\frac{1}{2}, 0, 0]$	[145, 146, 147, 148, 149, 150, 151, 152, 153, 154, 155, 156, 157, 158, 159, 160, 161, 162, 163, 164, 165, 166, 167, 168]
8	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[169, 170, 171, 172, 173, 174, 175, 176, 177, 178, 179, 180, 181, 182, 183, 184, 185, 186, 187, 188, 189, 190, 191, 192]

Table 2: Wyckoff site: 8b, site symmetry: $4'32'$

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

Table 3: Wyckoff site: 24c, site symmetry: $4'2'.2$

No.	position	mapping
1	$[0, \frac{1}{4}, \frac{1}{4}]$	[1, 13, 32, 38, 99, 105, 122, 130]
2	$[0, \frac{3}{4}, \frac{1}{4}]$	[2, 10, 27, 33, 104, 110, 121, 133]
3	$[0, \frac{1}{4}, \frac{3}{4}]$	[3, 9, 26, 34, 97, 109, 128, 134]
4	$[\frac{1}{4}, \frac{1}{4}, 0]$	[4, 18, 88, 93, 135, 143, 149, 163]
5	$[\frac{3}{4}, \frac{1}{4}, 0]$	[5, 19, 87, 95, 136, 141, 148, 162]
6	$[\frac{3}{4}, 0, \frac{1}{4}]$	[6, 20, 59, 70, 108, 120, 151, 161]
7	$[\frac{1}{4}, 0, \frac{1}{4}]$	[7, 17, 60, 72, 107, 118, 150, 164]
8	$[0, \frac{3}{4}, \frac{3}{4}]$	[8, 14, 25, 37, 98, 106, 123, 129]
9	$[\frac{1}{4}, 0, \frac{3}{4}]$	[11, 22, 54, 68, 103, 113, 156, 168]
10	$[\frac{3}{4}, 0, \frac{3}{4}]$	[12, 24, 55, 65, 102, 116, 155, 166]
11	$[\frac{1}{4}, \frac{3}{4}, 0]$	[15, 23, 77, 91, 124, 138, 160, 165]
12	$[\frac{3}{4}, \frac{3}{4}, 0]$	[16, 21, 76, 90, 125, 139, 159, 167]
13	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}]$	[28, 42, 64, 69, 111, 119, 173, 187]
14	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}]$	[29, 43, 63, 71, 112, 117, 172, 186]
15	$[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}]$	[30, 44, 83, 94, 132, 144, 175, 185]

continued ...

Table 3

No.	position	mapping
16	$[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}]$	[31, 41, 84, 96, 131, 142, 174, 188]
17	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$	[35, 46, 78, 92, 127, 137, 180, 192]
18	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$	[36, 48, 79, 89, 126, 140, 179, 190]
19	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$	[39, 47, 53, 67, 100, 114, 184, 189]
20	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	[40, 45, 52, 66, 101, 115, 183, 191]
21	$[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[49, 61, 80, 86, 147, 153, 170, 178]
22	$[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[50, 58, 75, 81, 152, 158, 169, 181]
23	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[51, 57, 74, 82, 145, 157, 176, 182]
24	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[56, 62, 73, 85, 146, 154, 171, 177]

Table 4: Wyckoff site: 24d, site symmetry: $42'.2'$

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

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

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

continued ...

Table 5

No.	position	mapping
47	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[175, 180, 188, 190]
48	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[177, 178, 181, 182]

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

No.	position	mapping
1	$[x, \frac{1}{4}, \frac{1}{4}]$	[1, 32, 99, 122]
2	$[x, \frac{3}{4}, \frac{1}{4}]$	[2, 27, 104, 121]
3	$[x, \frac{1}{4}, \frac{3}{4}]$	[3, 26, 97, 128]
4	$[\frac{1}{4}, \frac{1}{4}, -x]$	[4, 88, 143, 163]
5	$[\frac{3}{4}, \frac{1}{4}, x]$	[5, 87, 141, 162]
6	$[\frac{3}{4}, x, \frac{1}{4}]$	[6, 59, 120, 161]
7	$[\frac{1}{4}, -x, \frac{1}{4}]$	[7, 60, 118, 164]
8	$[x, \frac{3}{4}, \frac{3}{4}]$	[8, 25, 98, 123]
9	$[-x, \frac{1}{4}, \frac{3}{4}]$	[9, 34, 109, 134]
10	$[-x, \frac{3}{4}, \frac{1}{4}]$	[10, 33, 110, 133]
11	$[\frac{1}{4}, x, \frac{3}{4}]$	[11, 54, 113, 168]
12	$[\frac{3}{4}, -x, \frac{3}{4}]$	[12, 55, 116, 166]
13	$[-x, \frac{1}{4}, \frac{1}{4}]$	[13, 38, 105, 130]
14	$[-x, \frac{3}{4}, \frac{3}{4}]$	[14, 37, 106, 129]
15	$[\frac{1}{4}, \frac{3}{4}, x]$	[15, 77, 138, 165]
16	$[\frac{3}{4}, \frac{3}{4}, -x]$	[16, 76, 139, 167]
17	$[\frac{1}{4}, x, \frac{1}{4}]$	[17, 72, 107, 150]
18	$[\frac{1}{4}, \frac{1}{4}, x]$	[18, 93, 135, 149]
19	$[\frac{3}{4}, \frac{1}{4}, -x]$	[19, 95, 136, 148]
20	$[\frac{3}{4}, -x, \frac{1}{4}]$	[20, 70, 108, 151]
21	$[\frac{3}{4}, \frac{3}{4}, x]$	[21, 90, 125, 159]
22	$[\frac{1}{4}, -x, \frac{3}{4}]$	[22, 68, 103, 156]
23	$[\frac{1}{4}, \frac{3}{4}, -x]$	[23, 91, 124, 160]
24	$[\frac{3}{4}, x, \frac{3}{4}]$	[24, 65, 102, 155]
25	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[28, 64, 119, 187]
26	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[29, 63, 117, 186]
27	$[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[30, 83, 144, 185]
28	$[\frac{1}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[31, 84, 142, 188]
29	$[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[35, 78, 137, 192]
30	$[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[36, 79, 140, 190]
31	$[\frac{1}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[39, 53, 114, 189]
32	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[40, 52, 115, 191]
33	$[\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[41, 96, 131, 174]
34	$[\frac{1}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[42, 69, 111, 173]
35	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[43, 71, 112, 172]
36	$[\frac{3}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[44, 94, 132, 175]
37	$[\frac{3}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[45, 66, 101, 183]
38	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[46, 92, 127, 180]

continued ...

