

MSG No. 221.97 $P\bar{1}m\bar{3}m$ [Type IV, cubic]

Table 1: Wyckoff site: 2a, site symmetry: $m\bar{3}m$

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

Table 2: Wyckoff site: 6b, site symmetry: $4/\bar{m}.m$

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

Table 3: Wyckoff site: 8c, site symmetry: $\bar{3}m$

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

Table 4: Wyckoff site: 12d, site symmetry: $\bar{4}'m.2'$

No.	position	mapping
1	$[\frac{1}{4}, 0, \frac{1}{2}]$	$[1, 8, 33, 34, 61, 62, 74, 75]$
2	$[\frac{1}{4}, \frac{1}{2}, 0]$	$[2, 3, 37, 38, 57, 58, 73, 80]$
3	$[\frac{1}{2}, 0, \frac{3}{4}]$	$[4, 16, 29, 39, 66, 69, 91, 95]$
4	$[\frac{1}{2}, 0, \frac{1}{4}]$	$[5, 15, 28, 40, 67, 71, 90, 93]$
5	$[0, \frac{1}{4}, \frac{1}{2}]$	$[6, 11, 31, 36, 68, 70, 89, 96]$
6	$[0, \frac{3}{4}, \frac{1}{2}]$	$[7, 12, 30, 35, 65, 72, 92, 94]$
7	$[\frac{3}{4}, 0, \frac{1}{2}]$	$[9, 10, 25, 32, 50, 51, 85, 86]$

continued ...

Table 4

No.	position	mapping
8	$[\frac{3}{4}, \frac{1}{2}, 0]$	$[13, 14, 26, 27, 49, 56, 81, 82]$
9	$[\frac{1}{2}, \frac{1}{4}, 0]$	$[17, 24, 44, 46, 55, 60, 78, 83]$
10	$[0, \frac{1}{2}, \frac{1}{4}]$	$[18, 21, 43, 47, 52, 64, 77, 87]$
11	$[0, \frac{1}{2}, \frac{3}{4}]$	$[19, 23, 42, 45, 53, 63, 76, 88]$
12	$[\frac{1}{2}, \frac{3}{4}, 0]$	$[20, 22, 41, 48, 54, 59, 79, 84]$

Table 5: Wyckoff site: 12e, site symmetry: $4\bar{m}.m$

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

Table 6: Wyckoff site: 16f, site symmetry: $\bar{3}m$

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

Table 7: Wyckoff site: 24g, site symmetry: $2mm..$

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

Table 8: Wyckoff site: 24h, site symmetry: $m..2m$

No.	position	mapping
1	$[0, y, y]$	$[1, 13, 32, 38]$
2	$[0, -y, y]$	$[2, 10, 27, 33]$
3	$[0, y, -y]$	$[3, 9, 26, 34]$
4	$[y, y, 0]$	$[4, 18, 40, 45]$
5	$[-y, y, 0]$	$[5, 19, 39, 47]$
6	$[-y, 0, y]$	$[6, 20, 35, 46]$
7	$[y, 0, y]$	$[7, 17, 36, 48]$
8	$[0, -y, -y]$	$[8, 14, 25, 37]$
9	$[y, 0, -y]$	$[11, 22, 30, 44]$
10	$[-y, 0, -y]$	$[12, 24, 31, 41]$
11	$[y, -y, 0]$	$[15, 23, 29, 43]$
12	$[-y, -y, 0]$	$[16, 21, 28, 42]$
13	$[\frac{1}{2}, y + \frac{1}{2}, y + \frac{1}{2}]$	$[49, 61, 80, 86]$
14	$[\frac{1}{2}, \frac{1}{2} - y, y + \frac{1}{2}]$	$[50, 58, 75, 81]$
15	$[\frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - y]$	$[51, 57, 74, 82]$

continued ...

