

# MSG No. 209.49 $F4321'$ [ Type II, cubic ]

Table 1: Wyckoff site: 4a, site symmetry:  $4321'$

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

Table 2: Wyckoff site: 4b, site symmetry:  $4321'$

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

Table 3: Wyckoff site: 8c, site symmetry:  $23.1'$

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

Table 4: Wyckoff site: 24d, site symmetry: 2..21'

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

Table 5: Wyckoff site: 24e, site symmetry: 4..1'

No.	position	mapping
1	$[x, 0, 0]$	[1, 2, 3, 8, 97, 98, 99, 104]
2	$[0, 0, -x]$	[4, 16, 19, 23, 100, 112, 115, 119]
3	$[0, 0, x]$	[5, 15, 18, 21, 101, 111, 114, 117]
4	$[0, x, 0]$	[6, 11, 17, 24, 102, 107, 113, 120]
5	$[0, -x, 0]$	[7, 12, 20, 22, 103, 108, 116, 118]
6	$[-x, 0, 0]$	[9, 10, 13, 14, 105, 106, 109, 110]
7	$[x, \frac{1}{2}, \frac{1}{2}]$	[25, 26, 27, 32, 121, 122, 123, 128]
8	$[0, \frac{1}{2}, \frac{1}{2} - x]$	[28, 40, 43, 47, 124, 136, 139, 143]
9	$[0, \frac{1}{2}, x + \frac{1}{2}]$	[29, 39, 42, 45, 125, 135, 138, 141]
10	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[30, 35, 41, 48, 126, 131, 137, 144]
11	$[0, \frac{1}{2} - x, \frac{1}{2}]$	[31, 36, 44, 46, 127, 132, 140, 142]
12	$[-x, \frac{1}{2}, \frac{1}{2}]$	[33, 34, 37, 38, 129, 130, 133, 134]
13	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	[49, 50, 51, 56, 145, 146, 147, 152]
14	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[52, 64, 67, 71, 148, 160, 163, 167]
15	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[53, 63, 66, 69, 149, 159, 162, 165]

*continued ...*

Table 5

No.	position	mapping
16	$[\frac{1}{2}, x, \frac{1}{2}]$	[54, 59, 65, 72, 150, 155, 161, 168]
17	$[\frac{1}{2}, -x, \frac{1}{2}]$	[55, 60, 68, 70, 151, 156, 164, 166]
18	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[57, 58, 61, 62, 153, 154, 157, 158]
19	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[73, 74, 75, 80, 169, 170, 171, 176]
20	$[\frac{1}{2}, \frac{1}{2}, -x]$	[76, 88, 91, 95, 172, 184, 187, 191]
21	$[\frac{1}{2}, \frac{1}{2}, x]$	[77, 87, 90, 93, 173, 183, 186, 189]
22	$[\frac{1}{2}, x + \frac{1}{2}, 0]$	[78, 83, 89, 96, 174, 179, 185, 192]
23	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	[79, 84, 92, 94, 175, 180, 188, 190]
24	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[81, 82, 85, 86, 177, 178, 181, 182]

Table 6: Wyckoff site: 32f, site symmetry: .3.1'

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

continued ...

Table 6

No.	position	mapping
32	$[\frac{1}{2} - x, \frac{1}{2} - x, -x]$	[84, 86, 88, 180, 182, 184]

Table 7: Wyckoff site: 48g, site symmetry: . . 21'

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

*continued ...*

Table 7

No.	position	mapping
40	$[y + \frac{1}{2}, y + \frac{1}{2}, 0]$	[76, 90, 172, 186]
41	$[\frac{1}{2} - y, y + \frac{1}{2}, 0]$	[77, 91, 173, 187]
42	$[\frac{1}{2} - y, \frac{1}{2}, y]$	[78, 92, 174, 188]
43	$[y + \frac{1}{2}, \frac{1}{2}, y]$	[79, 89, 175, 185]
44	$[\frac{1}{2}, \frac{1}{2} - y, -y]$	[80, 86, 176, 182]
45	$[y + \frac{1}{2}, \frac{1}{2}, -y]$	[83, 94, 179, 190]
46	$[\frac{1}{2} - y, \frac{1}{2}, -y]$	[84, 96, 180, 192]
47	$[y + \frac{1}{2}, \frac{1}{2} - y, 0]$	[87, 95, 183, 191]
48	$[\frac{1}{2} - y, \frac{1}{2} - y, 0]$	[88, 93, 184, 189]