Table 6

No.	position	mapping
39	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[47, 67, 100, 184]
40	$[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[48, 89, 126, 179]
41	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[49, 80, 147, 170]
42	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[50, 75, 152, 169]
43	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[51, 74, 145, 176]
44	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[56, 73, 146, 171]
45	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[57, 82, 157, 182]
46	$[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$	[58, 81, 158, 181]
47	$[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$	[61, 86, 153, 178]
48	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]$	[62, 85, 154, 177]

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

No.	position	mapping
1	$[x, x, x]$	[1, 17, 18]
2	$[x, -x, x]$	[2, 7, 15]
3	$[x, x, -x]$	[3, 4, 11]
4	$[-x, x, x]$	[5, 6, 13]
5	$[x, -x, -x]$	[8, 22, 23]
6	$[-x, x, -x]$	[9, 19, 24]
7	$[-x, -x, x]$	[10, 20, 21]
8	$[-x, -x, -x]$	[12, 14, 16]
9	$[x, x + \frac{1}{2}, x + \frac{1}{2}]$	[25, 41, 42]
10	$[x, \frac{1}{2} - x, x + \frac{1}{2}]$	[26, 31, 39]
11	$[x, x + \frac{1}{2}, \frac{1}{2} - x]$	[27, 28, 35]
12	$[-x, x + \frac{1}{2}, x + \frac{1}{2}]$	[29, 30, 37]
13	$[x, \frac{1}{2} - x, \frac{1}{2} - x]$	[32, 46, 47]
14	$[-x, x + \frac{1}{2}, \frac{1}{2} - x]$	[33, 43, 48]
15	$[-x, \frac{1}{2} - x, x + \frac{1}{2}]$	[34, 44, 45]
16	$[-x, \frac{1}{2} - x, \frac{1}{2} - x]$	[36, 38, 40]
17	$[x + \frac{1}{2}, x, x + \frac{1}{2}]$	[49, 65, 66]
18	$[x + \frac{1}{2}, -x, x + \frac{1}{2}]$	[50, 55, 63]
19	$[x + \frac{1}{2}, x, \frac{1}{2} - x]$	[51, 52, 59]
20	$[\frac{1}{2} - x, x, x + \frac{1}{2}]$	[53, 54, 61]
21	$[x + \frac{1}{2}, -x, \frac{1}{2} - x]$	[56, 70, 71]
22	$[\frac{1}{2} - x, x, \frac{1}{2} - x]$	[57, 67, 72]
23	$[\frac{1}{2} - x, -x, x + \frac{1}{2}]$	[58, 68, 69]
24	$[\frac{1}{2} - x, -x, \frac{1}{2} - x]$	[60, 62, 64]
25	$[x + \frac{1}{2}, x + \frac{1}{2}, x]$	[73, 89, 90]
26	$[x + \frac{1}{2}, \frac{1}{2} - x, x]$	[74, 79, 87]
27	$[x + \frac{1}{2}, x + \frac{1}{2}, -x]$	[75, 76, 83]
28	$[\frac{1}{2} - x, x + \frac{1}{2}, x]$	[77, 78, 85]
29	$[x + \frac{1}{2}, \frac{1}{2} - x, -x]$	[80, 94, 95]
30	$[\frac{1}{2} - x, x + \frac{1}{2}, -x]$	[81, 91, 96]

continued ...

Table 7

No.	position	mapping
31	$[\frac{1}{2} - x, \frac{1}{2} - x, x]$	[82, 92, 93]
32	$[\frac{1}{2} - x, \frac{1}{2} - x, -x]$	[84, 86, 88]
33	$[x, x, x + \frac{1}{2}]$	[97, 113, 114]
34	$[x, -x, x + \frac{1}{2}]$	[98, 103, 111]
35	$[x, x, \frac{1}{2} - x]$	[99, 100, 107]
36	$[-x, x, x + \frac{1}{2}]$	[101, 102, 109]
37	$[x, -x, \frac{1}{2} - x]$	[104, 118, 119]
38	$[-x, x, \frac{1}{2} - x]$	[105, 115, 120]
39	$[-x, -x, x + \frac{1}{2}]$	[106, 116, 117]
40	$[-x, -x, \frac{1}{2} - x]$	[108, 110, 112]
41	$[x, x + \frac{1}{2}, x]$	[121, 137, 138]
42	$[x, \frac{1}{2} - x, x]$	[122, 127, 135]
43	$[x, x + \frac{1}{2}, -x]$	[123, 124, 131]
44	$[-x, x + \frac{1}{2}, x]$	[125, 126, 133]
45	$[x, \frac{1}{2} - x, -x]$	[128, 142, 143]
46	$[-x, x + \frac{1}{2}, -x]$	[129, 139, 144]
47	$[-x, \frac{1}{2} - x, x]$	[130, 140, 141]
48	$[-x, \frac{1}{2} - x, -x]$	[132, 134, 136]
49	$[x + \frac{1}{2}, x, x]$	[145, 161, 162]
50	$[x + \frac{1}{2}, -x, x]$	[146, 151, 159]
51	$[x + \frac{1}{2}, x, -x]$	[147, 148, 155]
52	$[\frac{1}{2} - x, x, x]$	[149, 150, 157]
53	$[x + \frac{1}{2}, -x, -x]$	[152, 166, 167]
54	$[\frac{1}{2} - x, x, -x]$	[153, 163, 168]
55	$[\frac{1}{2} - x, -x, x]$	[154, 164, 165]
56	$[\frac{1}{2} - x, -x, -x]$	[156, 158, 160]
57	$[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}]$	[169, 185, 186]
58	$[x + \frac{1}{2}, \frac{1}{2} - x, x + \frac{1}{2}]$	[170, 175, 183]
59	$[x + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - x]$	[171, 172, 179]
60	$[\frac{1}{2} - x, x + \frac{1}{2}, x + \frac{1}{2}]$	[173, 174, 181]
61	$[x + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - x]$	[176, 190, 191]
62	$[\frac{1}{2} - x, x + \frac{1}{2}, \frac{1}{2} - x]$	[177, 187, 192]
63	$[\frac{1}{2} - x, \frac{1}{2} - x, x + \frac{1}{2}]$	[178, 188, 189]
64	$[\frac{1}{2} - x, \frac{1}{2} - x, \frac{1}{2} - x]$	[180, 182, 184]

