MSG No. 202.25 $F_Sm\bar{3}$ [Type IV, cubic]

Table 1: Wyckoff site: `8a`, site symmetry: `m-3.`

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	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	[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	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	[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	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	[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	$\left[0, 0, \frac{1}{2}\right]$	[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	$\left[0, \frac{1}{2}, 0\right]$	[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	$\left[\frac{1}{2}, 0, 0\right]$	[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	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	[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: `m'-3'.`

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

Table 3: Wyckoff site: `24c`, site symmetry: `mm'm'..`

No.	position	mapping
1	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	[1,14,26,37,99,112,124,135]
2	$\left[0, \frac{3}{4}, \frac{3}{4}\right]$	[2,13,25,38,100,111,123,136]
3	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	[3,16,28,39,97,110,122,133]
4	$\left[0, \frac{3}{4}, \frac{1}{4}\right]$	[4,15,27,40,98,109,121,134]
5	$\left[\frac{1}{4}, 0, \frac{1}{4}\right]$	[5,24,60,65,106,116,152,166]
6	$\left[\frac{1}{4}, \frac{1}{4}, 0\right]$	[6,21,81,90,131,139,151,167]
7	$\left[\frac{3}{4}, \frac{1}{4}, 0\right]$	[7,23,83,91,129,138,150,165]
8	$\left[\frac{3}{4}, 0, \frac{1}{4}\right]$	[8,22,58,68,108,113,149,168]
9	$\left[\frac{3}{4}, \frac{3}{4}, 0\right]$	[9,18,78,93,127,143,155,163]
10	$\left[\frac{1}{4}, 0, \frac{3}{4}\right]$	[10,20,56,70,101,120,156,161]
11	$\left[\frac{1}{4}, \frac{3}{4}, 0\right]$	[11,19,79,95,126,141,153,162]
12	$\left[\frac{3}{4}, 0, \frac{3}{4}\right]$	[12,17,53,72,104,118,154,164]
13	$\left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[29,48,84,89,130,140,176,190]
14	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[30,45,57,66,107,115,175,191]
15	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}\right]$	[31,47,59,67,105,114,174,189]

continued ...

Table 3

No.	position	mapping
16	$\left[\frac{3}{4}, \frac{1}{2}, \frac{3}{4}\right]$	[32,46,82,92,132,137,173,192]
17	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[33,42,54,69,103,119,179,187]
18	$\left[\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[34,44,80,94,125,144,180,185]
19	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right]$	[35,43,55,71,102,117,177,186]
20	$\left[\frac{3}{4}, \frac{1}{2}, \frac{1}{4}\right]$	[36,41,77,96,128,142,178,188]
21	$\left[\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[49,62,74,85,147,160,172,183]
22	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[50,61,73,86,148,159,171,184]
23	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[51,64,76,87,145,158,170,181]
24	$\left[\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[52,63,75,88,146,157,169,182]

Table 4: Wyckoff site: 24d, site symmetry: m'mm..

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

Table 5: Wyckoff site: `48e`, site symmetry: `2mm..`

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

continued ...

Table 5

No.	position	mapping
47	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}-x\right]$	[175,179,186,189]
48	$\left[\frac{1}{2}, \frac{1}{2}-x, \frac{1}{2}\right]$	[176,178,185,192]

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

No.	position	mapping
1	$\left[x, 0, \frac{1}{4}\right]$	[1,15,98,112]
2	$\left[x, 0, \frac{3}{4}\right]$	[2,16,97,111]
3	$\left[-x, 0, \frac{3}{4}\right]$	[3,13,100,110]
4	$\left[-x, 0, \frac{1}{4}\right]$	[4,14,99,109]
5	$\left[\frac{1}{4}, x, 0\right]$	[5,20,156,166]
6	$\left[0, \frac{1}{4}, x\right]$	[6,23,129,139]
7	$\left[0, \frac{1}{4}, -x\right]$	[7,21,131,138]
8	$\left[\frac{3}{4}, -x, 0\right]$	[8,17,154,168]
9	$\left[0, \frac{3}{4}, x\right]$	[9,19,126,143]
10	$\left[\frac{1}{4}, -x, 0\right]$	[10,24,152,161]
11	$\left[0, \frac{3}{4}, -x\right]$	[11,18,127,141]
12	$\left[\frac{3}{4}, x, 0\right]$	[12,22,149,164]
13	$\left[x, \frac{1}{2}, \frac{3}{4}\right]$	[25,39,122,136]
14	$\left[x, \frac{1}{2}, \frac{1}{4}\right]$	[26,40,121,135]
15	$\left[-x, \frac{1}{2}, \frac{1}{4}\right]$	[27,37,124,134]
16	$\left[-x, \frac{1}{2}, \frac{3}{4}\right]$	[28,38,123,133]
17	$\left[\frac{1}{4}, x+\frac{1}{2}, \frac{1}{2}\right]$	[29,44,180,190]
18	$\left[0, \frac{3}{4}, x+\frac{1}{2}\right]$	[30,47,105,115]
19	$\left[0, \frac{3}{4}, \frac{1}{2}-x\right]$	[31,45,107,114]
20	$\left[\frac{3}{4}, \frac{1}{2}-x, \frac{1}{2}\right]$	[32,41,178,192]
21	$\left[0, \frac{1}{4}, x+\frac{1}{2}\right]$	[33,43,102,119]
22	$\left[\frac{1}{4}, \frac{1}{2}-x, \frac{1}{2}\right]$	[34,48,176,185]
23	$\left[0, \frac{1}{4}, \frac{1}{2}-x\right]$	[35,42,103,117]
24	$\left[\frac{3}{4}, x+\frac{1}{2}, \frac{1}{2}\right]$	[36,46,173,188]
25	$\left[x+\frac{1}{2}, 0, \frac{3}{4}\right]$	[49,63,146,160]
26	$\left[x+\frac{1}{2}, 0, \frac{1}{4}\right]$	[50,64,145,159]
27	$\left[\frac{1}{2}-x, 0, \frac{1}{4}\right]$	[51,61,148,158]
28	$\left[\frac{1}{2}-x, 0, \frac{3}{4}\right]$	[52,62,147,157]
29	$\left[\frac{3}{4}, x, \frac{1}{2}\right]$	[53,68,108,118]
30	$\left[\frac{1}{2}, \frac{1}{4}, x+\frac{1}{2}\right]$	[54,71,177,187]
31	$\left[\frac{1}{2}, \frac{1}{4}, \frac{1}{2}-x\right]$	[55,69,179,186]
32	$\left[\frac{1}{4}, -x, \frac{1}{2}\right]$	[56,65,106,120]
33	$\left[\frac{1}{2}, \frac{3}{4}, x+\frac{1}{2}\right]$	[57,67,174,191]
34	$\left[\frac{3}{4}, -x, \frac{1}{2}\right]$	[58,72,104,113]
35	$\left[\frac{1}{2}, \frac{3}{4}, \frac{1}{2}-x\right]$	[59,66,175,189]
36	$\left[\frac{1}{4}, x, \frac{1}{2}\right]$	[60,70,101,116]
37	$\left[x+\frac{1}{2}, \frac{1}{2}, \frac{1}{4}\right]$	[73,87,170,184]
38	$\left[x+\frac{1}{2}, \frac{1}{2}, \frac{3}{4}\right]$	[74,88,169,183]