Table 8: Wyckoff site: 48h, site symmetry: ...21'

No.	position	mapping
1	$[\frac{1}{2}, y, y]$	[1, 13, 97, 109]
2	$[\frac{1}{2}, -y, y]$	[2, 10, 98, 106]
3	$[\frac{1}{2}, y, -y]$	[3, 9, 99, 105]
4	$[y, y, \frac{1}{2}]$	[4, 18, 100, 114]
5	$[-y, y, \frac{1}{2}]$	[5, 19, 101, 115]
6	$[-y, \frac{1}{2}, y]$	[6, 20, 102, 116]
7	$[y, \frac{1}{2}, y]$	[7, 17, 103, 113]
8	$[\frac{1}{2}, -y, -y]$	[8, 14, 104, 110]
9	$[y, \frac{1}{2}, -y]$	[11, 22, 107, 118]
10	$[-y, \frac{1}{2}, -y]$	[12, 24, 108, 120]
11	$[y, -y, \frac{1}{2}]$	[15, 23, 111, 119]
12	$[-y, -y, \frac{1}{2}]$	[16, 21, 112, 117]
13	$[\frac{1}{2}, y + \frac{1}{2}, y + \frac{1}{2}]$	[25, 37, 121, 133]
14	$[\frac{1}{2}, \frac{1}{2} - y, y + \frac{1}{2}]$	[26, 34, 122, 130]
15	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - y]$	[27, 33, 123, 129]
16	$[y, y + \frac{1}{2}, 0]$	[28, 42, 124, 138]
17	$[-y, y + \frac{1}{2}, 0]$	[29, 43, 125, 139]
18	$[-y, 0, y + \frac{1}{2}]$	[30, 44, 126, 140]
19	$[y, 0, y + \frac{1}{2}]$	[31, 41, 127, 137]
20	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - y]$	[32, 38, 128, 134]
21	$[y, 0, \frac{1}{2} - y]$	[35, 46, 131, 142]
22	$[-y, 0, \frac{1}{2} - y]$	[36, 48, 132, 144]
23	$[y, \frac{1}{2} - y, 0]$	[39, 47, 135, 143]
24	$[-y, \frac{1}{2} - y, 0]$	[40, 45, 136, 141]
25	$[0, y, y + \frac{1}{2}]$	[49, 61, 145, 157]
26	$[0, -y, y + \frac{1}{2}]$	[50, 58, 146, 154]
27	$[0, y, \frac{1}{2} - y]$	[51, 57, 147, 153]
28	$[y + \frac{1}{2}, y, 0]$	[52, 66, 148, 162]
29	$[\frac{1}{2} - y, y, 0]$	[53, 67, 149, 163]
30	$[\frac{1}{2} - y, \frac{1}{2}, y + \frac{1}{2}]$	[54, 68, 150, 164]
31	$[y + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}]$	[55, 65, 151, 161]