Table 8

No.	position	mapping
16	$[y + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2}]$	[52,66,88,93]
17	$[\frac{1}{2} - y, y + \frac{1}{2}, \frac{1}{2}]$	[53,67,87,95]
18	$[\frac{1}{2} - y, \frac{1}{2}, y + \frac{1}{2}]$	[54,68,83,94]
19	$[y + \frac{1}{2}, \frac{1}{2}, y + \frac{1}{2}]$	[55,65,84,96]
20	$[\frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - y]$	[56,62,73,85]
21	$[y + \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - y]$	[59,70,78,92]
22	$[\frac{1}{2} - y, \frac{1}{2}, \frac{1}{2} - y]$	[60,72,79,89]
23	$[y + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2}]$	[63,71,77,91]
24	$[\frac{1}{2} - y, \frac{1}{2} - y, \frac{1}{2}]$	[64,69,76,90]

Table 9: Wyckoff site: 48i, site symmetry: $\dots 2'$

No.	position	mapping
1	$[\frac{1}{4}, y, \frac{1}{2} - y]$	[1,62]
2	$[\frac{1}{4}, y + \frac{1}{2}, y]$	[2,57]
3	$[\frac{1}{4}, \frac{1}{2} - y, -y]$	[3,58]
4	$[\frac{1}{2} - y, y, \frac{3}{4}]$	[4,69]
5	$[y + \frac{1}{2}, y, \frac{1}{4}]$	[5,71]
6	$[-y, \frac{1}{4}, \frac{1}{2} - y]$	[6,70]
7	$[y, \frac{3}{4}, \frac{1}{2} - y]$	[7,72]
8	$[\frac{1}{4}, -y, y + \frac{1}{2}]$	[8,61]
9	$[\frac{3}{4}, y, y + \frac{1}{2}]$	[9,50]
10	$[\frac{3}{4}, -y, \frac{1}{2} - y]$	[10,51]
11	$[y, \frac{1}{4}, y + \frac{1}{2}]$	[11,68]
12	$[-y, \frac{3}{4}, y + \frac{1}{2}]$	[12,65]
13	$[\frac{3}{4}, \frac{1}{2} - y, y]$	[13,56]
14	$[\frac{3}{4}, y + \frac{1}{2}, -y]$	[14,49]
15	$[\frac{1}{2} - y, -y, \frac{1}{4}]$	[15,67]
16	$[y + \frac{1}{2}, -y, \frac{3}{4}]$	[16,66]
17	$[\frac{1}{2} - y, \frac{1}{4}, y]$	[17,60]
18	$[y, \frac{1}{2} - y, \frac{1}{4}]$	[18,64]
19	$[-y, \frac{1}{2} - y, \frac{3}{4}]$	[19,63]
20	$[y + \frac{1}{2}, \frac{3}{4}, y]$	[20,59]
21	$[-y, y + \frac{1}{2}, \frac{1}{4}]$	[21,52]
22	$[\frac{1}{2} - y, \frac{3}{4}, -y]$	[22,54]
23	$[y, y + \frac{1}{2}, \frac{3}{4}]$	[23,53]
24	$[y + \frac{1}{2}, \frac{1}{4}, -y]$	[24,55]
25	$[\frac{3}{4}, -y, y + \frac{1}{2}]$	[25,86]
26	$[\frac{3}{4}, \frac{1}{2} - y, -y]$	[26,81]
27	$[\frac{3}{4}, y + \frac{1}{2}, y]$	[27,82]
28	$[y + \frac{1}{2}, -y, \frac{1}{4}]$	[28,93]
29	$[\frac{1}{2} - y, -y, \frac{3}{4}]$	[29,95]
30	$[y, \frac{3}{4}, y + \frac{1}{2}]$	[30,94]
31	$[-y, \frac{1}{4}, y + \frac{1}{2}]$	[31,96]

continued ...

Table 9

No.	position	mapping
32	$[\frac{3}{4}, y, \frac{1}{2} - y]$	[32,85]
33	$[\frac{1}{4}, -y, \frac{1}{2} - y]$	[33,74]
34	$[\frac{1}{4}, y, y + \frac{1}{2}]$	[34,75]
35	$[-y, \frac{3}{4}, \frac{1}{2} - y]$	[35,92]
36	$[y, \frac{1}{4}, \frac{1}{2} - y]$	[36,89]
37	$[\frac{1}{4}, y + \frac{1}{2}, -y]$	[37,80]
38	$[\frac{1}{4}, \frac{1}{2} - y, y]$	[38,73]
39	$[y + \frac{1}{2}, y, \frac{3}{4}]$	[39,91]
40	$[\frac{1}{2} - y, y, \frac{1}{4}]$	[40,90]
41	$[y + \frac{1}{2}, \frac{3}{4}, -y]$	[41,84]
42	$[-y, y + \frac{1}{2}, \frac{3}{4}]$	[42,88]
43	$[y, y + \frac{1}{2}, \frac{1}{4}]$	[43,87]
44	$[\frac{1}{2} - y, \frac{1}{4}, -y]$	[44,83]
45	$[y, \frac{1}{2} - y, \frac{3}{4}]$	[45,76]
46	$[y + \frac{1}{2}, \frac{1}{4}, y]$	[46,78]
47	$[-y, \frac{1}{2} - y, \frac{1}{4}]$	[47,77]
48	$[\frac{1}{2} - y, \frac{3}{4}, y]$	[48,79]