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

No.	position	mapping
1	$[x, \frac{1}{4}, 0]$	[1, 128]
2	$[x, 0, \frac{1}{4}]$	[2, 99]
3	$[x, 0, \frac{3}{4}]$	[3, 98]
4	$[0, \frac{1}{4}, -x]$	[4, 136]
5	$[0, \frac{1}{4}, x]$	[5, 135]
6	$[\frac{3}{4}, x, 0]$	[6, 155]

continued ...

Table 8

No.	position	mapping
7	$[\frac{1}{4}, -x, 0]$	[7, 156]
8	$[x, \frac{3}{4}, 0]$	[8, 121]
9	$[-x, \frac{1}{4}, 0]$	[9, 130]
10	$[-x, \frac{3}{4}, 0]$	[10, 129]
11	$[\frac{1}{4}, x, 0]$	[11, 150]
12	$[\frac{3}{4}, -x, 0]$	[12, 151]
13	$[-x, 0, \frac{1}{4}]$	[13, 110]
14	$[-x, 0, \frac{3}{4}]$	[14, 109]
15	$[0, \frac{3}{4}, x]$	[15, 125]
16	$[0, \frac{3}{4}, -x]$	[16, 124]
17	$[0, x, \frac{1}{4}]$	[17, 120]
18	$[\frac{1}{4}, 0, x]$	[18, 165]
19	$[\frac{3}{4}, 0, -x]$	[19, 167]
20	$[0, -x, \frac{1}{4}]$	[20, 118]
21	$[\frac{3}{4}, 0, x]$	[21, 162]
22	$[0, -x, \frac{3}{4}]$	[22, 116]
23	$[\frac{1}{4}, 0, -x]$	[23, 163]
24	$[0, x, \frac{3}{4}]$	[24, 113]
25	$[x, \frac{3}{4}, \frac{1}{2}]$	[25, 104]
26	$[x, \frac{1}{2}, \frac{3}{4}]$	[26, 123]
27	$[x, \frac{1}{2}, \frac{1}{4}]$	[27, 122]
28	$[0, \frac{3}{4}, \frac{1}{2} - x]$	[28, 112]
29	$[0, \frac{3}{4}, x + \frac{1}{2}]$	[29, 111]
30	$[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{2}]$	[30, 179]
31	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{2}]$	[31, 180]
32	$[x, \frac{1}{4}, \frac{1}{2}]$	[32, 97]
33	$[-x, \frac{3}{4}, \frac{1}{2}]$	[33, 106]
34	$[-x, \frac{1}{4}, \frac{1}{2}]$	[34, 105]
35	$[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{2}]$	[35, 174]
36	$[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{2}]$	[36, 175]
37	$[-x, \frac{1}{2}, \frac{3}{4}]$	[37, 134]
38	$[-x, \frac{1}{2}, \frac{1}{4}]$	[38, 133]
39	$[0, \frac{1}{4}, x + \frac{1}{2}]$	[39, 101]
40	$[0, \frac{1}{4}, \frac{1}{2} - x]$	[40, 100]
41	$[0, x + \frac{1}{2}, \frac{3}{4}]$	[41, 144]
42	$[\frac{1}{4}, \frac{1}{2}, x + \frac{1}{2}]$	[42, 189]
43	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{2} - x]$	[43, 191]
44	$[0, \frac{1}{2} - x, \frac{3}{4}]$	[44, 142]
45	$[\frac{3}{4}, \frac{1}{2}, x + \frac{1}{2}]$	[45, 186]
46	$[0, \frac{1}{2} - x, \frac{1}{4}]$	[46, 140]
47	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{2} - x]$	[47, 187]
48	$[0, x + \frac{1}{2}, \frac{1}{4}]$	[48, 137]
49	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{2}]$	[49, 176]
50	$[x + \frac{1}{2}, 0, \frac{3}{4}]$	[50, 147]
51	$[x + \frac{1}{2}, 0, \frac{1}{4}]$	[51, 146]
52	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2} - x]$	[52, 184]
53	$[\frac{1}{2}, \frac{1}{4}, x + \frac{1}{2}]$	[53, 183]

continued ...