continued ...

Table 6

No.	position	mapping
39	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{3}{4}\right]$	[75,85,172,182]
40	$\left[\frac{1}{2}-x,\ \frac{1}{2},\ \frac{1}{4}\right]$	[76,86,171,181]
41	$\left[\frac{3}{4},\ x+\frac{1}{2},\ 0\right]$	[77,92,132,142]
42	$\left[\frac{1}{2},\ \frac{3}{4},\ x\right]$	[78,95,153,163]
43	$\left[\frac{1}{2},\ \frac{3}{4},\ -x\right]$	[79,93,155,162]
44	$\left[\frac{1}{4},\ \frac{1}{2}-x,\ 0\right]$	[80,89,130,144]
45	$\left[\frac{1}{2},\ \frac{1}{4},\ x\right]$	[81,91,150,167]
46	$\left[\frac{3}{4},\ \frac{1}{2}-x,\ 0\right]$	[82,96,128,137]
47	$\left[\frac{1}{2},\ \frac{1}{4},\ -x\right]$	[83,90,151,165]
48	$\left[\frac{1}{4},\ x+\frac{1}{2},\ 0\right]$	[84,94,125,140]

Table 7: Wyckoff site: 48g, site symmetry: 2'm'm..

No.	position	mapping
1	$\left[x,\ \frac{1}{4},\ 0\right]$	[1,16,122,135]
2	$\left[x,\ \frac{3}{4},\ 0\right]$	[2,15,121,136]
3	$\left[-x,\ \frac{1}{4},\ 0\right]$	[3,14,124,133]
4	$\left[-x,\ \frac{3}{4},\ 0\right]$	[4,13,123,134]
5	$\left[0,\ x,\ \frac{1}{4}\right]$	[5,22,108,116]
6	$\left[\frac{1}{4},\ 0,\ x\right]$	[6,19,153,167]
7	$\left[\frac{3}{4},\ 0,\ -x\right]$	[7,18,155,165]
8	$\left[0,\ -x,\ \frac{1}{4}\right]$	[8,24,106,113]
9	$\left[\frac{3}{4},\ 0,\ x\right]$	[9,23,150,163]
10	$\left[0,\ -x,\ \frac{3}{4}\right]$	[10,17,104,120]
11	$\left[\frac{1}{4},\ 0,\ -x\right]$	[11,21,151,162]
12	$\left[0,\ x,\ \frac{3}{4}\right]$	[12,20,101,118]
13	$\left[x,\ \frac{3}{4},\ \frac{1}{2}\right]$	[25,40,98,111]
14	$\left[x,\ \frac{1}{4},\ \frac{1}{2}\right]$	[26,39,97,112]
15	$\left[-x,\ \frac{3}{4},\ \frac{1}{2}\right]$	[27,38,100,109]
16	$\left[-x,\ \frac{1}{4},\ \frac{1}{2}\right]$	[28,37,99,110]
17	$\left[0,\ x+\frac{1}{2},\ \frac{3}{4}\right]$	[29,46,132,140]
18	$\left[\frac{1}{4},\ \frac{1}{2},\ x+\frac{1}{2}\right]$	[30,43,177,191]
19	$\left[\frac{3}{4},\ \frac{1}{2},\ \frac{1}{2}-x\right]$	[31,42,179,189]
20	$\left[0,\ \frac{1}{2}-x,\ \frac{3}{4}\right]$	[32,48,130,137]
21	$\left[\frac{3}{4},\ \frac{1}{2},\ x+\frac{1}{2}\right]$	[33,47,174,187]
22	$\left[0,\ \frac{1}{2}-x,\ \frac{1}{4}\right]$	[34,41,128,144]
23	$\left[\frac{1}{4},\ \frac{1}{2},\ \frac{1}{2}-x\right]$	[35,45,175,186]
24	$\left[0,\ x+\frac{1}{2},\ \frac{1}{4}\right]$	[36,44,125,142]
25	$\left[x+\frac{1}{2},\ \frac{1}{4},\ \frac{1}{2}\right]$	[49,64,170,183]
26	$\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{1}{2}\right]$	[50,63,169,184]
27	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{1}{2}\right]$	[51,62,172,181]
28	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ \frac{1}{2}\right]$	[52,61,171,182]
29	$\left[\frac{1}{2},\ x,\ \frac{3}{4}\right]$	[53,70,156,164]
30	$\left[\frac{3}{4},\ 0,\ x+\frac{1}{2}\right]$	[54,67,105,119]

continued ...

