MSG No. 140.550 I_c4/mcm [Type IV, tetragonal]

Table 1: Wyckoff site: `4a`, site symmetry: `4/mm'm'`

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	[1,8,25,32,46,47,54,55]
2	$\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{4}\right]$	[2,4,26,28,43,45,51,53]

continued ...

Table 5

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

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

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

Table 7: Wyckoff site: 8g, site symmetry: 4m'm'

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

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

No.	position	mapping
1	$\left[0, \frac{1}{2}, z\right]$	[1,6,31,32,44,45,50,51]
2	$\left[\frac{1}{2}, 0, z\right]$	[2,3,28,29,47,48,49,54]
3	$\left[0, \frac{1}{2}, \frac{1}{2} - z\right]$	[4,5,26,27,41,46,55,56]
4	$\left[\frac{1}{2}, 0, \frac{1}{2} - z\right]$	[7,8,25,30,42,43,52,53]
5	$\left[0, \frac{1}{2}, -z\right]$	[9,14,23,24,36,37,58,59]

continued ...

Table 8

No.	position	mapping
6	$\left[\frac{1}{2}, 0, -z\right]$	[10,11,20,21,39,40,57,62]
7	$\left[0, \frac{1}{2}, z+\frac{1}{2}\right]$	[12,13,18,19,33,38,63,64]
8	$\left[\frac{1}{2}, 0, z+\frac{1}{2}\right]$	[15,16,17,22,34,35,60,61]

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

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

Table 10: Wyckoff site: 16j, site symmetry: mm'2'.

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

continued ...

Table 10

No.	position	mapping
16	$\left[\frac{1}{2}-y,\ \frac{1}{2},\ 0\right]$	[24,31,50,59]

Table 11: Wyckoff site: 16k, site symmetry: m'm'2.

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ \frac{1}{4}\right]$	`[1,32,46,55]`

continued ...

Table 15

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

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	$\left[x,\, -y,\, \frac{1}{2}\right]$	[4,13]
5	$\left[-x,\, y,\, \frac{1}{2}\right]$	[5,12]
6	$[-x,\, -y,\, 0]$	[6,9]
7	$\left[y,\, x,\, \frac{1}{2}\right]$	[7,16]
8	$\left[-y,\, -x,\, \frac{1}{2}\right]$	[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	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, 0\right]$	[20,29]
13	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, 0\right]$	[21,28]
14	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[22,25]
15	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, 0\right]$	[23,32]
16	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, 0\right]$	[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	$[x,\, -y,\, 0]$	[36,45]
21	$[-x,\, y,\, 0]$	[37,44]
22	$\left[-x,\, -y,\, \frac{1}{2}\right]$	[38,41]
23	$[y,\, x,\, 0]$	[39,48]
24	$[-y,\, -x,\, 0]$	[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	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}\right]$	[52,61]
29	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}\right]$	[53,60]
30	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, 0\right]$	[54,57]
31	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{2}\right]$	[55,64]
32	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{1}{2}\right]$	[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	$\left[x,\, -y,\, \frac{1}{4}\right]$	[4,45]
5	$\left[-x,\, y,\, \frac{1}{4}\right]$	[5,44]
6	$\left[-x,\, -y,\, \frac{1}{4}\right]$	[6,41]
7	$\left[y,\, x,\, \frac{1}{4}\right]$	[7,48]
8	$\left[-y,\, -x,\, \frac{1}{4}\right]$	[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	$\left[-x,\, y,\, \frac{3}{4}\right]$	[12,37]
13	$\left[x,\, -y,\, \frac{3}{4}\right]$	[13,36]
14	$\left[x,\, y,\, \frac{3}{4}\right]$	[14,33]
15	$\left[-y,\, -x,\, \frac{3}{4}\right]$	[15,40]
16	$\left[y,\, x,\, \frac{3}{4}\right]$	[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	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{3}{4}\right]$	[20,61]
21	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{3}{4}\right]$	[21,60]
22	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{3}{4}\right]$	[22,57]
23	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{3}{4}\right]$	[23,64]
24	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{3}{4}\right]$	[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	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{4}\right]$	[28,53]
29	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{4}\right]$	[29,52]
30	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{4}\right]$	[30,49]
31	$\left[\frac{1}{2}-y,\, \frac{1}{2}-x,\, \frac{1}{4}\right]$	[31,56]
32	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, \frac{1}{4}\right]$	[32,55]

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

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

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

No.	position	mapping
1	$[x,\ x,\ z]$	`[1,48]`
2	$[-x,\ x,\ z]$	`[2,44]`
3	$[x,\ -x,\ z]$	`[3,45]`
4	$\left[x,\ -x,\ \frac{1}{2}-z\right]$	`[4,42]`
5	$\left[-x,\ x,\ \frac{1}{2}-z\right]$	`[5,43]`
6	$[-x,\ -x,\ z]$	`[6,47]`
7	$\left[x,\ x,\ \frac{1}{2}-z\right]$	`[7,46]`

continued ...

