

MSG No. 196.6  $F_{S23}$  [ Type IV, cubic ]

Table 1: Wyckoff site: 8a, site symmetry: 23.

No.	position	mapping
1	[0, 0, 0]	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12]
2	[0, $\frac{1}{2}$ , $\frac{1}{2}$ ]	[13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]
3	[ $\frac{1}{2}$ , 0, $\frac{1}{2}$ ]	[25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36]
4	[ $\frac{1}{2}$ , $\frac{1}{2}$ , 0]	[37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48]
5	[0, 0, $\frac{1}{2}$ ]	[49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60]
6	[0, $\frac{1}{2}$ , 0]	[61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72]
7	[ $\frac{1}{2}$ , 0, 0]	[73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84]
8	[ $\frac{1}{2}$ , $\frac{1}{2}$ , $\frac{1}{2}$ ]	[85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96]

Table 2: Wyckoff site: 8b, site symmetry: 23.

No.	position	mapping
1	[ $\frac{1}{4}$ , $\frac{1}{4}$ , $\frac{1}{4}$ ]	[1, 5, 6, 14, 22, 23, 27, 31, 36, 40, 44, 45]
2	[ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{3}{4}$ ]	[2, 10, 11, 13, 17, 18, 28, 32, 33, 39, 43, 48]
3	[ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{3}{4}$ ]	[3, 7, 12, 16, 20, 21, 25, 29, 30, 38, 46, 47]
4	[ $\frac{3}{4}$ , $\frac{3}{4}$ , $\frac{1}{4}$ ]	[4, 8, 9, 15, 19, 24, 26, 34, 35, 37, 41, 42]
5	[ $\frac{1}{4}$ , $\frac{1}{4}$ , $\frac{3}{4}$ ]	[49, 53, 54, 62, 70, 71, 75, 79, 84, 88, 92, 93]
6	[ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{4}$ ]	[50, 58, 59, 61, 65, 66, 76, 80, 81, 87, 91, 96]
7	[ $\frac{3}{4}$ , $\frac{1}{4}$ , $\frac{1}{4}$ ]	[51, 55, 60, 64, 68, 69, 73, 77, 78, 86, 94, 95]
8	[ $\frac{3}{4}$ , $\frac{3}{4}$ , $\frac{3}{4}$ ]	[52, 56, 57, 63, 67, 72, 74, 82, 83, 85, 89, 90]

Table 3: Wyckoff site: 24c, site symmetry: 22'2'..

No.	position	mapping
1	[0, $\frac{1}{4}$ , $\frac{1}{4}$ ]	[1, 14, 51, 64]
2	[0, $\frac{3}{4}$ , $\frac{3}{4}$ ]	[2, 13, 52, 63]
3	[0, $\frac{1}{4}$ , $\frac{3}{4}$ ]	[3, 16, 49, 62]
4	[0, $\frac{3}{4}$ , $\frac{1}{4}$ ]	[4, 15, 50, 61]
5	[ $\frac{1}{4}$ , 0, $\frac{1}{4}$ ]	[5, 36, 58, 80]
6	[ $\frac{1}{4}$ , $\frac{1}{4}$ , 0]	[6, 45, 71, 79]
7	[ $\frac{3}{4}$ , $\frac{1}{4}$ , 0]	[7, 47, 69, 78]
8	[ $\frac{3}{4}$ , 0, $\frac{1}{4}$ ]	[8, 34, 60, 77]
9	[ $\frac{3}{4}$ , $\frac{3}{4}$ , 0]	[9, 42, 67, 83]
10	[ $\frac{1}{4}$ , 0, $\frac{3}{4}$ ]	[10, 32, 53, 84]
11	[ $\frac{1}{4}$ , $\frac{3}{4}$ , 0]	[11, 43, 66, 81]
12	[ $\frac{3}{4}$ , 0, $\frac{3}{4}$ ]	[12, 29, 56, 82]
13	[ $\frac{1}{4}$ , $\frac{1}{2}$ , $\frac{3}{4}$ ]	[17, 48, 70, 92]
14	[ $\frac{1}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ]	[18, 33, 59, 91]
15	[ $\frac{3}{4}$ , $\frac{3}{4}$ , $\frac{1}{2}$ ]	[19, 35, 57, 90]