Table 7

No.	position	mapping
31	$\left[\frac{1}{4}, 0, \frac{1}{2} - x\right]$	[55,66,107,117]
32	$\left[\frac{1}{2}, -x, \frac{3}{4}\right]$	[56,72,154,161]
33	$\left[\frac{1}{4}, 0, x + \frac{1}{2}\right]$	[57,71,102,115]
34	$\left[\frac{1}{2}, -x, \frac{1}{4}\right]$	[58,65,152,168]
35	$\left[\frac{3}{4}, 0, \frac{1}{2} - x\right]$	[59,69,103,114]
36	$\left[\frac{1}{2}, x, \frac{1}{4}\right]$	[60,68,149,166]
37	$\left[x + \frac{1}{2}, \frac{3}{4}, 0\right]$	[73,88,146,159]
38	$\left[x + \frac{1}{2}, \frac{1}{4}, 0\right]$	[74,87,145,160]
39	$\left[\frac{1}{2} - x, \frac{3}{4}, 0\right]$	[75,86,148,157]
40	$\left[\frac{1}{2} - x, \frac{1}{4}, 0\right]$	[76,85,147,158]
41	$\left[\frac{1}{2}, x + \frac{1}{2}, \frac{1}{4}\right]$	[77,94,180,188]
42	$\left[\frac{3}{4}, \frac{1}{2}, x\right]$	[78,91,129,143]
43	$\left[\frac{1}{4}, \frac{1}{2}, -x\right]$	[79,90,131,141]
44	$\left[\frac{1}{2}, \frac{1}{2} - x, \frac{1}{4}\right]$	[80,96,178,185]
45	$\left[\frac{1}{4}, \frac{1}{2}, x\right]$	[81,95,126,139]
46	$\left[\frac{1}{2}, \frac{1}{2} - x, \frac{3}{4}\right]$	[82,89,176,192]
47	$\left[\frac{3}{4}, \frac{1}{2}, -x\right]$	[83,93,127,138]
48	$\left[\frac{1}{2}, x + \frac{1}{2}, \frac{3}{4}\right]$	[84,92,173,190]

Table 8: Wyckoff site: 48h, site symmetry: 2m'm'..

No.	position	mapping
1	$\left[x, \frac{1}{4}, \frac{1}{4}\right]$	[1,26,112,135]
2	$\left[x, \frac{3}{4}, \frac{3}{4}\right]$	[2,25,111,136]
3	$\left[-x, \frac{1}{4}, \frac{3}{4}\right]$	[3,28,110,133]
4	$\left[-x, \frac{3}{4}, \frac{1}{4}\right]$	[4,27,109,134]
5	$\left[\frac{1}{4}, x, \frac{1}{4}\right]$	[5,60,116,166]
6	$\left[\frac{1}{4}, \frac{1}{4}, x\right]$	[6,81,139,167]
7	$\left[\frac{3}{4}, \frac{1}{4}, -x\right]$	[7,83,138,165]
8	$\left[\frac{3}{4}, -x, \frac{1}{4}\right]$	[8,58,113,168]
9	$\left[\frac{3}{4}, \frac{3}{4}, x\right]$	[9,78,143,163]
10	$\left[\frac{1}{4}, -x, \frac{3}{4}\right]$	[10,56,120,161]
11	$\left[\frac{1}{4}, \frac{3}{4}, -x\right]$	[11,79,141,162]
12	$\left[\frac{3}{4}, x, \frac{3}{4}\right]$	[12,53,118,164]
13	$\left[-x, \frac{3}{4}, \frac{3}{4}\right]$	[13,38,100,123]
14	$\left[-x, \frac{1}{4}, \frac{1}{4}\right]$	[14,37,99,124]
15	$\left[x, \frac{3}{4}, \frac{1}{4}\right]$	[15,40,98,121]
16	$\left[x, \frac{1}{4}, \frac{3}{4}\right]$	[16,39,97,122]
17	$\left[\frac{3}{4}, -x, \frac{3}{4}\right]$	[17,72,104,154]
18	$\left[\frac{3}{4}, \frac{3}{4}, -x\right]$	[18,93,127,155]
19	$\left[\frac{1}{4}, \frac{3}{4}, x\right]$	[19,95,126,153]
20	$\left[\frac{1}{4}, x, \frac{3}{4}\right]$	[20,70,101,156]
21	$\left[\frac{1}{4}, \frac{1}{4}, -x\right]$	[21,90,131,151]
22	$\left[\frac{3}{4}, x, \frac{1}{4}\right]$	[22,68,108,149]

continued ...

