MSG No. 139.540 I_c4/mmm [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `4/mmm`

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

Table 2: Wyckoff site: `4b`, site symmetry: `4/m'mm`

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

Table 3: Wyckoff site: `4c`, site symmetry: `4'/mmm'`

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

Table 4: Wyckoff site: `4d`, site symmetry: `4'/m'mm'`

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

Table 5: Wyckoff site: `8e`, site symmetry: `m'.mm'`

No.	position	mapping
1	$\left[\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right]$	`[1,15,23,25,40,46,54,64]`
2	$\left[\frac{3}{4}, \frac{3}{4}, \frac{1}{4}\right]$	`[2,13,21,26,36,43,51,60]`

continued ...

Table 5

No.	position	mapping
3	$\left[\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\right]$	[3,12,20,27,37,42,50,61]
4	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[4,11,19,28,34,45,53,58]
5	$\left[\frac{1}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[5,10,18,29,35,44,52,59]
6	$\left[\frac{1}{4}, \frac{3}{4}, \frac{1}{4}\right]$	[6,16,24,30,39,41,49,63]
7	$\left[\frac{1}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[7,9,17,31,38,48,56,62]
8	$\left[\frac{3}{4}, \frac{1}{4}, \frac{3}{4}\right]$	[8,14,22,32,33,47,55,57]

Table 6: Wyckoff site: 8f, site symmetry: m.mm'

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

Table 7: Wyckoff site: 8g, site symmetry: 4mm

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

Table 8: Wyckoff site: 8h, site symmetry: 4'mm'

No.	position	mapping
1	$\left[0, \frac{1}{2}, z\right]$	[1,6,12,13,50,51,63,64]
2	$\left[\frac{1}{2}, 0, z\right]$	[2,3,15,16,49,54,60,61]
3	$\left[0, \frac{1}{2}, -z\right]$	[4,5,9,14,55,56,58,59]
4	$\left[\frac{1}{2}, 0, -z\right]$	[7,8,10,11,52,53,57,62]
5	$\left[\frac{1}{2}, 0, z+\frac{1}{2}\right]$	[17,22,28,29,34,35,47,48]

continued ...

Table 8

No.	position	mapping
6	$\left[0,\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[18,19,31,32,33,38,44,45]
7	$\left[\frac{1}{2},\ 0,\ \frac{1}{2}-z\right]$	[20,21,25,30,39,40,42,43]
8	$\left[0,\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[23,24,26,27,36,37,41,46]

Table 9: Wyckoff site: 16i, site symmetry: 2.mm

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

Table 10: Wyckoff site: 16j, site symmetry: mm2.

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

continued ...

Table 10

No.	position	mapping
16	$\left[\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	[52,54,57,61]

Table 11: Wyckoff site: 16k, site symmetry: m'm2'.

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

Table 12: Wyckoff site: 16l, site symmetry: m.2m

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

Table 13: Wyckoff site: `16m`, site symmetry: `m'.2'm`

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

Table 14: Wyckoff site: `16n`, site symmetry: `m.2'm'`

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

Table 15: Wyckoff site: `16o`, site symmetry: `m'.2m'`

No.	position	mapping
1	$\left[x,\, x+\frac{1}{2},\, \frac{1}{4}\right]$	`[1,23,46,64]`

continued ...

Table 15

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

Table 16: Wyckoff site: 32p, site symmetry: m..

No.	position	mapping
1	$[x,\, y,\, 0]$	[1,14]
2	$[-y,\, x,\, 0]$	[2,11]
3	$[y,\, -x,\, 0]$	[3,10]
4	$[x,\, -y,\, 0]$	[4,13]
5	$[-x,\, y,\, 0]$	[5,12]
6	$[-x,\, -y,\, 0]$	[6,9]
7	$[y,\, x,\, 0]$	[7,16]
8	$[-y,\, -x,\, 0]$	[8,15]
9	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[17,30]
10	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, \frac{1}{2}\right]$	[18,27]
11	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, \frac{1}{2}\right]$	[19,26]
12	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[20,29]
13	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[21,28]
14	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[22,25]
15	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}\right]$	[23,32]
16	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{1}{2}\right]$	[24,31]
17	$\left[x,\, y,\, \frac{1}{2}\right]$	[33,46]
18	$\left[-y,\, x,\, \frac{1}{2}\right]$	[34,43]
19	$\left[y,\, -x,\, \frac{1}{2}\right]$	[35,42]
20	$\left[x,\, -y,\, \frac{1}{2}\right]$	[36,45]
21	$\left[-x,\, y,\, \frac{1}{2}\right]$	[37,44]
22	$\left[-x,\, -y,\, \frac{1}{2}\right]$	[38,41]
23	$\left[y,\, x,\, \frac{1}{2}\right]$	[39,48]
24	$\left[-y,\, -x,\, \frac{1}{2}\right]$	[40,47]
25	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, 0\right]$	[49,62]

continued ...