*continued ...*

Table 3

No.	position	mapping
16	$[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}]$	[20, 46, 72, 89]
17	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}]$	[21, 30, 55, 95]
18	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}]$	[22, 44, 65, 96]
19	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}]$	[23, 31, 54, 93]
20	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}]$	[24, 41, 68, 94]
21	$[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[25, 38, 75, 88]
22	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[26, 37, 76, 87]
23	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[27, 40, 73, 86]
24	$[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[28, 39, 74, 85]

Table 4: Wyckoff site: 24d, site symmetry: 22'2'...

No.	position	mapping
1	$[\frac{1}{4}, 0, 0]$	[1, 2, 75, 76]
2	$[\frac{3}{4}, 0, 0]$	[3, 4, 73, 74]
3	$[0, \frac{1}{4}, 0]$	[5, 12, 68, 70]
4	$[0, 0, \frac{1}{4}]$	[6, 9, 55, 59]
5	$[0, 0, \frac{3}{4}]$	[7, 11, 54, 57]
6	$[0, \frac{3}{4}, 0]$	[8, 10, 65, 72]
7	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{2}]$	[13, 14, 87, 88]
8	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{2}]$	[15, 16, 85, 86]
9	$[0, \frac{3}{4}, \frac{1}{2}]$	[17, 24, 56, 58]
10	$[0, \frac{1}{2}, \frac{3}{4}]$	[18, 21, 67, 71]
11	$[0, \frac{1}{2}, \frac{1}{4}]$	[19, 23, 66, 69]
12	$[0, \frac{1}{4}, \frac{1}{2}]$	[20, 22, 53, 60]
13	$[\frac{3}{4}, 0, \frac{1}{2}]$	[25, 26, 51, 52]
14	$[\frac{1}{4}, 0, \frac{1}{2}]$	[27, 28, 49, 50]
15	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2}]$	[29, 36, 92, 94]
16	$[\frac{1}{2}, 0, \frac{3}{4}]$	[30, 33, 79, 83]
17	$[\frac{1}{2}, 0, \frac{1}{4}]$	[31, 35, 78, 81]
18	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{2}]$	[32, 34, 89, 96]
19	$[\frac{3}{4}, \frac{1}{2}, 0]$	[37, 38, 63, 64]
20	$[\frac{1}{4}, \frac{1}{2}, 0]$	[39, 40, 61, 62]
21	$[\frac{1}{2}, \frac{3}{4}, 0]$	[41, 48, 80, 82]
22	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[42, 45, 91, 95]
23	$[\frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[43, 47, 90, 93]
24	$[\frac{1}{2}, \frac{1}{4}, 0]$	[44, 46, 77, 84]

Table 5: Wyckoff site: 32e, site symmetry: .3.

