MSG No. 229.141 $Im\bar{3}m1'$ [Type II, cubic]

Table 1: Wyckoff site: `2a`, site symmetry: `m-3m1'`

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,
		97,98,99,100,101,102,103,104,105,106,107,108,109,110,111,112,113,114,115,116,117,118,119,120,
		121,122,123,124,125,126,127,128,129,130,131,132,133,134,135,136,137,138,139,140,141,142,143,144]
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,
		145,146,147,148,149,150,151,152,153,154,155,156,157,158,159,160,161,162,163,164,165,166,167,168,
		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: `6b`, site symmetry: `4/mm.m1'`

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

Table 3: Wyckoff site: `8c`, site symmetry: `.-3m1'`

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

Table 4: Wyckoff site: `12d`, site symmetry: `-4m.21'`

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

Table 5: Wyckoff site: `12e`, site symmetry: `4m.m1'`

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

Table 6: Wyckoff site: `16f`, site symmetry: `.3m1'`

No.	position	mapping
1	$[x, x, x]$	[1,17,18,36,38,40,97,113,114,132,134,136]
2	$[x, -x, x]$	[2,7,15,33,43,48,98,103,111,129,139,144]
3	$[x, x, -x]$	[3,4,11,34,44,45,99,100,107,130,140,141]
4	$[-x, x, x]$	[5,6,13,32,46,47,101,102,109,128,142,143]
5	$[x, -x, -x]$	[8,22,23,29,30,37,104,118,119,125,126,133]
6	$[-x, x, -x]$	[9,19,24,26,31,39,105,115,120,122,127,135]
7	$[-x, -x, x]$	[10,20,21,27,28,35,106,116,117,123,124,131]
8	$[-x, -x, -x]$	[12,14,16,25,41,42,108,110,112,121,137,138]
9	$\left[x + \frac{1}{2}, x + \frac{1}{2}, x + \frac{1}{2}\right]$	[49,65,66,84,86,88,145,161,162,180,182,184]

continued ...

Table 6

No.	position	mapping
10	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ x+\frac{1}{2}\right]$	[50,55,63,81,91,96,146,151,159,177,187,192]
11	$\left[x+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}-x\right]$	[51,52,59,82,92,93,147,148,155,178,188,189]
12	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ x+\frac{1}{2}\right]$	[53,54,61,80,94,95,149,150,157,176,190,191]
13	$\left[x+\frac{1}{2},\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	[56,70,71,77,78,85,152,166,167,173,174,181]
14	$\left[\frac{1}{2}-x,\ x+\frac{1}{2},\ \frac{1}{2}-x\right]$	[57,67,72,74,79,87,153,163,168,170,175,183]
15	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ x+\frac{1}{2}\right]$	[58,68,69,75,76,83,154,164,165,171,172,179]
16	$\left[\frac{1}{2}-x,\ \frac{1}{2}-x,\ \frac{1}{2}-x\right]$	[60,62,64,73,89,90,156,158,160,169,185,186]

Table 7: Wyckoff site: 24g, site symmetry: 2mm..1'

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

Table 8: Wyckoff site: 24h, site symmetry: m.2m1'

No.	position	mapping
1	$[0,\ y,\ y]$	[1,13,32,38,97,109,128,134]
2	$[0,\ -y,\ y]$	[2,10,27,33,98,106,123,129]
3	$[0,\ y,\ -y]$	[3,9,26,34,99,105,122,130]

continued ...

Table 8

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

Table 9: Wyckoff site: 48i, site symmetry: ..21'

No.	position	mapping
1	$\left[\frac{1}{4},\ y,\ \frac{1}{2}-y\right]$	[1,62,97,158]
2	$\left[\frac{1}{4},\ y+\frac{1}{2},\ y\right]$	[2,57,98,153]
3	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ -y\right]$	[3,58,99,154]
4	$\left[\frac{1}{2}-y,\ y,\ \frac{3}{4}\right]$	[4,69,100,165]
5	$\left[y+\frac{1}{2},\ y,\ \frac{1}{4}\right]$	[5,71,101,167]
6	$\left[-y,\ \frac{1}{4},\ \frac{1}{2}-y\right]$	[6,70,102,166]
7	$\left[y,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[7,72,103,168]
8	$\left[\frac{1}{4},\ -y,\ y+\frac{1}{2}\right]$	[8,61,104,157]
9	$\left[\frac{3}{4},\ y,\ y+\frac{1}{2}\right]$	[9,50,105,146]
10	$\left[\frac{3}{4},\ -y,\ \frac{1}{2}-y\right]$	[10,51,106,147]
11	$\left[y,\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[11,68,107,164]
12	$\left[-y,\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[12,65,108,161]
13	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ y\right]$	[13,56,109,152]
14	$\left[\frac{3}{4},\ y+\frac{1}{2},\ -y\right]$	[14,49,110,145]
15	$\left[\frac{1}{2}-y,\ -y,\ \frac{1}{4}\right]$	[15,67,111,163]
16	$\left[y+\frac{1}{2},\ -y,\ \frac{3}{4}\right]$	[16,66,112,162]
17	$\left[\frac{1}{2}-y,\ \frac{1}{4},\ y\right]$	[17,60,113,156]
18	$\left[y,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[18,64,114,160]
19	$\left[-y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[19,63,115,159]

continued ...