Table 8

No.	position	mapping
23	$\left[\frac{3}{4}, \frac{1}{4}, x\right]$	[23,91,129,150]
24	$\left[\frac{1}{4}, -x, \frac{1}{4}\right]$	[24,65,106,152]
25	$\left[\frac{1}{4}, x+\frac{1}{2}, \frac{3}{4}\right]$	[29,84,140,190]
26	$\left[\frac{1}{4}, \frac{3}{4}, x+\frac{1}{2}\right]$	[30,57,115,191]
27	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{2}-x\right]$	[31,59,114,189]
28	$\left[\frac{3}{4}, \frac{1}{2}-x, \frac{3}{4}\right]$	[32,82,137,192]
29	$\left[\frac{3}{4}, \frac{1}{4}, x+\frac{1}{2}\right]$	[33,54,119,187]
30	$\left[\frac{1}{4}, \frac{1}{2}-x, \frac{1}{4}\right]$	[34,80,144,185]
31	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{2}-x\right]$	[35,55,117,186]
32	$\left[\frac{3}{4}, x+\frac{1}{2}, \frac{1}{4}\right]$	[36,77,142,188]
33	$\left[\frac{3}{4}, \frac{1}{2}-x, \frac{1}{4}\right]$	[41,96,128,178]
34	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{2}-x\right]$	[42,69,103,179]
35	$\left[\frac{1}{4}, \frac{1}{4}, x+\frac{1}{2}\right]$	[43,71,102,177]
36	$\left[\frac{1}{4}, x+\frac{1}{2}, \frac{1}{4}\right]$	[44,94,125,180]
37	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{2}-x\right]$	[45,66,107,175]
38	$\left[\frac{3}{4}, x+\frac{1}{2}, \frac{3}{4}\right]$	[46,92,132,173]
39	$\left[\frac{3}{4}, \frac{3}{4}, x+\frac{1}{2}\right]$	[47,67,105,174]
40	$\left[\frac{1}{4}, \frac{1}{2}-x, \frac{3}{4}\right]$	[48,89,130,176]
41	$\left[x+\frac{1}{2}, \frac{1}{4}, \frac{3}{4}\right]$	[49,74,160,183]
42	$\left[x+\frac{1}{2}, \frac{3}{4}, \frac{1}{4}\right]$	[50,73,159,184]
43	$\left[\frac{1}{2}-x, \frac{1}{4}, \frac{1}{4}\right]$	[51,76,158,181]
44	$\left[\frac{1}{2}-x, \frac{3}{4}, \frac{3}{4}\right]$	[52,75,157,182]
45	$\left[\frac{1}{2}-x, \frac{3}{4}, \frac{1}{4}\right]$	[61,86,148,171]
46	$\left[\frac{1}{2}-x, \frac{1}{4}, \frac{3}{4}\right]$	[62,85,147,172]
47	$\left[x+\frac{1}{2}, \frac{3}{4}, \frac{3}{4}\right]$	[63,88,146,169]
48	$\left[x+\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right]$	[64,87,145,170]

Table 9: Wyckoff site: 64i, 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	$[-x, -x, -x]$	[13,17,18]
6	$[-x, x, x]$	[14,22,23]
7	$[x, -x, x]$	[15,19,24]
8	$[x, x, -x]$	[16,20,21]
9	$\left[x, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[25,29,30]
10	$\left[x, \frac{1}{2}-x, \frac{1}{2}-x\right]$	[26,34,35]
11	$\left[-x, x+\frac{1}{2}, \frac{1}{2}-x\right]$	[27,31,36]
12	$\left[-x, \frac{1}{2}-x, x+\frac{1}{2}\right]$	[28,32,33]
13	$\left[-x, \frac{1}{2}-x, \frac{1}{2}-x\right]$	[37,41,42]
14	$\left[-x, x+\frac{1}{2}, x+\frac{1}{2}\right]$	[38,46,47]

continued ...

Table 9

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

continued ...

Table 9

No.	position	mapping
62	$\left[\frac{1}{2}-x,\, x+\frac{1}{2},\, x+\frac{1}{2}\right]$	[182,190,191]
63	$\left[x+\frac{1}{2},\, \frac{1}{2}-x,\, x+\frac{1}{2}\right]$	[183,187,192]
64	$\left[x+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}-x\right]$	[184,188,189]

Table 10: Wyckoff site: 96j, site symmetry: m..

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

continued ...

Table 10

No.	position	mapping
38	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[74,85]
39	$\left[\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	[75,88]
40	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$	[76,87]
41	$\left[z+\frac{1}{2},\ \frac{1}{2},\ y\right]$	[77,96]
42	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ 0\right]$	[78,93]
43	$\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ 0\right]$	[79,95]
44	$\left[\frac{1}{2}-z,\ \frac{1}{2},\ y\right]$	[80,94]
45	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ 0\right]$	[81,90]
46	$\left[z+\frac{1}{2},\ \frac{1}{2},\ -y\right]$	[82,92]
47	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ 0\right]$	[83,91]
48	$\left[\frac{1}{2}-z,\ \frac{1}{2},\ -y\right]$	[84,89]
49	$\left[0,\ y,\ z+\frac{1}{2}\right]$	[97,110]
50	$\left[0,\ -y,\ \frac{1}{2}-z\right]$	[98,109]
51	$\left[0,\ y,\ \frac{1}{2}-z\right]$	[99,112]
52	$\left[0,\ -y,\ z+\frac{1}{2}\right]$	[100,111]
53	$\left[z,\ 0,\ y+\frac{1}{2}\right]$	[101,120]
54	$\left[y,\ z,\ \frac{1}{2}\right]$	[102,117]
55	$\left[-y,\ z,\ \frac{1}{2}\right]$	[103,119]
56	$\left[-z,\ 0,\ y+\frac{1}{2}\right]$	[104,118]
57	$\left[-y,\ -z,\ \frac{1}{2}\right]$	[105,114]
58	$\left[z,\ 0,\ \frac{1}{2}-y\right]$	[106,116]
59	$\left[y,\ -z,\ \frac{1}{2}\right]$	[107,115]
60	$\left[-z,\ 0,\ \frac{1}{2}-y\right]$	[108,113]
61	$\left[0,\ y+\frac{1}{2},\ z\right]$	[121,134]
62	$\left[0,\ \frac{1}{2}-y,\ -z\right]$	[122,133]
63	$\left[0,\ y+\frac{1}{2},\ -z\right]$	[123,136]
64	$\left[0,\ \frac{1}{2}-y,\ z\right]$	[124,135]
65	$\left[z,\ \frac{1}{2},\ y\right]$	[125,144]
66	$\left[y,\ z+\frac{1}{2},\ 0\right]$	[126,141]
67	$\left[-y,\ z+\frac{1}{2},\ 0\right]$	[127,143]
68	$\left[-z,\ \frac{1}{2},\ y\right]$	[128,142]
69	$\left[-y,\ \frac{1}{2}-z,\ 0\right]$	[129,138]
70	$\left[z,\ \frac{1}{2},\ -y\right]$	[130,140]
71	$\left[y,\ \frac{1}{2}-z,\ 0\right]$	[131,139]
72	$\left[-z,\ \frac{1}{2},\ -y\right]$	[132,137]
73	$\left[\frac{1}{2},\ y,\ z\right]$	[145,158]
74	$\left[\frac{1}{2},\ -y,\ -z\right]$	[146,157]
75	$\left[\frac{1}{2},\ y,\ -z\right]$	[147,160]
76	$\left[\frac{1}{2},\ -y,\ z\right]$	[148,159]
77	$\left[z+\frac{1}{2},\ 0,\ y\right]$	[149,168]
78	$\left[y+\frac{1}{2},\ z,\ 0\right]$	[150,165]
79	$\left[\frac{1}{2}-y,\ z,\ 0\right]$	[151,167]
80	$\left[\frac{1}{2}-z,\ 0,\ y\right]$	[152,166]
81	$\left[\frac{1}{2}-y,\ -z,\ 0\right]$	[153,162]
82	$\left[z+\frac{1}{2},\ 0,\ -y\right]$	[154,164]
83	$\left[y+\frac{1}{2},\ -z,\ 0\right]$	[155,163]
84	$\left[\frac{1}{2}-z,\ 0,\ -y\right]$	[156,161]