No.	position	mapping
1	[x, x, x]	[1, 5, 6]
2	[x, -x, -x]	[2, 10, 11]
3	[-x, x, -x]	[3, 7, 12]
4	[-x, -x, x]	[4, 8, 9]
5	[x, x + $\frac{1}{2}$ , x + $\frac{1}{2}$ ]	[13, 17, 18]
6	[x, $\frac{1}{2}$ - x, $\frac{1}{2}$ - x]	[14, 22, 23]
7	[-x, x + $\frac{1}{2}$ , $\frac{1}{2}$ - x]	[15, 19, 24]
8	[-x, $\frac{1}{2}$ - x, x + $\frac{1}{2}$ ]	[16, 20, 21]
9	[x + $\frac{1}{2}$ , x, x + $\frac{1}{2}$ ]	[25, 29, 30]
10	[x + $\frac{1}{2}$ , -x, $\frac{1}{2}$ - x]	[26, 34, 35]
11	[ $\frac{1}{2}$ - x, x, $\frac{1}{2}$ - x]	[27, 31, 36]
12	[ $\frac{1}{2}$ - x, -x, x + $\frac{1}{2}$ ]	[28, 32, 33]
13	[x + $\frac{1}{2}$ , x + $\frac{1}{2}$ , x]	[37, 41, 42]
14	[x + $\frac{1}{2}$ , $\frac{1}{2}$ - x, -x]	[38, 46, 47]
15	[ $\frac{1}{2}$ - x, x + $\frac{1}{2}$ , -x]	[39, 43, 48]
16	[ $\frac{1}{2}$ - x, $\frac{1}{2}$ - x, x]	[40, 44, 45]
17	[x, x, x + $\frac{1}{2}$ ]	[49, 53, 54]
18	[x, -x, $\frac{1}{2}$ - x]	[50, 58, 59]
19	[-x, x, $\frac{1}{2}$ - x]	[51, 55, 60]
20	[-x, -x, x + $\frac{1}{2}$ ]	[52, 56, 57]
21	[x, x + $\frac{1}{2}$ , x]	[61, 65, 66]
22	[x, $\frac{1}{2}$ - x, -x]	[62, 70, 71]
23	[-x, x + $\frac{1}{2}$ , -x]	[63, 67, 72]
24	[-x, $\frac{1}{2}$ - x, x]	[64, 68, 69]
25	[x + $\frac{1}{2}$ , x, x]	[73, 77, 78]
26	[x + $\frac{1}{2}$ , -x, -x]	[74, 82, 83]
27	[ $\frac{1}{2}$ - x, x, -x]	[75, 79, 84]
28	[ $\frac{1}{2}$ - x, -x, x]	[76, 80, 81]
29	[x + $\frac{1}{2}$ , x + $\frac{1}{2}$ , x + $\frac{1}{2}$ ]	[85, 89, 90]
30	[x + $\frac{1}{2}$ , $\frac{1}{2}$ - x, $\frac{1}{2}$ - x]	[86, 94, 95]
31	[ $\frac{1}{2}$ - x, x + $\frac{1}{2}$ , $\frac{1}{2}$ - x]	[87, 91, 96]
32	[ $\frac{1}{2}$ - x, $\frac{1}{2}$ - x, x + $\frac{1}{2}$ ]	[88, 92, 93]

Table 6: Wyckoff site: 48f, site symmetry: 2..

No.	position	mapping
1	[x, 0, 0]	[1, 2]
2	[-x, 0, 0]	[3, 4]
3	[0, x, 0]	[5, 12]
4	[0, 0, x]	[6, 9]
5	[0, 0, -x]	[7, 11]
6	[0, -x, 0]	[8, 10]
7	[x, $\frac{1}{2}$ , $\frac{1}{2}$ ]	[13, 14]