Table 19

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

Table 20: Wyckoff site: 32t, site symmetry: ..m

No.	position	mapping
1	$\left[x,\ x+\frac{1}{2},\ z\right]$	[1,32]
2	$\left[\frac{1}{2}-x,\ x,\ z\right]$	[2,28]
3	$\left[x+\frac{1}{2},\ -x,\ z\right]$	[3,29]
4	$\left[x,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[4,26]
5	$\left[-x,\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[5,27]
6	$\left[-x,\ \frac{1}{2}-x,\ z\right]$	[6,31]
7	$\left[x+\frac{1}{2},\ x,\ \frac{1}{2}-z\right]$	[7,30]
8	$\left[\frac{1}{2}-x,\ -x,\ \frac{1}{2}-z\right]$	[8,25]
9	$\left[-x,\ \frac{1}{2}-x,\ -z\right]$	[9,24]
10	$\left[x+\frac{1}{2},\ -x,\ -z\right]$	[10,20]
11	$\left[\frac{1}{2}-x,\ x,\ -z\right]$	[11,21]
12	$\left[-x,\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[12,18]
13	$\left[x,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	[13,19]
14	$\left[x,\ x+\frac{1}{2},\ -z\right]$	[14,23]
15	$\left[\frac{1}{2}-x,\ -x,\ z+\frac{1}{2}\right]$	[15,22]

continued ...

Table 20

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

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	$\left[x,\, -y,\, \frac{1}{2}-z\right]$	[4]
5	$\left[-x,\, y,\, \frac{1}{2}-z\right]$	[5]
6	$[-x,\, -y,\, z]$	[6]
7	$\left[y,\, x,\, \frac{1}{2}-z\right]$	[7]
8	$\left[-y,\, -x,\, \frac{1}{2}-z\right]$	[8]
9	$[-x,\, -y,\, -z]$	[9]
10	$[y,\, -x,\, -z]$	[10]
11	$[-y,\, x,\, -z]$	[11]
12	$\left[-x,\, y,\, z+\frac{1}{2}\right]$	[12]
13	$\left[x,\, -y,\, z+\frac{1}{2}\right]$	[13]
14	$[x,\, y,\, -z]$	[14]
15	$\left[-y,\, -x,\, z+\frac{1}{2}\right]$	[15]
16	$\left[y,\, x,\, z+\frac{1}{2}\right]$	[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	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, -z\right]$	[20]
21	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, -z\right]$	[21]
22	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[22]
23	$\left[y+\frac{1}{2},\, x+\frac{1}{2},\, -z\right]$	[23]

continued ...

Table 21

No.	position	mapping
24	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ -z\right]$	[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	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z\right]$	[28]
29	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z\right]$	[29]
30	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[30]
31	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z\right]$	[31]
32	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z\right]$	[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	$[x,\ -y,\ -z]$	[36]
37	$[-x,\ y,\ -z]$	[37]
38	$\left[-x,\ -y,\ z+\frac{1}{2}\right]$	[38]
39	$[y,\ x,\ -z]$	[39]
40	$[-y,\ -x,\ -z]$	[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	$[-x,\ y,\ z]$	[44]
45	$[x,\ -y,\ z]$	[45]
46	$\left[x,\ y,\ \frac{1}{2}-z\right]$	[46]
47	$[-y,\ -x,\ z]$	[47]
48	$[y,\ x,\ z]$	[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	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[52]
53	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[53]
54	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ z\right]$	[54]
55	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ \frac{1}{2}-z\right]$	[55]
56	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ \frac{1}{2}-z\right]$	[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	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[60]
61	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[61]
62	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ -z\right]$	[62]
63	$\left[\frac{1}{2}-y,\ \frac{1}{2}-x,\ z+\frac{1}{2}\right]$	[63]
64	$\left[y+\frac{1}{2},\ x+\frac{1}{2},\ z+\frac{1}{2}\right]$	[64]