Table 9

No.	position	mapping
20	$\left[y+\frac{1}{2},\ \frac{3}{4},\ y\right]$	[20,59,116,155]
21	$\left[-y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[21,52,117,148]
22	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ -y\right]$	[22,54,118,150]
23	$\left[y,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[23,53,119,149]
24	$\left[y+\frac{1}{2},\ \frac{1}{4},\ -y\right]$	[24,55,120,151]
25	$\left[\frac{3}{4},\ -y,\ y+\frac{1}{2}\right]$	[25,86,121,182]
26	$\left[\frac{3}{4},\ \frac{1}{2}-y,\ -y\right]$	[26,81,122,177]
27	$\left[\frac{3}{4},\ y+\frac{1}{2},\ y\right]$	[27,82,123,178]
28	$\left[y+\frac{1}{2},\ -y,\ \frac{1}{4}\right]$	[28,93,124,189]
29	$\left[\frac{1}{2}-y,\ -y,\ \frac{3}{4}\right]$	[29,95,125,191]
30	$\left[y,\ \frac{3}{4},\ y+\frac{1}{2}\right]$	[30,94,126,190]
31	$\left[-y,\ \frac{1}{4},\ y+\frac{1}{2}\right]$	[31,96,127,192]
32	$\left[\frac{3}{4},\ y,\ \frac{1}{2}-y\right]$	[32,85,128,181]
33	$\left[\frac{1}{4},\ -y,\ \frac{1}{2}-y\right]$	[33,74,129,170]
34	$\left[\frac{1}{4},\ y,\ y+\frac{1}{2}\right]$	[34,75,130,171]
35	$\left[-y,\ \frac{3}{4},\ \frac{1}{2}-y\right]$	[35,92,131,188]
36	$\left[y,\ \frac{1}{4},\ \frac{1}{2}-y\right]$	[36,89,132,185]
37	$\left[\frac{1}{4},\ y+\frac{1}{2},\ -y\right]$	[37,80,133,176]
38	$\left[\frac{1}{4},\ \frac{1}{2}-y,\ y\right]$	[38,73,134,169]
39	$\left[y+\frac{1}{2},\ y,\ \frac{3}{4}\right]$	[39,91,135,187]
40	$\left[\frac{1}{2}-y,\ y,\ \frac{1}{4}\right]$	[40,90,136,186]
41	$\left[y+\frac{1}{2},\ \frac{3}{4},\ -y\right]$	[41,84,137,180]
42	$\left[-y,\ y+\frac{1}{2},\ \frac{3}{4}\right]$	[42,88,138,184]
43	$\left[y,\ y+\frac{1}{2},\ \frac{1}{4}\right]$	[43,87,139,183]
44	$\left[\frac{1}{2}-y,\ \frac{1}{4},\ -y\right]$	[44,83,140,179]
45	$\left[y,\ \frac{1}{2}-y,\ \frac{3}{4}\right]$	[45,76,141,172]
46	$\left[y+\frac{1}{2},\ \frac{1}{4},\ y\right]$	[46,78,142,174]
47	$\left[-y,\ \frac{1}{2}-y,\ \frac{1}{4}\right]$	[47,77,143,173]
48	$\left[\frac{1}{2}-y,\ \frac{3}{4},\ y\right]$	[48,79,144,175]

Table 10: Wyckoff site: 48j, site symmetry: m..1'

No.	position	mapping
1	$[0,\ y,\ z]$	[1,32,97,128]
2	$[0,\ -z,\ y]$	[2,27,98,123]
3	$[0,\ z,\ -y]$	[3,26,99,122]
4	$[z,\ y,\ 0]$	[4,40,100,136]
5	$[-z,\ y,\ 0]$	[5,39,101,135]
6	$[-y,\ 0,\ z]$	[6,35,102,131]
7	$[y,\ 0,\ z]$	[7,36,103,132]
8	$[0,\ -y,\ -z]$	[8,25,104,121]
9	$[0,\ y,\ -z]$	[9,34,105,130]
10	$[0,\ -y,\ z]$	[10,33,106,129]
11	$[y,\ 0,\ -z]$	[11,30,107,126]

continued ...

Table 10

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

Table 11: Wyckoff site: `48k`, site symmetry: `..m1'`

No.	position	mapping
1	$[x,\ x,\ z]$	`[1,36,97,132]`
2	$[x,\ -z,\ x]$	`[2,43,98,139]`
3	$[x,\ z,\ -x]$	`[3,45,99,141]`

continued ...