Table 8

No.	position	mapping
54	$[\frac{1}{4}, x, \frac{1}{2}]$	[54,107]
55	$[\frac{3}{4}, -x, \frac{1}{2}]$	[55,108]
56	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{2}]$	[56,169]
57	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{2}]$	[57,178]
58	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{2}]$	[58,177]
59	$[\frac{3}{4}, x, \frac{1}{2}]$	[59,102]
60	$[\frac{1}{4}, -x, \frac{1}{2}]$	[60,103]
61	$[\frac{1}{2} - x, 0, \frac{3}{4}]$	[61,158]
62	$[\frac{1}{2} - x, 0, \frac{1}{4}]$	[62,157]
63	$[\frac{1}{2}, \frac{3}{4}, x + \frac{1}{2}]$	[63,173]
64	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{2} - x]$	[64,172]
65	$[\frac{1}{2}, x, \frac{3}{4}]$	[65,168]
66	$[\frac{3}{4}, 0, x + \frac{1}{2}]$	[66,117]
67	$[\frac{1}{4}, 0, \frac{1}{2} - x]$	[67,119]
68	$[\frac{1}{2}, -x, \frac{3}{4}]$	[68,166]
69	$[\frac{1}{4}, 0, x + \frac{1}{2}]$	[69,114]
70	$[\frac{1}{2}, -x, \frac{1}{4}]$	[70,164]
71	$[\frac{3}{4}, 0, \frac{1}{2} - x]$	[71,115]
72	$[\frac{1}{2}, x, \frac{1}{4}]$	[72,161]
73	$[x + \frac{1}{2}, \frac{3}{4}, 0]$	[73,152]
74	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[74,171]
75	$[x + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[75,170]
76	$[\frac{1}{2}, \frac{3}{4}, -x]$	[76,160]
77	$[\frac{1}{2}, \frac{3}{4}, x]$	[77,159]
78	$[\frac{1}{4}, x + \frac{1}{2}, 0]$	[78,131]
79	$[\frac{3}{4}, \frac{1}{2} - x, 0]$	[79,132]
80	$[x + \frac{1}{2}, \frac{1}{4}, 0]$	[80,145]
81	$[\frac{1}{2} - x, \frac{3}{4}, 0]$	[81,154]
82	$[\frac{1}{2} - x, \frac{1}{4}, 0]$	[82,153]
83	$[\frac{3}{4}, x + \frac{1}{2}, 0]$	[83,126]
84	$[\frac{1}{4}, \frac{1}{2} - x, 0]$	[84,127]
85	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{4}]$	[85,182]
86	$[\frac{1}{2} - x, \frac{1}{2}, \frac{3}{4}]$	[86,181]
87	$[\frac{1}{2}, \frac{1}{4}, x]$	[87,149]
88	$[\frac{1}{2}, \frac{1}{4}, -x]$	[88,148]
89	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[89,192]
90	$[\frac{3}{4}, \frac{1}{2}, x]$	[90,141]
91	$[\frac{1}{4}, \frac{1}{2}, -x]$	[91,143]
92	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}]$	[92,190]
93	$[\frac{1}{4}, \frac{1}{2}, x]$	[93,138]
94	$[\frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}]$	[94,188]
95	$[\frac{3}{4}, \frac{1}{2}, -x]$	[95,139]
96	$[\frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}]$	[96,185]

Table 9: Wyckoff site: 96i, site symmetry: . . 2

No.	position	mapping
1	$[0, y, y]$	[1, 13]
2	$[0, -y, y]$	[2, 10]
3	$[0, y, -y]$	[3, 9]
4	$[y, y, 0]$	[4, 18]
5	$[-y, y, 0]$	[5, 19]
6	$[-y, 0, y]$	[6, 20]
7	$[y, 0, y]$	[7, 17]
8	$[0, -y, -y]$	[8, 14]
9	$[y, 0, -y]$	[11, 22]
10	$[-y, 0, -y]$	[12, 24]
11	$[y, -y, 0]$	[15, 23]
12	$[-y, -y, 0]$	[16, 21]
13	$[0, y + \frac{1}{2}, y + \frac{1}{2}]$	[25, 37]
14	$[0, \frac{1}{2} - y, y + \frac{1}{2}]$	[26, 34]
15	$[0, y + \frac{1}{2}, \frac{1}{2} - y]$	[27, 33]
16	$[y, y + \frac{1}{2}, \frac{1}{2}]$	[28, 42]
17	$[-y, y + \frac{1}{2}, \frac{1}{2}]$	[29, 43]
18	$[-y, \frac{1}{2}, y + \frac{1}{2}]$	[30, 44]
19	$[y, \frac{1}{2}, y + \frac{1}{2}]$	[31, 41]
20	$[0, \frac{1}{2} - y, \frac{1}{2} - y]$	[32, 38]
21	$[y, \frac{1}{2}, \frac{1}{2} - y]$	[35, 46]
22	$[-y, \frac{1}{2}, \frac{1}{2} - y]$	[36, 48]
23	$[y, \frac{1}{2} - y, \frac{1}{2}]$	[39, 47]
24	$[-y, \frac{1}{2} - y, \frac{1}{2}]$	[40, 45]
25	$[\frac{1}{2}, y, y + \frac{1}{2}]$	[49, 61]
26	$[\frac{1}{2}, -y, y + \frac{1}{2}]$	[50, 58]
27	$[\frac{1}{2}, y, \frac{1}{2} - y]$	[51, 57]
28	$[y + \frac{1}{2}, y, \frac{1}{2}]$	[52, 66]
29	$[\frac{1}{2} - y, y, \frac{1}{2}]$	[53, 67]
30	$[\frac{1}{2} - y, 0, y + \frac{1}{2}]$	[54, 68]
31	$[y + \frac{1}{2}, 0, y + \frac{1}{2}]$	[55, 65]
32	$[\frac{1}{2}, -y, \frac{1}{2} - y]$	[56, 62]
33	$[y + \frac{1}{2}, 0, \frac{1}{2} - y]$	[59, 70]
34	$[\frac{1}{2} - y, 0, \frac{1}{2} - y]$	[60, 72]
35	$[y + \frac{1}{2}, -y, \frac{1}{2}]$	[63, 71]
36	$[\frac{1}{2} - y, -y, \frac{1}{2}]$	[64, 69]
37	$[\frac{1}{2}, y + \frac{1}{2}, y]$	[73, 85]
38	$[\frac{1}{2}, \frac{1}{2} - y, y]$	[74, 82]
39	$[\frac{1}{2}, y + \frac{1}{2}, -y]$	[75, 81]
40	$[y + \frac{1}{2}, y + \frac{1}{2}, 0]$	[76, 90]
41	$[\frac{1}{2} - y, y + \frac{1}{2}, 0]$	[77, 91]
42	$[\frac{1}{2} - y, \frac{1}{2}, y]$	[78, 92]
43	$[y + \frac{1}{2}, \frac{1}{2}, y]$	[79, 89]
44	$[\frac{1}{2}, \frac{1}{2} - y, -y]$	[80, 86]
45	$[y + \frac{1}{2}, \frac{1}{2}, -y]$	[83, 94]
46	$[\frac{1}{2} - y, \frac{1}{2}, -y]$	[84, 96]

continued ...