*continued ...*

Table 8

No.	position	mapping
32	$[0, -y, \frac{1}{2} - y]$	[56, 62, 152, 158]
33	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - y]$	[59, 70, 155, 166]
34	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - y]$	[60, 72, 156, 168]
35	$[y + \frac{1}{2}, -y, 0]$	[63, 71, 159, 167]
36	$[\frac{1}{2} - y, -y, 0]$	[64, 69, 160, 165]
37	$[0, y + \frac{1}{2}, y]$	[73, 85, 169, 181]
38	$[0, \frac{1}{2} - y, y]$	[74, 82, 170, 178]
39	$[0, y + \frac{1}{2}, -y]$	[75, 81, 171, 177]
40	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[76, 90, 172, 186]
41	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{2}]$	[77, 91, 173, 187]
42	$[\frac{1}{2} - y, 0, y]$	[78, 92, 174, 188]
43	$[y + \frac{1}{2}, 0, y]$	[79, 89, 175, 185]
44	$[0, \frac{1}{2} - y, -y]$	[80, 86, 176, 182]
45	$[y + \frac{1}{2}, 0, -y]$	[83, 94, 179, 190]
46	$[\frac{1}{2} - y, 0, -y]$	[84, 96, 180, 192]
47	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[87, 95, 183, 191]
48	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{2}]$	[88, 93, 184, 189]

Table 9: Wyckoff site: 48i, site symmetry: 2..1'

No.	position	mapping
1	$[x, \frac{1}{4}, \frac{1}{4}]$	[1, 32, 97, 128]
2	$[x, \frac{3}{4}, \frac{1}{4}]$	[2, 27, 98, 123]
3	$[x, \frac{1}{4}, \frac{3}{4}]$	[3, 26, 99, 122]
4	$[\frac{1}{4}, \frac{1}{4}, -x]$	[4, 88, 100, 184]
5	$[\frac{3}{4}, \frac{1}{4}, x]$	[5, 87, 101, 183]
6	$[\frac{3}{4}, x, \frac{1}{4}]$	[6, 59, 102, 155]
7	$[\frac{1}{4}, -x, \frac{1}{4}]$	[7, 60, 103, 156]
8	$[x, \frac{3}{4}, \frac{3}{4}]$	[8, 25, 104, 121]
9	$[-x, \frac{1}{4}, \frac{3}{4}]$	[9, 34, 105, 130]
10	$[-x, \frac{3}{4}, \frac{1}{4}]$	[10, 33, 106, 129]
11	$[\frac{1}{4}, x, \frac{3}{4}]$	[11, 54, 107, 150]
12	$[\frac{3}{4}, -x, \frac{3}{4}]$	[12, 55, 108, 151]
13	$[-x, \frac{1}{4}, \frac{1}{4}]$	[13, 38, 109, 134]
14	$[-x, \frac{3}{4}, \frac{3}{4}]$	[14, 37, 110, 133]
15	$[\frac{1}{4}, \frac{3}{4}, x]$	[15, 77, 111, 173]
16	$[\frac{3}{4}, \frac{3}{4}, -x]$	[16, 76, 112, 172]
17	$[\frac{1}{4}, x, \frac{1}{4}]$	[17, 72, 113, 168]
18	$[\frac{1}{4}, \frac{1}{4}, x]$	[18, 93, 114, 189]
19	$[\frac{3}{4}, \frac{1}{4}, -x]$	[19, 95, 115, 191]
20	$[\frac{3}{4}, -x, \frac{1}{4}]$	[20, 70, 116, 166]
21	$[\frac{3}{4}, \frac{3}{4}, x]$	[21, 90, 117, 186]
22	$[\frac{1}{4}, -x, \frac{3}{4}]$	[22, 68, 118, 164]
23	$[\frac{1}{4}, \frac{3}{4}, -x]$	[23, 91, 119, 187]

*continued ...*

Table 9

No.	position	mapping
24	$[\frac{3}{4}, x, \frac{3}{4}]$	[24,65,120,161]
25	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[28,64,124,160]
26	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[29,63,125,159]
27	$[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[30,83,126,179]
28	$[\frac{1}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[31,84,127,180]
29	$[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[35,78,131,174]
30	$[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[36,79,132,175]
31	$[\frac{1}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[39,53,135,149]
32	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[40,52,136,148]
33	$[\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[41,96,137,192]
34	$[\frac{1}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[42,69,138,165]
35	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[43,71,139,167]
36	$[\frac{3}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[44,94,140,190]
37	$[\frac{3}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[45,66,141,162]
38	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[46,92,142,188]
39	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[47,67,143,163]
40	$[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[48,89,144,185]
41	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[49,80,145,176]
42	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[50,75,146,171]
43	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[51,74,147,170]
44	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[56,73,152,169]
45	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[57,82,153,178]
46	$[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$	[58,81,154,177]
47	$[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$	[61,86,157,182]
48	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]$	[62,85,158,181]