*continued ...*

Table 6

No.	position	mapping
8	$[-x, \frac{1}{2}, \frac{1}{2}]$	[15,16]
9	$[0, x + \frac{1}{2}, \frac{1}{2}]$	[17,24]
10	$[0, \frac{1}{2}, x + \frac{1}{2}]$	[18,21]
11	$[0, \frac{1}{2}, \frac{1}{2} - x]$	[19,23]
12	$[0, \frac{1}{2} - x, \frac{1}{2}]$	[20,22]
13	$[x + \frac{1}{2}, 0, \frac{1}{2}]$	[25,26]
14	$[\frac{1}{2} - x, 0, \frac{1}{2}]$	[27,28]
15	$[\frac{1}{2}, x, \frac{1}{2}]$	[29,36]
16	$[\frac{1}{2}, 0, x + \frac{1}{2}]$	[30,33]
17	$[\frac{1}{2}, 0, \frac{1}{2} - x]$	[31,35]
18	$[\frac{1}{2}, -x, \frac{1}{2}]$	[32,34]
19	$[x + \frac{1}{2}, \frac{1}{2}, 0]$	[37,38]
20	$[\frac{1}{2} - x, \frac{1}{2}, 0]$	[39,40]
21	$[\frac{1}{2}, x + \frac{1}{2}, 0]$	[41,48]
22	$[\frac{1}{2}, \frac{1}{2}, x]$	[42,45]
23	$[\frac{1}{2}, \frac{1}{2}, -x]$	[43,47]
24	$[\frac{1}{2}, \frac{1}{2} - x, 0]$	[44,46]
25	$[x, 0, \frac{1}{2}]$	[49,50]
26	$[-x, 0, \frac{1}{2}]$	[51,52]
27	$[0, x, \frac{1}{2}]$	[53,60]
28	$[0, 0, x + \frac{1}{2}]$	[54,57]
29	$[0, 0, \frac{1}{2} - x]$	[55,59]
30	$[0, -x, \frac{1}{2}]$	[56,58]
31	$[x, \frac{1}{2}, 0]$	[61,62]
32	$[-x, \frac{1}{2}, 0]$	[63,64]
33	$[0, x + \frac{1}{2}, 0]$	[65,72]
34	$[0, \frac{1}{2}, x]$	[66,69]
35	$[0, \frac{1}{2}, -x]$	[67,71]
36	$[0, \frac{1}{2} - x, 0]$	[68,70]
37	$[x + \frac{1}{2}, 0, 0]$	[73,74]
38	$[\frac{1}{2} - x, 0, 0]$	[75,76]
39	$[\frac{1}{2}, x, 0]$	[77,84]
40	$[\frac{1}{2}, 0, x]$	[78,81]
41	$[\frac{1}{2}, 0, -x]$	[79,83]
42	$[\frac{1}{2}, -x, 0]$	[80,82]
43	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[85,86]
44	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{2}]$	[87,88]
45	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{2}]$	[89,96]
46	$[\frac{1}{2}, \frac{1}{2}, x + \frac{1}{2}]$	[90,93]
47	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - x]$	[91,95]
48	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{2}]$	[92,94]

Table 7: Wyckoff site: 48g, site symmetry:  $2' \dots$ 

No.	position	mapping
1	$[x, 0, \frac{1}{4}]$	[1,50]
2	$[x, 0, \frac{3}{4}]$	[2,49]
3	$[-x, 0, \frac{3}{4}]$	[3,52]
4	$[-x, 0, \frac{1}{4}]$	[4,51]
5	$[\frac{1}{4}, x, 0]$	[5,84]
6	$[0, \frac{1}{4}, x]$	[6,69]
7	$[0, \frac{1}{4}, -x]$	[7,71]
8	$[\frac{3}{4}, -x, 0]$	[8,82]
9	$[0, \frac{3}{4}, x]$	[9,66]
10	$[\frac{1}{4}, -x, 0]$	[10,80]
11	$[0, \frac{3}{4}, -x]$	[11,67]
12	$[\frac{3}{4}, x, 0]$	[12,77]
13	$[x, \frac{1}{2}, \frac{3}{4}]$	[13,62]
14	$[x, \frac{1}{2}, \frac{1}{4}]$	[14,61]
15	$[-x, \frac{1}{2}, \frac{1}{4}]$	[15,64]
16	$[-x, \frac{1}{2}, \frac{3}{4}]$	[16,63]
17	$[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{2}]$	[17,96]
18	$[0, \frac{3}{4}, x + \frac{1}{2}]$	[18,57]
19	$[0, \frac{3}{4}, \frac{1}{2} - x]$	[19,59]
20	$[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{2}]$	[20,94]
21	$[0, \frac{1}{4}, x + \frac{1}{2}]$	[21,54]
22	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{2}]$	[22,92]
23	$[0, \frac{1}{4}, \frac{1}{2} - x]$	[23,55]
24	$[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{2}]$	[24,89]
25	$[x + \frac{1}{2}, 0, \frac{3}{4}]$	[25,74]
26	$[x + \frac{1}{2}, 0, \frac{1}{4}]$	[26,73]
27	$[\frac{1}{2} - x, 0, \frac{1}{4}]$	[27,76]
28	$[\frac{1}{2} - x, 0, \frac{3}{4}]$	[28,75]
29	$[\frac{3}{4}, x, \frac{1}{2}]$	[29,60]
30	$[\frac{1}{2}, \frac{1}{4}, x + \frac{1}{2}]$	[30,93]
31	$[\frac{1}{2}, \frac{1}{4}, \frac{1}{2} - x]$	[31,95]
32	$[\frac{1}{4}, -x, \frac{1}{2}]$	[32,58]
33	$[\frac{1}{2}, \frac{3}{4}, x + \frac{1}{2}]$	[33,90]
34	$[\frac{3}{4}, -x, \frac{1}{2}]$	[34,56]
35	$[\frac{1}{2}, \frac{3}{4}, \frac{1}{2} - x]$	[35,91]
36	$[\frac{1}{4}, x, \frac{1}{2}]$	[36,53]
37	$[x + \frac{1}{2}, \frac{1}{2}, \frac{1}{4}]$	[37,86]
38	$[x + \frac{1}{2}, \frac{1}{2}, \frac{3}{4}]$	[38,85]
39	$[\frac{1}{2} - x, \frac{1}{2}, \frac{3}{4}]$	[39,88]
40	$[\frac{1}{2} - x, \frac{1}{2}, \frac{1}{4}]$	[40,87]
41	$[\frac{3}{4}, x + \frac{1}{2}, 0]$	[41,72]
42	$[\frac{1}{2}, \frac{3}{4}, x]$	[42,81]
43	$[\frac{1}{2}, \frac{3}{4}, -x]$	[43,83]
44	$[\frac{1}{4}, \frac{1}{2} - x, 0]$	[44,70]
45	$[\frac{1}{2}, \frac{1}{4}, x]$	[45,78]
46	$[\frac{3}{4}, \frac{1}{2} - x, 0]$	[46,68]