Table 9

No.	position	mapping
47	$[y + \frac{1}{2}, \frac{1}{2} - y, 0]$	[87,95]
48	$[\frac{1}{2} - y, \frac{1}{2} - y, 0]$	[88,93]
49	$[0, y, y + \frac{1}{2}]$	[97,109]
50	$[0, -y, y + \frac{1}{2}]$	[98,106]
51	$[0, y, \frac{1}{2} - y]$	[99,105]
52	$[y, y, \frac{1}{2}]$	[100,114]
53	$[-y, y, \frac{1}{2}]$	[101,115]
54	$[-y, 0, y + \frac{1}{2}]$	[102,116]
55	$[y, 0, y + \frac{1}{2}]$	[103,113]
56	$[0, -y, \frac{1}{2} - y]$	[104,110]
57	$[y, 0, \frac{1}{2} - y]$	[107,118]
58	$[-y, 0, \frac{1}{2} - y]$	[108,120]
59	$[y, -y, \frac{1}{2}]$	[111,119]
60	$[-y, -y, \frac{1}{2}]$	[112,117]
61	$[0, y + \frac{1}{2}, y]$	[121,133]
62	$[0, \frac{1}{2} - y, y]$	[122,130]
63	$[0, y + \frac{1}{2}, -y]$	[123,129]
64	$[y, y + \frac{1}{2}, 0]$	[124,138]
65	$[-y, y + \frac{1}{2}, 0]$	[125,139]
66	$[-y, \frac{1}{2}, y]$	[126,140]
67	$[y, \frac{1}{2}, y]$	[127,137]
68	$[0, \frac{1}{2} - y, -y]$	[128,134]
69	$[y, \frac{1}{2}, -y]$	[131,142]
70	$[-y, \frac{1}{2}, -y]$	[132,144]
71	$[y, \frac{1}{2} - y, 0]$	[135,143]
72	$[-y, \frac{1}{2} - y, 0]$	[136,141]
73	$[\frac{1}{2}, y, y]$	[145,157]
74	$[\frac{1}{2}, -y, y]$	[146,154]
75	$[\frac{1}{2}, y, -y]$	[147,153]
76	$[y + \frac{1}{2}, y, 0]$	[148,162]
77	$[\frac{1}{2} - y, y, 0]$	[149,163]
78	$[\frac{1}{2} - y, 0, y]$	[150,164]
79	$[y + \frac{1}{2}, 0, y]$	[151,161]
80	$[\frac{1}{2}, -y, -y]$	[152,158]
81	$[y + \frac{1}{2}, 0, -y]$	[155,166]
82	$[\frac{1}{2} - y, 0, -y]$	[156,168]
83	$[y + \frac{1}{2}, -y, 0]$	[159,167]
84	$[\frac{1}{2} - y, -y, 0]$	[160,165]
85	$[\frac{1}{2}, y + \frac{1}{2}, y + \frac{1}{2}]$	[169,181]
86	$[\frac{1}{2}, \frac{1}{2} - y, y + \frac{1}{2}]$	[170,178]
87	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - y]$	[171,177]
88	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[172,186]
89	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{2}]$	[173,187]
90	$[\frac{1}{2} - y, \frac{1}{2}, y + \frac{1}{2}]$	[174,188]
91	$[y + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}]$	[175,185]
92	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - y]$	[176,182]
93	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - y]$	[179,190]

continued ...

Table 9

No.	position	mapping
94	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - y]$	[180,192]
95	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[183,191]
96	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{2}]$	[184,189]

Table 10: Wyckoff site: 96j, site symmetry: $\dots 2'$

No.	position	mapping
1	$[\frac{1}{4}, y, y]$	[1,157]
2	$[\frac{1}{4}, -y, y]$	[2,154]
3	$[\frac{1}{4}, y, -y]$	[3,153]
4	$[y, y, \frac{3}{4}]$	[4,114]
5	$[-y, y, \frac{1}{4}]$	[5,115]
6	$[-y, \frac{1}{4}, y]$	[6,140]
7	$[y, \frac{3}{4}, y]$	[7,137]
8	$[\frac{1}{4}, -y, -y]$	[8,158]
9	$[\frac{3}{4}, y, -y]$	[9,147]
10	$[\frac{3}{4}, -y, y]$	[10,146]
11	$[y, \frac{1}{4}, -y]$	[11,142]
12	$[-y, \frac{3}{4}, -y]$	[12,144]
13	$[\frac{3}{4}, y, y]$	[13,145]
14	$[\frac{3}{4}, -y, -y]$	[14,152]
15	$[y, -y, \frac{1}{4}]$	[15,119]
16	$[-y, -y, \frac{3}{4}]$	[16,117]
17	$[y, \frac{1}{4}, y]$	[17,127]
18	$[y, y, \frac{1}{4}]$	[18,100]
19	$[-y, y, \frac{3}{4}]$	[19,101]
20	$[-y, \frac{3}{4}, y]$	[20,126]
21	$[-y, -y, \frac{1}{4}]$	[21,112]
22	$[y, \frac{3}{4}, -y]$	[22,131]
23	$[y, -y, \frac{3}{4}]$	[23,111]
24	$[-y, \frac{1}{4}, -y]$	[24,132]
25	$[\frac{1}{4}, y + \frac{1}{2}, y + \frac{1}{2}]$	[25,181]
26	$[\frac{1}{4}, \frac{1}{2} - y, y + \frac{1}{2}]$	[26,178]
27	$[\frac{1}{4}, y + \frac{1}{2}, \frac{1}{2} - y]$	[27,177]
28	$[y, y + \frac{1}{2}, \frac{1}{4}]$	[28,138]
29	$[-y, y + \frac{1}{2}, \frac{3}{4}]$	[29,139]
30	$[-y, \frac{3}{4}, y + \frac{1}{2}]$	[30,116]
31	$[y, \frac{1}{4}, y + \frac{1}{2}]$	[31,113]
32	$[\frac{1}{4}, \frac{1}{2} - y, \frac{1}{2} - y]$	[32,182]
33	$[\frac{3}{4}, y + \frac{1}{2}, \frac{1}{2} - y]$	[33,171]
34	$[\frac{3}{4}, \frac{1}{2} - y, y + \frac{1}{2}]$	[34,170]
35	$[y, \frac{3}{4}, \frac{1}{2} - y]$	[35,118]
36	$[-y, \frac{1}{4}, \frac{1}{2} - y]$	[36,120]
37	$[\frac{3}{4}, y + \frac{1}{2}, y + \frac{1}{2}]$	[37,169]

continued ...