Table 16

No.	position	mapping
26	$\left[\frac{1}{2}-y,\ x+\frac{1}{2},\ 0\right]$	[50,59]
27	$\left[y+\frac{1}{2},\ \frac{1}{2}-x,\ 0\right]$	[51,58]
28	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ 0\right]$	[52,61]
29	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ 0\right]$	[53,60]
30	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ 0\right]$	[54,57]
31	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ 0\right]$	[55,64]
32	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ 0\right]$	[56,63]

Table 17: Wyckoff site: 32q, site symmetry: m'..

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

Table 18: Wyckoff site: `32r`, site symmetry: `.m.`

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

Table 19: Wyckoff site: `32s`, site symmetry: `..m`

No.	position	mapping
1	$[x,\ x,\ z]$	`[1,16]`
2	$[-x,\ x,\ z]$	`[2,12]`
3	$[x,\ -x,\ z]$	`[3,13]`
4	$[x,\ -x,\ -z]$	`[4,10]`
5	$[-x,\ x,\ -z]$	`[5,11]`
6	$[-x,\ -x,\ z]$	`[6,15]`
7	$[x,\ x,\ -z]$	`[7,14]`

continued ...

Table 19

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

Table 20: Wyckoff site: 32t, site symmetry: ..m'

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ z\right]$	[1,64]
2	$\left[\frac{1}{2}-x,\ x,\ z\right]$	[2,60]
3	$\left[x+\frac{1}{2},\ -x,\ z\right]$	[3,61]
4	$\left[x,\ \frac{1}{2}-x,\ -z\right]$	[4,58]
5	$\left[-x,\ x+\frac{1}{2},\ -z\right]$	[5,59]
6	$\left[-x,\ \frac{1}{2}-x,\ z\right]$	[6,63]
7	$\left[x+\frac{1}{2},\ x,\ -z\right]$	[7,62]
8	$\left[\frac{1}{2}-x,\ -x,\ -z\right]$	[8,57]
9	$\left[-x,\ \frac{1}{2}-x,\ -z\right]$	[9,56]
10	$\left[x+\frac{1}{2},\ -x,\ -z\right]$	[10,52]
11	$\left[\frac{1}{2}-x,\ x,\ -z\right]$	[11,53]
12	$\left[-x,\ x+\frac{1}{2},\ z\right]$	[12,50]
13	$\left[x,\ \frac{1}{2}-x,\ z\right]$	[13,51]
14	$\left[x,\ x+\frac{1}{2},\ -z\right]$	[14,55]
15	$\left[\frac{1}{2}-x,\ -x,\ z\right]$	[15,54]

continued ...

Table 20

No.	position	mapping
16	$\left[x+\frac{1}{2},\, x,\, z\right]$	[16,49]
17	$\left[x+\frac{1}{2},\, x,\, z+\frac{1}{2}\right]$	[17,48]
18	$\left[-x,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[18,44]
19	$\left[x,\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$	[19,45]
20	$\left[x+\frac{1}{2},\, -x,\, \frac{1}{2}-z\right]$	[20,42]
21	$\left[\frac{1}{2}-x,\, x,\, \frac{1}{2}-z\right]$	[21,43]
22	$\left[\frac{1}{2}-x,\, -x,\, z+\frac{1}{2}\right]$	[22,47]
23	$\left[x,\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[23,46]
24	$\left[-x,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[24,41]
25	$\left[\frac{1}{2}-x,\, -x,\, \frac{1}{2}-z\right]$	[25,40]
26	$\left[x,\, \frac{1}{2}-x,\, \frac{1}{2}-z\right]$	[26,36]
27	$\left[-x,\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[27,37]
28	$\left[\frac{1}{2}-x,\, x,\, z+\frac{1}{2}\right]$	[28,34]
29	$\left[x+\frac{1}{2},\, -x,\, z+\frac{1}{2}\right]$	[29,35]
30	$\left[x+\frac{1}{2},\, x,\, \frac{1}{2}-z\right]$	[30,39]
31	$\left[-x,\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$	[31,38]
32	$\left[x,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[32,33]

Table 21: Wyckoff site: 64u, site symmetry: 1

No.	position	mapping
1	$[x,\, y,\, z]$	[1]
2	$[-y,\, x,\, z]$	[2]
3	$[y,\, -x,\, z]$	[3]
4	$[x,\, -y,\, -z]$	[4]
5	$[-x,\, y,\, -z]$	[5]
6	$[-x,\, -y,\, z]$	[6]
7	$[y,\, x,\, -z]$	[7]
8	$[-y,\, -x,\, -z]$	[8]
9	$[-x,\, -y,\, -z]$	[9]
10	$[y,\, -x,\, -z]$	[10]
11	$[-y,\, x,\, -z]$	[11]
12	$[-x,\, y,\, z]$	[12]
13	$[x,\, -y,\, z]$	[13]
14	$[x,\, y,\, -z]$	[14]
15	$[-y,\, -x,\, z]$	[15]
16	$[y,\, x,\, z]$	[16]
17	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[17]
18	$\left[\frac{1}{2}-y,\, x+\frac{1}{2},\, z+\frac{1}{2}\right]$	[18]
19	$\left[y+\frac{1}{2},\, \frac{1}{2}-x,\, z+\frac{1}{2}\right]$	[19]
20	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[20]
21	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[21]
22	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[22]
23	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}-z\right]$	[23]

continued ...

Table 21

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