Table 10: Wyckoff site: 48j, site symmetry: $m..$

No.	position	mapping
1	$[0, y, z]$	[1,32]
2	$[0, -z, y]$	[2,27]
3	$[0, z, -y]$	[3,26]
4	$[z, y, 0]$	[4,40]
5	$[-z, y, 0]$	[5,39]
6	$[-y, 0, z]$	[6,35]
7	$[y, 0, z]$	[7,36]
8	$[0, -y, -z]$	[8,25]
9	$[0, y, -z]$	[9,34]
10	$[0, -y, z]$	[10,33]
11	$[y, 0, -z]$	[11,30]
12	$[-y, 0, -z]$	[12,31]
13	$[0, z, y]$	[13,38]
14	$[0, -z, -y]$	[14,37]
15	$[z, -y, 0]$	[15,29]
16	$[-z, -y, 0]$	[16,28]
17	$[z, 0, y]$	[17,48]
18	$[y, z, 0]$	[18,45]
19	$[-y, z, 0]$	[19,47]
20	$[-z, 0, y]$	[20,46]
21	$[-y, -z, 0]$	[21,42]
22	$[z, 0, -y]$	[22,44]
23	$[y, -z, 0]$	[23,43]

continued ...

Table 10

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

Table 11: Wyckoff site: 48k, site symmetry: $\bar{3}m$

No.	position	mapping
1	$[x, x, z]$	[1,36]
2	$[x, -z, x]$	[2,43]
3	$[x, z, -x]$	[3,45]
4	$[z, x, -x]$	[4,44]
5	$[-z, x, x]$	[5,46]
6	$[-x, x, z]$	[6,32]
7	$[x, -x, z]$	[7,33]
8	$[x, -x, -z]$	[8,30]
9	$[-x, x, -z]$	[9,31]
10	$[-x, -x, z]$	[10,35]
11	$[x, x, -z]$	[11,34]
12	$[-x, -x, -z]$	[12,25]
13	$[-x, z, x]$	[13,47]
14	$[-x, -z, -x]$	[14,42]
15	$[z, -x, x]$	[15,48]

continued ...

Table 11

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

Table 12: Wyckoff site: 961, 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]

continued ...

Table 12

No.	position	mapping
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	$[-x, -y, -z]$	[25]
26	$[-x, z, -y]$	[26]
27	$[-x, -z, y]$	[27]
28	$[-z, -y, x]$	[28]
29	$[z, -y, -x]$	[29]
30	$[y, -x, -z]$	[30]
31	$[-y, x, -z]$	[31]
32	$[-x, y, z]$	[32]
33	$[x, -y, z]$	[33]
34	$[x, y, -z]$	[34]
35	$[-y, -x, z]$	[35]
36	$[y, x, z]$	[36]
37	$[x, -z, -y]$	[37]
38	$[x, z, y]$	[38]
39	$[-z, y, -x]$	[39]
40	$[z, y, x]$	[40]
41	$[-z, -x, -y]$	[41]
42	$[-y, -z, -x]$	[42]
43	$[y, -z, x]$	[43]
44	$[z, x, -y]$	[44]
45	$[y, z, -x]$	[45]
46	$[-z, x, y]$	[46]
47	$[-y, z, x]$	[47]
48	$[z, -x, y]$	[48]
49	$[x + \frac{1}{2}, y + \frac{1}{2}, z + \frac{1}{2}]$	[49]
50	$[x + \frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[50]
51	$[x + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[51]
52	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - x]$	[52]
53	$[\frac{1}{2} - z, y + \frac{1}{2}, x + \frac{1}{2}]$	[53]
54	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[54]

continued ...