Table 10

No.	position	mapping
38	$[\frac{3}{4}, \frac{1}{2} - y, \frac{1}{2} - y]$	[38, 176]
39	$[y, \frac{1}{2} - y, \frac{3}{4}]$	[39, 143]
40	$[-y, \frac{1}{2} - y, \frac{1}{4}]$	[40, 141]
41	$[y, \frac{3}{4}, y + \frac{1}{2}]$	[41, 103]
42	$[y, y + \frac{1}{2}, \frac{3}{4}]$	[42, 124]
43	$[-y, y + \frac{1}{2}, \frac{1}{4}]$	[43, 125]
44	$[-y, \frac{1}{4}, y + \frac{1}{2}]$	[44, 102]
45	$[-y, \frac{1}{2} - y, \frac{3}{4}]$	[45, 136]
46	$[y, \frac{1}{4}, \frac{1}{2} - y]$	[46, 107]
47	$[y, \frac{1}{2} - y, \frac{1}{4}]$	[47, 135]
48	$[-y, \frac{3}{4}, \frac{1}{2} - y]$	[48, 108]
49	$[\frac{3}{4}, y, y + \frac{1}{2}]$	[49, 109]
50	$[\frac{3}{4}, -y, y + \frac{1}{2}]$	[50, 106]
51	$[\frac{3}{4}, y, \frac{1}{2} - y]$	[51, 105]
52	$[y + \frac{1}{2}, y, \frac{1}{4}]$	[52, 162]
53	$[\frac{1}{2} - y, y, \frac{3}{4}]$	[53, 163]
54	$[\frac{1}{2} - y, \frac{1}{4}, y + \frac{1}{2}]$	[54, 188]
55	$[y + \frac{1}{2}, \frac{3}{4}, y + \frac{1}{2}]$	[55, 185]
56	$[\frac{3}{4}, -y, \frac{1}{2} - y]$	[56, 110]
57	$[\frac{1}{4}, y, \frac{1}{2} - y]$	[57, 99]
58	$[\frac{1}{4}, -y, y + \frac{1}{2}]$	[58, 98]
59	$[y + \frac{1}{2}, \frac{1}{4}, \frac{1}{2} - y]$	[59, 190]
60	$[\frac{1}{2} - y, \frac{3}{4}, \frac{1}{2} - y]$	[60, 192]
61	$[\frac{1}{4}, y, y + \frac{1}{2}]$	[61, 97]
62	$[\frac{1}{4}, -y, \frac{1}{2} - y]$	[62, 104]
63	$[y + \frac{1}{2}, -y, \frac{3}{4}]$	[63, 167]
64	$[\frac{1}{2} - y, -y, \frac{1}{4}]$	[64, 165]
65	$[y + \frac{1}{2}, \frac{1}{4}, y + \frac{1}{2}]$	[65, 175]
66	$[y + \frac{1}{2}, y, \frac{3}{4}]$	[66, 148]
67	$[\frac{1}{2} - y, y, \frac{1}{4}]$	[67, 149]
68	$[\frac{1}{2} - y, \frac{3}{4}, y + \frac{1}{2}]$	[68, 174]
69	$[\frac{1}{2} - y, -y, \frac{3}{4}]$	[69, 160]
70	$[y + \frac{1}{2}, \frac{3}{4}, \frac{1}{2} - y]$	[70, 179]
71	$[y + \frac{1}{2}, -y, \frac{1}{4}]$	[71, 159]
72	$[\frac{1}{2} - y, \frac{1}{4}, \frac{1}{2} - y]$	[72, 180]
73	$[\frac{3}{4}, y + \frac{1}{2}, y]$	[73, 133]
74	$[\frac{3}{4}, \frac{1}{2} - y, y]$	[74, 130]
75	$[\frac{3}{4}, y + \frac{1}{2}, -y]$	[75, 129]
76	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{3}{4}]$	[76, 186]
77	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{4}]$	[77, 187]
78	$[\frac{1}{2} - y, \frac{3}{4}, y]$	[78, 164]
79	$[y + \frac{1}{2}, \frac{1}{4}, y]$	[79, 161]
80	$[\frac{3}{4}, \frac{1}{2} - y, -y]$	[80, 134]
81	$[\frac{1}{4}, y + \frac{1}{2}, -y]$	[81, 123]
82	$[\frac{1}{4}, \frac{1}{2} - y, y]$	[82, 122]
83	$[y + \frac{1}{2}, \frac{3}{4}, -y]$	[83, 166]
84	$[\frac{1}{2} - y, \frac{1}{4}, -y]$	[84, 168]

continued ...

Table 10

No.	position	mapping
85	$[\frac{1}{4}, y + \frac{1}{2}, y]$	[85, 121]
86	$[\frac{1}{4}, \frac{1}{2} - y, -y]$	[86, 128]
87	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{4}]$	[87, 191]
88	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{3}{4}]$	[88, 189]
89	$[y + \frac{1}{2}, \frac{3}{4}, y]$	[89, 151]
90	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{4}]$	[90, 172]
91	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{3}{4}]$	[91, 173]
92	$[\frac{1}{2} - y, \frac{1}{4}, y]$	[92, 150]
93	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{4}]$	[93, 184]
94	$[y + \frac{1}{2}, \frac{1}{4}, -y]$	[94, 155]
95	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{3}{4}]$	[95, 183]
96	$[\frac{1}{2} - y, \frac{3}{4}, -y]$	[96, 156]

Table 11: Wyckoff site: 192k, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x, -z, y]$	[2]
3	$[x, z, -y]$	[3]
4	$[z, y, -x]$	[4]
5	$[-z, y, x]$	[5]
6	$[-y, x, z]$	[6]
7	$[y, -x, z]$	[7]
8	$[x, -y, -z]$	[8]
9	$[-x, y, -z]$	[9]
10	$[-x, -y, z]$	[10]
11	$[y, x, -z]$	[11]
12	$[-y, -x, -z]$	[12]
13	$[-x, z, y]$	[13]
14	$[-x, -z, -y]$	[14]
15	$[z, -y, x]$	[15]
16	$[-z, -y, -x]$	[16]
17	$[z, x, y]$	[17]
18	$[y, z, x]$	[18]
19	$[-y, z, -x]$	[19]
20	$[-z, -x, y]$	[20]
21	$[-y, -z, x]$	[21]
22	$[z, -x, -y]$	[22]
23	$[y, -z, -x]$	[23]
24	$[-z, x, -y]$	[24]
25	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[25]
26	$[x, \frac{1}{2} - z, y + \frac{1}{2}]$	[26]
27	$[x, z + \frac{1}{2}, \frac{1}{2} - y]$	[27]
28	$[z, y + \frac{1}{2}, \frac{1}{2} - x]$	[28]

continued ...