continued ...

Table 10

No.	position	mapping
85	$\left[\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[169,182]
86	$\left[\frac{1}{2}, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[170,181]
87	$\left[\frac{1}{2}, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[171,184]
88	$\left[\frac{1}{2}, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[172,183]
89	$\left[z+\frac{1}{2}, \frac{1}{2}, y+\frac{1}{2}\right]$	[173,192]
90	$\left[y+\frac{1}{2}, z+\frac{1}{2}, \frac{1}{2}\right]$	[174,189]
91	$\left[\frac{1}{2}-y, z+\frac{1}{2}, \frac{1}{2}\right]$	[175,191]
92	$\left[\frac{1}{2}-z, \frac{1}{2}, y+\frac{1}{2}\right]$	[176,190]
93	$\left[\frac{1}{2}-y, \frac{1}{2}-z, \frac{1}{2}\right]$	[177,186]
94	$\left[z+\frac{1}{2}, \frac{1}{2}, \frac{1}{2}-y\right]$	[178,188]
95	$\left[y+\frac{1}{2}, \frac{1}{2}-z, \frac{1}{2}\right]$	[179,187]
96	$\left[\frac{1}{2}-z, \frac{1}{2}, \frac{1}{2}-y\right]$	[180,185]

Table 11: Wyckoff site: 96k, site symmetry: m'..

No.	position	mapping
1	$\left[\frac{1}{4}, y, z\right]$	[1,158]
2	$\left[\frac{1}{4}, -y, -z\right]$	[2,157]
3	$\left[\frac{3}{4}, y, -z\right]$	[3,160]
4	$\left[\frac{3}{4}, -y, z\right]$	[4,159]
5	$\left[z, \frac{1}{4}, y\right]$	[5,144]
6	$\left[y, z, \frac{1}{4}\right]$	[6,117]
7	$\left[-y, z, \frac{3}{4}\right]$	[7,119]
8	$\left[-z, \frac{3}{4}, y\right]$	[8,142]
9	$\left[-y, -z, \frac{1}{4}\right]$	[9,114]
10	$\left[z, \frac{3}{4}, -y\right]$	[10,140]
11	$\left[y, -z, \frac{3}{4}\right]$	[11,115]
12	$\left[-z, \frac{1}{4}, -y\right]$	[12,137]
13	$\left[\frac{3}{4}, -y, -z\right]$	[13,146]
14	$\left[\frac{3}{4}, y, z\right]$	[14,145]
15	$\left[\frac{1}{4}, -y, z\right]$	[15,148]
16	$\left[\frac{1}{4}, y, -z\right]$	[16,147]
17	$\left[-z, \frac{3}{4}, -y\right]$	[17,132]
18	$\left[-y, -z, \frac{3}{4}\right]$	[18,105]
19	$\left[y, -z, \frac{1}{4}\right]$	[19,107]
20	$\left[z, \frac{1}{4}, -y\right]$	[20,130]
21	$\left[y, z, \frac{3}{4}\right]$	[21,102]
22	$\left[-z, \frac{1}{4}, y\right]$	[22,128]
23	$\left[-y, z, \frac{1}{4}\right]$	[23,103]
24	$\left[z, \frac{3}{4}, y\right]$	[24,125]
25	$\left[\frac{1}{4}, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[25,182]
26	$\left[\frac{1}{4}, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[26,181]
27	$\left[\frac{3}{4}, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[27,184]
28	$\left[\frac{3}{4}, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[28,183]

continued ...