*continued ...*

Table 7

No.	position	mapping
47	$[\frac{1}{2}, \frac{1}{4}, -x]$	[47, 79]
48	$[\frac{1}{4}, x + \frac{1}{2}, 0]$	[48, 65]

Table 8: Wyckoff site: 48h, site symmetry:  $2' \dots$ 

No.	position	mapping
1	$[x, \frac{1}{4}, 0]$	[1, 62]
2	$[x, \frac{3}{4}, 0]$	[2, 61]
3	$[-x, \frac{1}{4}, 0]$	[3, 64]
4	$[-x, \frac{3}{4}, 0]$	[4, 63]
5	$[0, x, \frac{1}{4}]$	[5, 60]
6	$[\frac{1}{4}, 0, x]$	[6, 81]
7	$[\frac{3}{4}, 0, -x]$	[7, 83]
8	$[0, -x, \frac{1}{4}]$	[8, 58]
9	$[\frac{3}{4}, 0, x]$	[9, 78]
10	$[0, -x, \frac{3}{4}]$	[10, 56]
11	$[\frac{1}{4}, 0, -x]$	[11, 79]
12	$[0, x, \frac{3}{4}]$	[12, 53]
13	$[x, \frac{3}{4}, \frac{1}{2}]$	[13, 50]
14	$[x, \frac{1}{4}, \frac{1}{2}]$	[14, 49]
15	$[-x, \frac{3}{4}, \frac{1}{2}]$	[15, 52]
16	$[-x, \frac{1}{4}, \frac{1}{2}]$	[16, 51]
17	$[0, x + \frac{1}{2}, \frac{3}{4}]$	[17, 72]
18	$[\frac{1}{4}, \frac{1}{2}, x + \frac{1}{2}]$	[18, 93]
19	$[\frac{3}{4}, \frac{1}{2}, \frac{1}{2} - x]$	[19, 95]
20	$[0, \frac{1}{2} - x, \frac{3}{4}]$	[20, 70]
21	$[\frac{3}{4}, \frac{1}{2}, x + \frac{1}{2}]$	[21, 90]
22	$[0, \frac{1}{2} - x, \frac{1}{4}]$	[22, 68]
23	$[\frac{1}{4}, \frac{1}{2}, \frac{1}{2} - x]$	[23, 91]
24	$[0, x + \frac{1}{2}, \frac{1}{4}]$	[24, 65]
25	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{2}]$	[25, 86]
26	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{2}]$	[26, 85]
27	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{2}]$	[27, 88]
28	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{2}]$	[28, 87]
29	$[\frac{1}{2}, x, \frac{3}{4}]$	[29, 84]
30	$[\frac{3}{4}, 0, x + \frac{1}{2}]$	[30, 57]
31	$[\frac{1}{4}, 0, \frac{1}{2} - x]$	[31, 59]
32	$[\frac{1}{2}, -x, \frac{3}{4}]$	[32, 82]
33	$[\frac{1}{4}, 0, x + \frac{1}{2}]$	[33, 54]
34	$[\frac{1}{2}, -x, \frac{1}{4}]$	[34, 80]
35	$[\frac{3}{4}, 0, \frac{1}{2} - x]$	[35, 55]
36	$[\frac{1}{2}, x, \frac{1}{4}]$	[36, 77]
37	$[x + \frac{1}{2}, \frac{3}{4}, 0]$	[37, 74]
38	$[x + \frac{1}{2}, \frac{1}{4}, 0]$	[38, 73]