Table 11

No.	position	mapping
29	$[-z, y + \frac{1}{2}, x + \frac{1}{2}]$	[29]
30	$[-y, x + \frac{1}{2}, z + \frac{1}{2}]$	[30]
31	$[y, \frac{1}{2} - x, z + \frac{1}{2}]$	[31]
32	$[x, \frac{1}{2} - y, \frac{1}{2} - z]$	[32]
33	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[33]
34	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[34]
35	$[y, x + \frac{1}{2}, \frac{1}{2} - z]$	[35]
36	$[-y, \frac{1}{2} - x, \frac{1}{2} - z]$	[36]
37	$[-x, z + \frac{1}{2}, y + \frac{1}{2}]$	[37]
38	$[-x, \frac{1}{2} - z, \frac{1}{2} - y]$	[38]
39	$[z, \frac{1}{2} - y, x + \frac{1}{2}]$	[39]
40	$[-z, \frac{1}{2} - y, \frac{1}{2} - x]$	[40]
41	$[z, x + \frac{1}{2}, y + \frac{1}{2}]$	[41]
42	$[y, z + \frac{1}{2}, x + \frac{1}{2}]$	[42]
43	$[-y, z + \frac{1}{2}, \frac{1}{2} - x]$	[43]
44	$[-z, \frac{1}{2} - x, y + \frac{1}{2}]$	[44]
45	$[-y, \frac{1}{2} - z, x + \frac{1}{2}]$	[45]
46	$[z, \frac{1}{2} - x, \frac{1}{2} - y]$	[46]
47	$[y, \frac{1}{2} - z, \frac{1}{2} - x]$	[47]
48	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[48]
49	$[x + \frac{1}{2}, y, z + \frac{1}{2}]$	[49]
50	$[x + \frac{1}{2}, -z, y + \frac{1}{2}]$	[50]
51	$[x + \frac{1}{2}, z, \frac{1}{2} - y]$	[51]
52	$[z + \frac{1}{2}, y, \frac{1}{2} - x]$	[52]
53	$[\frac{1}{2} - z, y, x + \frac{1}{2}]$	[53]
54	$[\frac{1}{2} - y, x, z + \frac{1}{2}]$	[54]
55	$[y + \frac{1}{2}, -x, z + \frac{1}{2}]$	[55]
56	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[56]
57	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[57]
58	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[58]
59	$[y + \frac{1}{2}, x, \frac{1}{2} - z]$	[59]
60	$[\frac{1}{2} - y, -x, \frac{1}{2} - z]$	[60]
61	$[\frac{1}{2} - x, z, y + \frac{1}{2}]$	[61]
62	$[\frac{1}{2} - x, -z, \frac{1}{2} - y]$	[62]
63	$[z + \frac{1}{2}, -y, x + \frac{1}{2}]$	[63]
64	$[\frac{1}{2} - z, -y, \frac{1}{2} - x]$	[64]
65	$[z + \frac{1}{2}, x, y + \frac{1}{2}]$	[65]
66	$[y + \frac{1}{2}, z, x + \frac{1}{2}]$	[66]
67	$[\frac{1}{2} - y, z, \frac{1}{2} - x]$	[67]
68	$[\frac{1}{2} - z, -x, y + \frac{1}{2}]$	[68]
69	$[\frac{1}{2} - y, -z, x + \frac{1}{2}]$	[69]
70	$[z + \frac{1}{2}, -x, \frac{1}{2} - y]$	[70]
71	$[y + \frac{1}{2}, -z, \frac{1}{2} - x]$	[71]
72	$[\frac{1}{2} - z, x, \frac{1}{2} - y]$	[72]
73	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[73]
74	$[x + \frac{1}{2}, \frac{1}{2} - z, y]$	[74]
75	$[x + \frac{1}{2}, z + \frac{1}{2}, -y]$	[75]

continued ...