Table 11

No.	position	mapping
29	$\left[z,\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[29,120]
30	$\left[y,\ z+\frac{1}{2},\ \frac{3}{4}\right]$	[30,141]
31	$\left[-y,\ z+\frac{1}{2},\ \frac{1}{4}\right]$	[31,143]
32	$\left[-z,\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[32,118]
33	$\left[-y,\ \frac{1}{2}-z,\ \frac{3}{4}\right]$	[33,138]
34	$\left[z,\ \frac{1}{4},\ \frac{1}{2}-y\right]$	[34,116]
35	$\left[y,\ \frac{1}{2}-z,\ \frac{1}{4}\right]$	[35,139]
36	$\left[-z,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[36,113]
37	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[37,170]
38	$\left[\frac{3}{4},\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[38,169]
39	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[39,172]
40	$\left[\frac{1}{4},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[40,171]
41	$\left[-z,\ \frac{1}{4},\ \frac{1}{2}-y\right]$	[41,108]
42	$\left[-y,\ \frac{1}{2}-z,\ \frac{1}{4}\right]$	[42,129]
43	$\left[y,\ \frac{1}{2}-z,\ \frac{3}{4}\right]$	[43,131]
44	$\left[z,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[44,106]
45	$\left[y,\ z+\frac{1}{2},\ \frac{1}{4}\right]$	[45,126]
46	$\left[-z,\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[46,104]
47	$\left[-y,\ z+\frac{1}{2},\ \frac{3}{4}\right]$	[47,127]
48	$\left[z,\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[48,101]
49	$\left[\frac{3}{4},\ y,\ z+\frac{1}{2}\right]$	[49,110]
50	$\left[\frac{3}{4},\ -y,\ \frac{1}{2}-z\right]$	[50,109]
51	$\left[\frac{1}{4},\ y,\ \frac{1}{2}-z\right]$	[51,112]
52	$\left[\frac{1}{4},\ -y,\ z+\frac{1}{2}\right]$	[52,111]
53	$\left[z+\frac{1}{2},\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[53,192]
54	$\left[y+\frac{1}{2},\ z,\ \frac{3}{4}\right]$	[54,165]
55	$\left[\frac{1}{2}-y,\ z,\ \frac{1}{4}\right]$	[55,167]
56	$\left[\frac{1}{2}-z,\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[56,190]
57	$\left[\frac{1}{2}-y,\ -z,\ \frac{3}{4}\right]$	[57,162]
58	$\left[z+\frac{1}{2},\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[58,188]
59	$\left[y+\frac{1}{2},\ -z,\ \frac{1}{4}\right]$	[59,163]
60	$\left[\frac{1}{2}-z,\ \frac{1}{4},\ \frac{1}{2}-y\right]$	[60,185]
61	$\left[\frac{1}{4},\ -y,\ \frac{1}{2}-z\right]$	[61,98]
62	$\left[\frac{1}{4},\ y,\ z+\frac{1}{2}\right]$	[62,97]
63	$\left[\frac{3}{4},\ -y,\ z+\frac{1}{2}\right]$	[63,100]
64	$\left[\frac{3}{4},\ y,\ \frac{1}{2}-z\right]$	[64,99]
65	$\left[\frac{1}{2}-z,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[65,180]
66	$\left[\frac{1}{2}-y,\ -z,\ \frac{1}{4}\right]$	[66,153]
67	$\left[y+\frac{1}{2},\ -z,\ \frac{3}{4}\right]$	[67,155]
68	$\left[z+\frac{1}{2},\ \frac{1}{4},\ \frac{1}{2}-y\right]$	[68,178]
69	$\left[y+\frac{1}{2},\ z,\ \frac{1}{4}\right]$	[69,150]
70	$\left[\frac{1}{2}-z,\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[70,176]
71	$\left[\frac{1}{2}-y,\ z,\ \frac{3}{4}\right]$	[71,151]
72	$\left[z+\frac{1}{2},\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[72,173]
73	$\left[\frac{3}{4},\ y+\frac{1}{2},\ z\right]$	[73,134]
74	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ -z\right]$	[74,133]
75	$\left[\frac{1}{4},\ y+\frac{1}{2},\ -z\right]$	[75,136]

continued ...

Table 11

No.	position	mapping
76	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ z\right]$	[76,135]
77	$\left[z+\frac{1}{2},\ \frac{3}{4},\ y\right]$	[77,168]
78	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ \frac{1}{4}\right]$	[78,189]
79	$\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ \frac{3}{4}\right]$	[79,191]
80	$\left[\frac{1}{2}-z,\ \frac{1}{4},\ y\right]$	[80,166]
81	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ \frac{1}{4}\right]$	[81,186]
82	$\left[z+\frac{1}{2},\ \frac{1}{4},\ -y\right]$	[82,164]
83	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ \frac{3}{4}\right]$	[83,187]
84	$\left[\frac{1}{2}-z,\ \frac{3}{4},\ -y\right]$	[84,161]
85	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ -z\right]$	[85,122]
86	$\left[\frac{1}{4},\ y+\frac{1}{2},\ z\right]$	[86,121]
87	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ z\right]$	[87,124]
88	$\left[\frac{3}{4},\ y+\frac{1}{2},\ -z\right]$	[88,123]
89	$\left[\frac{1}{2}-z,\ \frac{1}{4},\ -y\right]$	[89,156]
90	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ \frac{3}{4}\right]$	[90,177]
91	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ \frac{1}{4}\right]$	[91,179]
92	$\left[z+\frac{1}{2},\ \frac{3}{4},\ -y\right]$	[92,154]
93	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ \frac{3}{4}\right]$	[93,174]
94	$\left[\frac{1}{2}-z,\ \frac{3}{4},\ y\right]$	[94,152]
95	$\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ \frac{1}{4}\right]$	[95,175]
96	$\left[z+\frac{1}{2},\ \frac{1}{4},\ y\right]$	[96,149]

Table 12: Wyckoff site: 192l, 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	$[-x,\ -y,\ -z]$	[13]
14	$[-x,\ y,\ z]$	[14]
15	$[x,\ -y,\ z]$	[15]
16	$[x,\ y,\ -z]$	[16]
17	$[-z,\ -x,\ -y]$	[17]
18	$[-y,\ -z,\ -x]$	[18]
19	$[y,\ -z,\ x]$	[19]

continued ...

Table 12

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

continued ...