*continued ...*

Table 8

No.	position	mapping
39	$[\frac{1}{2} - x, \frac{3}{4}, 0]$	[39,76]
40	$[\frac{1}{2} - x, \frac{1}{4}, 0]$	[40,75]
41	$[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}]$	[41,96]
42	$[\frac{3}{4}, \frac{1}{2}, x]$	[42,69]
43	$[\frac{1}{4}, \frac{1}{2}, -x]$	[43,71]
44	$[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}]$	[44,94]
45	$[\frac{1}{4}, \frac{1}{2}, x]$	[45,66]
46	$[\frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}]$	[46,92]
47	$[\frac{3}{4}, \frac{1}{2}, -x]$	[47,67]
48	$[\frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}]$	[48,89]

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

No.	position	mapping
1	$[x, \frac{1}{4}, \frac{1}{4}]$	[1,14]
2	$[x, \frac{3}{4}, \frac{3}{4}]$	[2,13]
3	$[-x, \frac{1}{4}, \frac{3}{4}]$	[3,16]
4	$[-x, \frac{3}{4}, \frac{1}{4}]$	[4,15]
5	$[\frac{1}{4}, x, \frac{1}{4}]$	[5,36]
6	$[\frac{1}{4}, \frac{1}{4}, x]$	[6,45]
7	$[\frac{3}{4}, \frac{1}{4}, -x]$	[7,47]
8	$[\frac{3}{4}, -x, \frac{1}{4}]$	[8,34]
9	$[\frac{3}{4}, \frac{3}{4}, x]$	[9,42]
10	$[\frac{1}{4}, -x, \frac{3}{4}]$	[10,32]
11	$[\frac{1}{4}, \frac{3}{4}, -x]$	[11,43]
12	$[\frac{3}{4}, x, \frac{3}{4}]$	[12,29]
13	$[\frac{1}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[17,48]
14	$[\frac{1}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[18,33]
15	$[\frac{3}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[19,35]
16	$[\frac{3}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[20,46]
17	$[\frac{3}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[21,30]
18	$[\frac{1}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[22,44]
19	$[\frac{1}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[23,31]
20	$[\frac{3}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[24,41]
21	$[x + \frac{1}{2}, \frac{1}{4}, \frac{3}{4}]$	[25,38]
22	$[x + \frac{1}{2}, \frac{3}{4}, \frac{1}{4}]$	[26,37]
23	$[\frac{1}{2} - x, \frac{1}{4}, \frac{1}{4}]$	[27,40]
24	$[\frac{1}{2} - x, \frac{3}{4}, \frac{3}{4}]$	[28,39]
25	$[x, \frac{1}{4}, \frac{3}{4}]$	[49,62]
26	$[x, \frac{3}{4}, \frac{1}{4}]$	[50,61]
27	$[-x, \frac{1}{4}, \frac{1}{4}]$	[51,64]
28	$[-x, \frac{3}{4}, \frac{3}{4}]$	[52,63]
29	$[\frac{1}{4}, x, \frac{3}{4}]$	[53,84]
30	$[\frac{1}{4}, \frac{1}{4}, x + \frac{1}{2}]$	[54,93]

continued ...