Table 11

No.	position	mapping
76	$[z + \frac{1}{2}, y + \frac{1}{2}, -x]$	[76]
77	$[\frac{1}{2} - z, y + \frac{1}{2}, x]$	[77]
78	$[\frac{1}{2} - y, x + \frac{1}{2}, z]$	[78]
79	$[y + \frac{1}{2}, \frac{1}{2} - x, z]$	[79]
80	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[80]
81	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[81]
82	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[82]
83	$[y + \frac{1}{2}, x + \frac{1}{2}, -z]$	[83]
84	$[\frac{1}{2} - y, \frac{1}{2} - x, -z]$	[84]
85	$[\frac{1}{2} - x, z + \frac{1}{2}, y]$	[85]
86	$[\frac{1}{2} - x, \frac{1}{2} - z, -y]$	[86]
87	$[z + \frac{1}{2}, \frac{1}{2} - y, x]$	[87]
88	$[\frac{1}{2} - z, \frac{1}{2} - y, -x]$	[88]
89	$[z + \frac{1}{2}, x + \frac{1}{2}, y]$	[89]
90	$[y + \frac{1}{2}, z + \frac{1}{2}, x]$	[90]
91	$[\frac{1}{2} - y, z + \frac{1}{2}, -x]$	[91]
92	$[\frac{1}{2} - z, \frac{1}{2} - x, y]$	[92]
93	$[\frac{1}{2} - y, \frac{1}{2} - z, x]$	[93]
94	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[94]
95	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[95]
96	$[\frac{1}{2} - z, x + \frac{1}{2}, -y]$	[96]
97	$[x, y, z + \frac{1}{2}]$	[97]
98	$[x, -z, y + \frac{1}{2}]$	[98]
99	$[x, z, \frac{1}{2} - y]$	[99]
100	$[z, y, \frac{1}{2} - x]$	[100]
101	$[-z, y, x + \frac{1}{2}]$	[101]
102	$[-y, x, z + \frac{1}{2}]$	[102]
103	$[y, -x, z + \frac{1}{2}]$	[103]
104	$[x, -y, \frac{1}{2} - z]$	[104]
105	$[-x, y, \frac{1}{2} - z]$	[105]
106	$[-x, -y, z + \frac{1}{2}]$	[106]
107	$[y, x, \frac{1}{2} - z]$	[107]
108	$[-y, -x, \frac{1}{2} - z]$	[108]
109	$[-x, z, y + \frac{1}{2}]$	[109]
110	$[-x, -z, \frac{1}{2} - y]$	[110]
111	$[z, -y, x + \frac{1}{2}]$	[111]
112	$[-z, -y, \frac{1}{2} - x]$	[112]
113	$[z, x, y + \frac{1}{2}]$	[113]
114	$[y, z, x + \frac{1}{2}]$	[114]
115	$[-y, z, \frac{1}{2} - x]$	[115]
116	$[-z, -x, y + \frac{1}{2}]$	[116]
117	$[-y, -z, x + \frac{1}{2}]$	[117]
118	$[z, -x, \frac{1}{2} - y]$	[118]
119	$[y, -z, \frac{1}{2} - x]$	[119]
120	$[-z, x, \frac{1}{2} - y]$	[120]
121	$[x, y + \frac{1}{2}, z]$	[121]
122	$[x, \frac{1}{2} - z, y]$	[122]

continued ...

Table 11

No.	position	mapping
123	$[x, z + \frac{1}{2}, -y]$	[123]
124	$[z, y + \frac{1}{2}, -x]$	[124]
125	$[-z, y + \frac{1}{2}, x]$	[125]
126	$[-y, x + \frac{1}{2}, z]$	[126]
127	$[y, \frac{1}{2} - x, z]$	[127]
128	$[x, \frac{1}{2} - y, -z]$	[128]
129	$[-x, y + \frac{1}{2}, -z]$	[129]
130	$[-x, \frac{1}{2} - y, z]$	[130]
131	$[y, x + \frac{1}{2}, -z]$	[131]
132	$[-y, \frac{1}{2} - x, -z]$	[132]
133	$[-x, z + \frac{1}{2}, y]$	[133]
134	$[-x, \frac{1}{2} - z, -y]$	[134]
135	$[z, \frac{1}{2} - y, x]$	[135]
136	$[-z, \frac{1}{2} - y, -x]$	[136]
137	$[z, x + \frac{1}{2}, y]$	[137]
138	$[y, z + \frac{1}{2}, x]$	[138]
139	$[-y, z + \frac{1}{2}, -x]$	[139]
140	$[-z, \frac{1}{2} - x, y]$	[140]
141	$[-y, \frac{1}{2} - z, x]$	[141]
142	$[z, \frac{1}{2} - x, -y]$	[142]
143	$[y, \frac{1}{2} - z, -x]$	[143]
144	$[-z, x + \frac{1}{2}, -y]$	[144]
145	$[x + \frac{1}{2}, y, z]$	[145]
146	$[x + \frac{1}{2}, -z, y]$	[146]
147	$[x + \frac{1}{2}, z, -y]$	[147]
148	$[z + \frac{1}{2}, y, -x]$	[148]
149	$[\frac{1}{2} - z, y, x]$	[149]
150	$[\frac{1}{2} - y, x, z]$	[150]
151	$[y + \frac{1}{2}, -x, z]$	[151]
152	$[x + \frac{1}{2}, -y, -z]$	[152]
153	$[\frac{1}{2} - x, y, -z]$	[153]
154	$[\frac{1}{2} - x, -y, z]$	[154]
155	$[y + \frac{1}{2}, x, -z]$	[155]
156	$[\frac{1}{2} - y, -x, -z]$	[156]
157	$[\frac{1}{2} - x, z, y]$	[157]
158	$[\frac{1}{2} - x, -z, -y]$	[158]
159	$[z + \frac{1}{2}, -y, x]$	[159]
160	$[\frac{1}{2} - z, -y, -x]$	[160]
161	$[z + \frac{1}{2}, x, y]$	[161]
162	$[y + \frac{1}{2}, z, x]$	[162]
163	$[\frac{1}{2} - y, z, -x]$	[163]
164	$[\frac{1}{2} - z, -x, y]$	[164]
165	$[\frac{1}{2} - y, -z, x]$	[165]
166	$[z + \frac{1}{2}, -x, -y]$	[166]
167	$[y + \frac{1}{2}, -z, -x]$	[167]
168	$[\frac{1}{2} - z, x, -y]$	[168]
169	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[169]

continued ...

Table 11

No.	position	mapping
170	$[x + \frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[170]
171	$[x + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[171]
172	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - x]$	[172]
173	$[\frac{1}{2} - z, y + \frac{1}{2}, x + \frac{1}{2}]$	[173]
174	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[174]
175	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[175]
176	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[176]
177	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[177]
178	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[178]
179	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[179]
180	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[180]
181	$[\frac{1}{2} - x, z + \frac{1}{2}, y + \frac{1}{2}]$	[181]
182	$[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y]$	[182]
183	$[z + \frac{1}{2}, \frac{1}{2} - y, x + \frac{1}{2}]$	[183]
184	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2} - x]$	[184]
185	$[z + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}]$	[185]
186	$[y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}]$	[186]
187	$[\frac{1}{2} - y, z + \frac{1}{2}, \frac{1}{2} - x]$	[187]
188	$[\frac{1}{2} - z, \frac{1}{2} - x, y + \frac{1}{2}]$	[188]
189	$[\frac{1}{2} - y, \frac{1}{2} - z, x + \frac{1}{2}]$	[189]
190	$[z + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - y]$	[190]
191	$[y + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - x]$	[191]
192	$[\frac{1}{2} - z, x + \frac{1}{2}, \frac{1}{2} - y]$	[192]