Table 11

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

Table 12: Wyckoff site: `961`, 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]`
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	$[-x, -y, -z]$	`[25,121]`
26	$[-x, z, -y]$	`[26,122]`
27	$[-x, -z, y]$	`[27,123]`
28	$[-z, -y, x]$	`[28,124]`
29	$[z, -y, -x]$	`[29,125]`
30	$[y, -x, -z]$	`[30,126]`
31	$[-y, x, -z]$	`[31,127]`
32	$[-x, y, z]$	`[32,128]`
33	$[x, -y, z]$	`[33,129]`
34	$[x, y, -z]$	`[34,130]`
35	$[-y, -x, z]$	`[35,131]`
36	$[y, x, z]$	`[36,132]`
37	$[x, -z, -y]$	`[37,133]`
38	$[x, z, y]$	`[38,134]`
39	$[-z, y, -x]$	`[39,135]`
40	$[z, y, x]$	`[40,136]`
41	$[-z, -x, -y]$	`[41,137]`
42	$[-y, -z, -x]$	`[42,138]`
43	$[y, -z, x]$	`[43,139]`
44	$[z, x, -y]$	`[44,140]`
45	$[y, z, -x]$	`[45,141]`
46	$[-z, x, y]$	`[46,142]`

continued ...

Table 12

No.	position	mapping
47	$[-y,\, z,\, x]$	[47,143]
48	$[z,\, -x,\, y]$	[48,144]
49	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[49,145]
50	$\left[x+\frac{1}{2},\, \frac{1}{2}-z,\, y+\frac{1}{2}\right]$	[50,146]
51	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, \frac{1}{2}-y\right]$	[51,147]
52	$\left[z+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}-x\right]$	[52,148]
53	$\left[\frac{1}{2}-z,\, y+\frac{1}{2},\, x+\frac{1}{2}\right]$	[53,149]
54	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[54,150]
55	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$	[55,151]
56	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[56,152]
57	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[57,153]
58	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[58,154]
59	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[59,155]
60	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[60,156]
61	$\left[\frac{1}{2}-x,\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[61,157]
62	$\left[\frac{1}{2}-x,\, \frac{1}{2}-z,\, \frac{1}{2}-y\right]$	[62,158]
63	$\left[z+\frac{1}{2},\, \frac{1}{2}-y,\, x+\frac{1}{2}\right]$	[63,159]
64	$\left[\frac{1}{2}-z,\, \frac{1}{2}-y,\, \frac{1}{2}-x\right]$	[64,160]
65	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[65,161]
66	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[66,162]
67	$\left[\frac{1}{2}-y,\, z+\frac{1}{2},\, \frac{1}{2}-x\right]$	[67,163]
68	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, y+\frac{1}{2}\right]$	[68,164]
69	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, x+\frac{1}{2}\right]$	[69,165]
70	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, \frac{1}{2}-y\right]$	[70,166]
71	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, \frac{1}{2}-x\right]$	[71,167]
72	$\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, \frac{1}{2}-y\right]$	[72,168]
73	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[73,169]
74	$\left[\frac{1}{2}-x,\, z+\frac{1}{2},\, \frac{1}{2}-y\right]$	[74,170]
75	$\left[\frac{1}{2}-x,\, \frac{1}{2}-z,\, y+\frac{1}{2}\right]$	[75,171]
76	$\left[\frac{1}{2}-z,\, \frac{1}{2}-y,\, x+\frac{1}{2}\right]$	[76,172]
77	$\left[z+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}-x\right]$	[77,173]
78	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[78,174]
79	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[79,175]
80	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[80,176]
81	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[81,177]
82	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[82,178]
83	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$	[83,179]
84	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[84,180]
85	$\left[x+\frac{1}{2},\, \frac{1}{2}-z,\, \frac{1}{2}-y\right]$	[85,181]
86	$\left[x+\frac{1}{2},\, z+\frac{1}{2},\, y+\frac{1}{2}\right]$	[86,182]
87	$\left[\frac{1}{2}-z,\, y+\frac{1}{2},\, \frac{1}{2}-x\right]$	[87,183]
88	$\left[z+\frac{1}{2},\, y+\frac{1}{2},\, x+\frac{1}{2}\right]$	[88,184]
89	$\left[\frac{1}{2}-z,\, \frac{1}{2}-x,\, \frac{1}{2}-y\right]$	[89,185]
90	$\left[\frac{1}{2}-y,\, \frac{1}{2}-z,\, \frac{1}{2}-x\right]$	[90,186]
91	$\left[y+\frac{1}{2},\, \frac{1}{2}-z,\, x+\frac{1}{2}\right]$	[91,187]
92	$\left[z+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}-y\right]$	[92,188]
93	$\left[y+\frac{1}{2},\, z+\frac{1}{2},\, \frac{1}{2}-x\right]$	[93,189]

continued ...

Table 12

No.	position	mapping
94	$\left[\frac{1}{2}-z,\, x+\frac{1}{2},\, y+\frac{1}{2}\right]$	[94,190]
95	$\left[\frac{1}{2}-y,\, z+\frac{1}{2},\, x+\frac{1}{2}\right]$	[95,191]
96	$\left[z+\frac{1}{2},\, \frac{1}{2}-x,\, y+\frac{1}{2}\right]$	[96,192]