Table 12

No.	position	mapping
55	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[55]
56	$[x + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - z]$	[56]
57	$[\frac{1}{2} - x, y + \frac{1}{2}, \frac{1}{2} - z]$	[57]
58	$[\frac{1}{2} - x, \frac{1}{2} - y, z + \frac{1}{2}]$	[58]
59	$[y + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - z]$	[59]
60	$[\frac{1}{2} - y, \frac{1}{2} - x, \frac{1}{2} - z]$	[60]
61	$[\frac{1}{2} - x, z + \frac{1}{2}, y + \frac{1}{2}]$	[61]
62	$[\frac{1}{2} - x, \frac{1}{2} - z, \frac{1}{2} - y]$	[62]
63	$[z + \frac{1}{2}, \frac{1}{2} - y, x + \frac{1}{2}]$	[63]
64	$[\frac{1}{2} - z, \frac{1}{2} - y, \frac{1}{2} - x]$	[64]
65	$[z + \frac{1}{2}, x + \frac{1}{2}, y + \frac{1}{2}]$	[65]
66	$[y + \frac{1}{2}, z + \frac{1}{2}, x + \frac{1}{2}]$	[66]
67	$[\frac{1}{2} - y, z + \frac{1}{2}, \frac{1}{2} - x]$	[67]
68	$[\frac{1}{2} - z, \frac{1}{2} - x, y + \frac{1}{2}]$	[68]
69	$[\frac{1}{2} - y, \frac{1}{2} - z, x + \frac{1}{2}]$	[69]
70	$[z + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - y]$	[70]
71	$[y + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - x]$	[71]
72	$[\frac{1}{2} - z, x + \frac{1}{2}, \frac{1}{2} - y]$	[72]
73	$[\frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} - z]$	[73]
74	$[\frac{1}{2} - x, z + \frac{1}{2}, \frac{1}{2} - y]$	[74]
75	$[\frac{1}{2} - x, \frac{1}{2} - z, y + \frac{1}{2}]$	[75]
76	$[\frac{1}{2} - z, \frac{1}{2} - y, x + \frac{1}{2}]$	[76]
77	$[z + \frac{1}{2}, \frac{1}{2} - y, \frac{1}{2} - x]$	[77]
78	$[y + \frac{1}{2}, \frac{1}{2} - x, \frac{1}{2} - z]$	[78]
79	$[\frac{1}{2} - y, x + \frac{1}{2}, \frac{1}{2} - z]$	[79]
80	$[\frac{1}{2} - x, y + \frac{1}{2}, z + \frac{1}{2}]$	[80]
81	$[x + \frac{1}{2}, \frac{1}{2} - y, z + \frac{1}{2}]$	[81]
82	$[x + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - z]$	[82]
83	$[\frac{1}{2} - y, \frac{1}{2} - x, z + \frac{1}{2}]$	[83]
84	$[y + \frac{1}{2}, x + \frac{1}{2}, z + \frac{1}{2}]$	[84]
85	$[x + \frac{1}{2}, \frac{1}{2} - z, \frac{1}{2} - y]$	[85]
86	$[x + \frac{1}{2}, z + \frac{1}{2}, y + \frac{1}{2}]$	[86]
87	$[\frac{1}{2} - z, y + \frac{1}{2}, \frac{1}{2} - x]$	[87]
88	$[z + \frac{1}{2}, y + \frac{1}{2}, x + \frac{1}{2}]$	[88]
89	$[\frac{1}{2} - z, \frac{1}{2} - x, \frac{1}{2} - y]$	[89]
90	$[\frac{1}{2} - y, \frac{1}{2} - z, \frac{1}{2} - x]$	[90]
91	$[y + \frac{1}{2}, \frac{1}{2} - z, x + \frac{1}{2}]$	[91]
92	$[z + \frac{1}{2}, x + \frac{1}{2}, \frac{1}{2} - y]$	[92]
93	$[y + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - x]$	[93]
94	$[\frac{1}{2} - z, x + \frac{1}{2}, y + \frac{1}{2}]$	[94]
95	$[\frac{1}{2} - y, z + \frac{1}{2}, x + \frac{1}{2}]$	[95]
96	$[z + \frac{1}{2}, \frac{1}{2} - x, y + \frac{1}{2}]$	[96]