Table 12

No.	position	mapping
67	$\left[y+\frac{1}{2},\ -z,\ x+\frac{1}{2}\right]$	[67]
68	$\left[z+\frac{1}{2},\ x,\ \frac{1}{2}-y\right]$	[68]
69	$\left[y+\frac{1}{2},\ z,\ \frac{1}{2}-x\right]$	[69]
70	$\left[\frac{1}{2}-z,\ x,\ y+\frac{1}{2}\right]$	[70]
71	$\left[\frac{1}{2}-y,\ z,\ x+\frac{1}{2}\right]$	[71]
72	$\left[z+\frac{1}{2},\ -x,\ y+\frac{1}{2}\right]$	[72]
73	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ z\right]$	[73]
74	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[74]
75	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ -z\right]$	[75]
76	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	[76]
77	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ y\right]$	[77]
78	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ x\right]$	[78]
79	$\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ -x\right]$	[79]
80	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ y\right]$	[80]
81	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ x\right]$	[81]
82	$\left[z+\frac{1}{2},\ \frac{1}{2}-x,\ -y\right]$	[82]
83	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ -x\right]$	[83]
84	$\left[\frac{1}{2}-z,\ x+\frac{1}{2},\ -y\right]$	[84]
85	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ -z\right]$	[85]
86	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z\right]$	[86]
87	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$	[87]
88	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	[88]
89	$\left[\frac{1}{2}-z,\ \frac{1}{2}-x,\ -y\right]$	[89]
90	$\left[\frac{1}{2}-y,\ \frac{1}{2}-z,\ -x\right]$	[90]
91	$\left[y+\frac{1}{2},\ \frac{1}{2}-z,\ x\right]$	[91]
92	$\left[z+\frac{1}{2},\ x+\frac{1}{2},\ -y\right]$	[92]
93	$\left[y+\frac{1}{2},\ z+\frac{1}{2},\ -x\right]$	[93]
94	$\left[\frac{1}{2}-z,\ x+\frac{1}{2},\ y\right]$	[94]
95	$\left[\frac{1}{2}-y,\ z+\frac{1}{2},\ x\right]$	[95]
96	$\left[z+\frac{1}{2},\ \frac{1}{2}-x,\ y\right]$	[96]
97	$\left[x,\ y,\ z+\frac{1}{2}\right]$	[97]
98	$\left[x,\ -y,\ \frac{1}{2}-z\right]$	[98]
99	$\left[-x,\ y,\ \frac{1}{2}-z\right]$	[99]
100	$\left[-x,\ -y,\ z+\frac{1}{2}\right]$	[100]
101	$\left[z,\ x,\ y+\frac{1}{2}\right]$	[101]
102	$\left[y,\ z,\ x+\frac{1}{2}\right]$	[102]
103	$\left[-y,\ z,\ \frac{1}{2}-x\right]$	[103]
104	$\left[-z,\ -x,\ y+\frac{1}{2}\right]$	[104]
105	$\left[-y,\ -z,\ x+\frac{1}{2}\right]$	[105]
106	$\left[z,\ -x,\ \frac{1}{2}-y\right]$	[106]
107	$\left[y,\ -z,\ \frac{1}{2}-x\right]$	[107]
108	$\left[-z,\ x,\ \frac{1}{2}-y\right]$	[108]
109	$\left[-x,\ -y,\ \frac{1}{2}-z\right]$	[109]
110	$\left[-x,\ y,\ z+\frac{1}{2}\right]$	[110]
111	$\left[x,\ -y,\ z+\frac{1}{2}\right]$	[111]
112	$\left[x,\ y,\ \frac{1}{2}-z\right]$	[112]
113	$\left[-z,\ -x,\ \frac{1}{2}-y\right]$	[113]

continued ...

Table 12

No.	position	mapping
114	$\left[-y,\, -z,\, \frac{1}{2}-x\right]$	[114]
115	$\left[y,\, -z,\, x+\frac{1}{2}\right]$	[115]
116	$\left[z,\, x,\, \frac{1}{2}-y\right]$	[116]
117	$\left[y,\, z,\, \frac{1}{2}-x\right]$	[117]
118	$\left[-z,\, x,\, y+\frac{1}{2}\right]$	[118]
119	$\left[-y,\, z,\, x+\frac{1}{2}\right]$	[119]
120	$\left[z,\, -x,\, y+\frac{1}{2}\right]$	[120]
121	$\left[x,\, y+\frac{1}{2},\, z\right]$	[121]
122	$\left[x,\, \frac{1}{2}-y,\, -z\right]$	[122]
123	$\left[-x,\, y+\frac{1}{2},\, -z\right]$	[123]
124	$\left[-x,\, \frac{1}{2}-y,\, z\right]$	[124]
125	$\left[z,\, x+\frac{1}{2},\, y\right]$	[125]
126	$\left[y,\, z+\frac{1}{2},\, x\right]$	[126]
127	$\left[-y,\, z+\frac{1}{2},\, -x\right]$	[127]
128	$\left[-z,\, \frac{1}{2}-x,\, y\right]$	[128]
129	$\left[-y,\, \frac{1}{2}-z,\, x\right]$	[129]
130	$\left[z,\, \frac{1}{2}-x,\, -y\right]$	[130]
131	$\left[y,\, \frac{1}{2}-z,\, -x\right]$	[131]
132	$\left[-z,\, x+\frac{1}{2},\, -y\right]$	[132]
133	$\left[-x,\, \frac{1}{2}-y,\, -z\right]$	[133]
134	$\left[-x,\, y+\frac{1}{2},\, z\right]$	[134]
135	$\left[x,\, \frac{1}{2}-y,\, z\right]$	[135]
136	$\left[x,\, y+\frac{1}{2},\, -z\right]$	[136]
137	$\left[-z,\, \frac{1}{2}-x,\, -y\right]$	[137]
138	$\left[-y,\, \frac{1}{2}-z,\, -x\right]$	[138]
139	$\left[y,\, \frac{1}{2}-z,\, x\right]$	[139]
140	$\left[z,\, x+\frac{1}{2},\, -y\right]$	[140]
141	$\left[y,\, z+\frac{1}{2},\, -x\right]$	[141]
142	$\left[-z,\, x+\frac{1}{2},\, y\right]$	[142]
143	$\left[-y,\, z+\frac{1}{2},\, x\right]$	[143]
144	$\left[z,\, \frac{1}{2}-x,\, y\right]$	[144]
145	$\left[x+\frac{1}{2},\, y,\, z\right]$	[145]
146	$\left[x+\frac{1}{2},\, -y,\, -z\right]$	[146]
147	$\left[\frac{1}{2}-x,\, y,\, -z\right]$	[147]
148	$\left[\frac{1}{2}-x,\, -y,\, z\right]$	[148]
149	$\left[z+\frac{1}{2},\, x,\, y\right]$	[149]
150	$\left[y+\frac{1}{2},\, z,\, x\right]$	[150]
151	$\left[\frac{1}{2}-y,\, z,\, -x\right]$	[151]
152	$\left[\frac{1}{2}-z,\, -x,\, y\right]$	[152]
153	$\left[\frac{1}{2}-y,\, -z,\, x\right]$	[153]
154	$\left[z+\frac{1}{2},\, -x,\, -y\right]$	[154]
155	$\left[y+\frac{1}{2},\, -z,\, -x\right]$	[155]
156	$\left[\frac{1}{2}-z,\, x,\, -y\right]$	[156]
157	$\left[\frac{1}{2}-x,\, -y,\, -z\right]$	[157]
158	$\left[\frac{1}{2}-x,\, y,\, z\right]$	[158]
159	$\left[x+\frac{1}{2},\, -y,\, z\right]$	[159]
160	$\left[x+\frac{1}{2},\, y,\, -z\right]$	[160]