Table 10: Wyckoff site: 96j, site symmetry: 11'

No.	position	mapping
1	$[x, y, z]$	[1,97]
2	$[x, -z, y]$	[2,98]
3	$[x, z, -y]$	[3,99]
4	$[z, y, -x]$	[4,100]
5	$[-z, y, x]$	[5,101]
6	$[-y, x, z]$	[6,102]
7	$[y, -x, z]$	[7,103]
8	$[x, -y, -z]$	[8,104]
9	$[-x, y, -z]$	[9,105]
10	$[-x, -y, z]$	[10,106]
11	$[y, x, -z]$	[11,107]
12	$[-y, -x, -z]$	[12,108]
13	$[-x, z, y]$	[13,109]
14	$[-x, -z, -y]$	[14,110]
15	$[z, -y, x]$	[15,111]

*continued ...*

Table 10

No.	position	mapping
16	$[-z, -y, -x]$	[16,112]
17	$[z, x, y]$	[17,113]
18	$[y, z, x]$	[18,114]
19	$[-y, z, -x]$	[19,115]
20	$[-z, -x, y]$	[20,116]
21	$[-y, -z, x]$	[21,117]
22	$[z, -x, -y]$	[22,118]
23	$[y, -z, -x]$	[23,119]
24	$[-z, x, -y]$	[24,120]
25	$[x, y + \frac{1}{2}, z + \frac{1}{2}]$	[25,121]
26	$[x, \frac{1}{2} - z, y + \frac{1}{2}]$	[26,122]
27	$[x, z + \frac{1}{2}, \frac{1}{2} - y]$	[27,123]
28	$[z, y + \frac{1}{2}, \frac{1}{2} - x]$	[28,124]
29	$[-z, y + \frac{1}{2}, x + \frac{1}{2}]$	[29,125]
30	$[-y, x + \frac{1}{2}, z + \frac{1}{2}]$	[30,126]
31	$[y, \frac{1}{2} - x, z + \frac{1}{2}]$	[31,127]
32	$[x, \frac{1}{2} - y, \frac{1}{2} - z]$	[32,128]
33	$[-x, y + \frac{1}{2}, \frac{1}{2} - z]$	[33,129]
34	$[-x, \frac{1}{2} - y, z + \frac{1}{2}]$	[34,130]
35	$[y, x + \frac{1}{2}, \frac{1}{2} - z]$	[35,131]
36	$[-y, \frac{1}{2} - x, \frac{1}{2} - z]$	[36,132]
37	$[-x, z + \frac{1}{2}, y + \frac{1}{2}]$	[37,133]
38	$[-x, \frac{1}{2} - z, \frac{1}{2} - y]$	[38,134]
39	$[z, \frac{1}{2} - y, x + \frac{1}{2}]$	[39,135]
40	$[-z, \frac{1}{2} - y, \frac{1}{2} - x]$	[40,136]
41	$[z, x + \frac{1}{2}, y + \frac{1}{2}]$	[41,137]
42	$[y, z + \frac{1}{2}, x + \frac{1}{2}]$	[42,138]
43	$[-y, z + \frac{1}{2}, \frac{1}{2} - x]$	[43,139]
44	$[-z, \frac{1}{2} - x, y + \frac{1}{2}]$	[44,140]
45	$[-y, \frac{1}{2} - z, x + \frac{1}{2}]$	[45,141]
46	$[z, \frac{1}{2} - x, \frac{1}{2} - y]$	[46,142]
47	$[y, \frac{1}{2} - z, \frac{1}{2} - x]$	[47,143]
48	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[48,144]
49	$[x + \frac{1}{2}, y, z + \frac{1}{2}]$	[49,145]
50	$[x + \frac{1}{2}, -z, y + \frac{1}{2}]$	[50,146]
51	$[x + \frac{1}{2}, z, \frac{1}{2} - y]$	[51,147]
52	$[z + \frac{1}{2}, y, \frac{1}{2} - x]$	[52,148]
53	$[\frac{1}{2} - z, y, x + \frac{1}{2}]$	[53,149]
54	$[\frac{1}{2} - y, x, z + \frac{1}{2}]$	[54,150]
55	$[y + \frac{1}{2}, -x, z + \frac{1}{2}]$	[55,151]
56	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[56,152]
57	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[57,153]
58	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[58,154]
59	$[y + \frac{1}{2}, x, \frac{1}{2} - z]$	[59,155]
60	$[\frac{1}{2} - y, -x, \frac{1}{2} - z]$	[60,156]
61	$[\frac{1}{2} - x, z, y + \frac{1}{2}]$	[61,157]
62	$[\frac{1}{2} - x, -z, \frac{1}{2} - y]$	[62,158]