Table 9

No.	position	mapping
31	$[\frac{3}{4}, \frac{1}{4}, \frac{1}{2} - x]$	[55,95]
32	$[\frac{3}{4}, -x, \frac{3}{4}]$	[56,82]
33	$[\frac{3}{4}, \frac{3}{4}, x + \frac{1}{2}]$	[57,90]
34	$[\frac{1}{4}, -x, \frac{1}{4}]$	[58,80]
35	$[\frac{1}{4}, \frac{3}{4}, \frac{1}{2} - x]$	[59,91]
36	$[\frac{3}{4}, x, \frac{1}{4}]$	[60,77]
37	$[\frac{1}{4}, x + \frac{1}{2}, \frac{1}{4}]$	[65,96]
38	$[\frac{1}{4}, \frac{3}{4}, x]$	[66,81]
39	$[\frac{3}{4}, \frac{3}{4}, -x]$	[67,83]
40	$[\frac{3}{4}, \frac{1}{2} - x, \frac{1}{4}]$	[68,94]
41	$[\frac{3}{4}, \frac{1}{4}, x]$	[69,78]
42	$[\frac{1}{4}, \frac{1}{2} - x, \frac{3}{4}]$	[70,92]
43	$[\frac{1}{4}, \frac{1}{4}, -x]$	[71,79]
44	$[\frac{3}{4}, x + \frac{1}{2}, \frac{3}{4}]$	[72,89]
45	$[x + \frac{1}{2}, \frac{1}{4}, \frac{1}{4}]$	[73,86]
46	$[x + \frac{1}{2}, \frac{3}{4}, \frac{3}{4}]$	[74,85]
47	$[\frac{1}{2} - x, \frac{1}{4}, \frac{3}{4}]$	[75,88]
48	$[\frac{1}{2} - x, \frac{3}{4}, \frac{1}{4}]$	[76,87]

Table 10: Wyckoff site: 96j, site symmetry: 1

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

continued ...