continued ...

Table 12

No.	position	mapping
161	$\left[\frac{1}{2}-z,\,-x,\,-y\right]$	[161]
162	$\left[\frac{1}{2}-y,\,-z,\,-x\right]$	[162]
163	$\left[y+\frac{1}{2},\,-z,\,x\right]$	[163]
164	$\left[z+\frac{1}{2},\,x,\,-y\right]$	[164]
165	$\left[y+\frac{1}{2},\,z,\,-x\right]$	[165]
166	$\left[\frac{1}{2}-z,\,x,\,y\right]$	[166]
167	$\left[\frac{1}{2}-y,\,z,\,x\right]$	[167]
168	$\left[z+\frac{1}{2},\,-x,\,y\right]$	[168]
169	$\left[x+\frac{1}{2},\,y+\frac{1}{2},\,z+\frac{1}{2}\right]$	[169]
170	$\left[x+\frac{1}{2},\,\frac{1}{2}-y,\,\frac{1}{2}-z\right]$	[170]
171	$\left[\frac{1}{2}-x,\,y+\frac{1}{2},\,\frac{1}{2}-z\right]$	[171]
172	$\left[\frac{1}{2}-x,\,\frac{1}{2}-y,\,z+\frac{1}{2}\right]$	[172]
173	$\left[z+\frac{1}{2},\,x+\frac{1}{2},\,y+\frac{1}{2}\right]$	[173]
174	$\left[y+\frac{1}{2},\,z+\frac{1}{2},\,x+\frac{1}{2}\right]$	[174]
175	$\left[\frac{1}{2}-y,\,z+\frac{1}{2},\,\frac{1}{2}-x\right]$	[175]
176	$\left[\frac{1}{2}-z,\,\frac{1}{2}-x,\,y+\frac{1}{2}\right]$	[176]
177	$\left[\frac{1}{2}-y,\,\frac{1}{2}-z,\,x+\frac{1}{2}\right]$	[177]
178	$\left[z+\frac{1}{2},\,\frac{1}{2}-x,\,\frac{1}{2}-y\right]$	[178]
179	$\left[y+\frac{1}{2},\,\frac{1}{2}-z,\,\frac{1}{2}-x\right]$	[179]
180	$\left[\frac{1}{2}-z,\,x+\frac{1}{2},\,\frac{1}{2}-y\right]$	[180]
181	$\left[\frac{1}{2}-x,\,\frac{1}{2}-y,\,\frac{1}{2}-z\right]$	[181]
182	$\left[\frac{1}{2}-x,\,y+\frac{1}{2},\,z+\frac{1}{2}\right]$	[182]
183	$\left[x+\frac{1}{2},\,\frac{1}{2}-y,\,z+\frac{1}{2}\right]$	[183]
184	$\left[x+\frac{1}{2},\,y+\frac{1}{2},\,\frac{1}{2}-z\right]$	[184]
185	$\left[\frac{1}{2}-z,\,\frac{1}{2}-x,\,\frac{1}{2}-y\right]$	[185]
186	$\left[\frac{1}{2}-y,\,\frac{1}{2}-z,\,\frac{1}{2}-x\right]$	[186]
187	$\left[y+\frac{1}{2},\,\frac{1}{2}-z,\,x+\frac{1}{2}\right]$	[187]
188	$\left[z+\frac{1}{2},\,x+\frac{1}{2},\,\frac{1}{2}-y\right]$	[188]
189	$\left[y+\frac{1}{2},\,z+\frac{1}{2},\,\frac{1}{2}-x\right]$	[189]
190	$\left[\frac{1}{2}-z,\,x+\frac{1}{2},\,y+\frac{1}{2}\right]$	[190]
191	$\left[\frac{1}{2}-y,\,z+\frac{1}{2},\,x+\frac{1}{2}\right]$	[191]
192	$\left[z+\frac{1}{2},\,\frac{1}{2}-x,\,y+\frac{1}{2}\right]$	[192]