*continued ...*

Table 10

No.	position	mapping
63	$[z + \frac{1}{2}, -y, x + \frac{1}{2}]$	[63,159]
64	$[\frac{1}{2} - z, -y, \frac{1}{2} - x]$	[64,160]
65	$[z + \frac{1}{2}, x, y + \frac{1}{2}]$	[65,161]
66	$[y + \frac{1}{2}, z, x + \frac{1}{2}]$	[66,162]
67	$[\frac{1}{2} - y, z, \frac{1}{2} - x]$	[67,163]
68	$[\frac{1}{2} - z, -x, y + \frac{1}{2}]$	[68,164]
69	$[\frac{1}{2} - y, -z, x + \frac{1}{2}]$	[69,165]
70	$[z + \frac{1}{2}, -x, \frac{1}{2} - y]$	[70,166]
71	$[y + \frac{1}{2}, -z, \frac{1}{2} - x]$	[71,167]
72	$[\frac{1}{2} - z, x, \frac{1}{2} - y]$	[72,168]
73	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[73,169]
74	$[x + \frac{1}{2}, \frac{1}{2} - z, y]$	[74,170]
75	$[x + \frac{1}{2}, z + \frac{1}{2}, -y]$	[75,171]
76	$[z + \frac{1}{2}, y + \frac{1}{2}, -x]$	[76,172]
77	$[\frac{1}{2} - z, y + \frac{1}{2}, x]$	[77,173]
78	$[\frac{1}{2} - y, x + \frac{1}{2}, z]$	[78,174]
79	$[y + \frac{1}{2}, \frac{1}{2} - x, z]$	[79,175]
80	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[80,176]
81	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[81,177]
82	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[82,178]
83	$[y + \frac{1}{2}, x + \frac{1}{2}, -z]$	[83,179]
84	$[\frac{1}{2} - y, \frac{1}{2} - x, -z]$	[84,180]
85	$[\frac{1}{2} - x, z + \frac{1}{2}, y]$	[85,181]
86	$[\frac{1}{2} - x, \frac{1}{2} - z, -y]$	[86,182]
87	$[z + \frac{1}{2}, \frac{1}{2} - y, x]$	[87,183]
88	$[\frac{1}{2} - z, \frac{1}{2} - y, -x]$	[88,184]
89	$[z + \frac{1}{2}, x + \frac{1}{2}, y]$	[89,185]
90	$[y + \frac{1}{2}, z + \frac{1}{2}, x]$	[90,186]
91	$[\frac{1}{2} - y, z + \frac{1}{2}, -x]$	[91,187]
92	$[\frac{1}{2} - z, \frac{1}{2} - x, y]$	[92,188]
93	$[\frac{1}{2} - y, \frac{1}{2} - z, x]$	[93,189]
94	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[94,190]
95	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[95,191]
96	$[\frac{1}{2} - z, x + \frac{1}{2}, -y]$	[96,192]