Table 10

No.	position	mapping
23	$[y, \frac{1}{2} - z, \frac{1}{2} - x]$	[23]
24	$[-z, x + \frac{1}{2}, \frac{1}{2} - y]$	[24]
25	$[x + \frac{1}{2}, y, z + \frac{1}{2}]$	[25]
26	$[x + \frac{1}{2}, -y, \frac{1}{2} - z]$	[26]
27	$[\frac{1}{2} - x, y, \frac{1}{2} - z]$	[27]
28	$[\frac{1}{2} - x, -y, z + \frac{1}{2}]$	[28]
29	$[z + \frac{1}{2}, x, y + \frac{1}{2}]$	[29]
30	$[y + \frac{1}{2}, z, x + \frac{1}{2}]$	[30]
31	$[\frac{1}{2} - y, z, \frac{1}{2} - x]$	[31]
32	$[\frac{1}{2} - z, -x, y + \frac{1}{2}]$	[32]
33	$[\frac{1}{2} - y, -z, x + \frac{1}{2}]$	[33]
34	$[z + \frac{1}{2}, -x, \frac{1}{2} - y]$	[34]
35	$[y + \frac{1}{2}, -z, \frac{1}{2} - x]$	[35]
36	$[\frac{1}{2} - z, x, \frac{1}{2} - y]$	[36]
37	$[x + \frac{1}{2}, y + \frac{1}{2}, z]$	[37]
38	$[x + \frac{1}{2}, \frac{1}{2} - y, -z]$	[38]
39	$[\frac{1}{2} - x, y + \frac{1}{2}, -z]$	[39]
40	$[\frac{1}{2} - x, \frac{1}{2} - y, z]$	[40]
41	$[z + \frac{1}{2}, x + \frac{1}{2}, y]$	[41]
42	$[y + \frac{1}{2}, z + \frac{1}{2}, x]$	[42]
43	$[\frac{1}{2} - y, z + \frac{1}{2}, -x]$	[43]
44	$[\frac{1}{2} - z, \frac{1}{2} - x, y]$	[44]
45	$[\frac{1}{2} - y, \frac{1}{2} - z, x]$	[45]
46	$[z + \frac{1}{2}, \frac{1}{2} - x, -y]$	[46]
47	$[y + \frac{1}{2}, \frac{1}{2} - z, -x]$	[47]
48	$[\frac{1}{2} - z, x + \frac{1}{2}, -y]$	[48]
49	$[x, y, z + \frac{1}{2}]$	[49]
50	$[x, -y, \frac{1}{2} - z]$	[50]
51	$[-x, y, \frac{1}{2} - z]$	[51]
52	$[-x, -y, z + \frac{1}{2}]$	[52]
53	$[z, x, y + \frac{1}{2}]$	[53]
54	$[y, z, x + \frac{1}{2}]$	[54]
55	$[-y, z, \frac{1}{2} - x]$	[55]
56	$[-z, -x, y + \frac{1}{2}]$	[56]
57	$[-y, -z, x + \frac{1}{2}]$	[57]
58	$[z, -x, \frac{1}{2} - y]$	[58]
59	$[y, -z, \frac{1}{2} - x]$	[59]
60	$[-z, x, \frac{1}{2} - y]$	[60]
61	$[x, y + \frac{1}{2}, z]$	[61]
62	$[x, \frac{1}{2} - y, -z]$	[62]
63	$[-x, y + \frac{1}{2}, -z]$	[63]
64	$[-x, \frac{1}{2} - y, z]$	[64]
65	$[z, x + \frac{1}{2}, y]$	[65]
66	$[y, z + \frac{1}{2}, x]$	[66]
67	$[-y, z + \frac{1}{2}, -x]$	[67]
68	$[-z, \frac{1}{2} - x, y]$	[68]
69	$[-y, \frac{1}{2} - z, x]$	[69]

*continued ...*

Table 10

No.	position	mapping
70	$[z, \frac{1}{2} - x, -y]$	[70]
71	$[y, \frac{1}{2} - z, -x]$	[71]
72	$[-z, x + \frac{1}{2}, -y]$	[72]
73	$[x + \frac{1}{2}, y, z]$	[73]
74	$[x + \frac{1}{2}, -y, -z]$	[74]
75	$[\frac{1}{2} - x, y, -z]$	[75]
76	$[\frac{1}{2} - x, -y, z]$	[76]
77	$[z + \frac{1}{2}, x, y]$	[77]
78	$[y + \frac{1}{2}, z, x]$	[78]
79	$[\frac{1}{2} - y, z, -x]$	[79]
80	$[\frac{1}{2} - z, -x, y]$	[80]
81	$[\frac{1}{2} - y, -z, x]$	[81]
82	$[z + \frac{1}{2}, -x, -y]$	[82]
83	$[y + \frac{1}{2}, -z, -x]$	[83]
84	$[\frac{1}{2} - z, x, -y]$	[84]
85	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[85]
86	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[86]
87	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[87]
88	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[88]
89	$[z + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}]$	[89]
90	$[y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}]$	[90]
91	$[\frac{1}{2} - y, z + \frac{1}{2}, \frac{1}{2} - x]$	[91]
92	$[\frac{1}{2} - z, \frac{1}{2} - x, y + \frac{1}{2}]$	[92]
93	$[\frac{1}{2} - y, \frac{1}{2} - z, x + \frac{1}{2}]$	[93]
94	$[z + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - y]$	[94]
95	$[y + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - x]$	[95]
96	$[\frac{1}{2} - z, x + \frac{1}{2}, \frac{1}{2} - y]$	[96]