MSG No. 69.526 F_Smmm [Type IV, orthorhombic]

Table 1: Wyckoff site: `8a`, site symmetry: `mmm`

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

Table 2: Wyckoff site: `8b`, site symmetry: `m'mm`

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

Table 3: Wyckoff site: `8c`, site symmetry: `mmm'`

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

Table 4: Wyckoff site: 8d, site symmetry: m'mm'

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

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

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

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

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

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

No.	position	mapping
1	$\left[0, \frac{1}{4}, \frac{1}{4}\right]$	[1,6,10,13,35,40,44,47]
2	$\left[0, \frac{3}{4}, \frac{3}{4}\right]$	[2,5,9,14,36,39,43,48]
3	$\left[0, \frac{1}{4}, \frac{3}{4}\right]$	[3,8,12,15,33,38,42,45]

continued ...

Table 7

No.	position	mapping
4	$\left[0,\ \frac{3}{4},\ \frac{1}{4}\right]$	`[4,7,11,16,34,37,41,46]`
5	$\left[\frac{1}{2},\ \frac{1}{4},\ \frac{3}{4}\right]$	`[17,22,26,29,51,56,60,63]`
6	$\left[\frac{1}{2},\ \frac{3}{4},\ \frac{1}{4}\right]$	`[18,21,25,30,52,55,59,64]`
7	$\left[\frac{1}{2},\ \frac{1}{4},\ \frac{1}{4}\right]$	`[19,24,28,31,49,54,58,61]`
8	$\left[\frac{1}{2},\ \frac{3}{4},\ \frac{3}{4}\right]$	`[20,23,27,32,50,53,57,62]`

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

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

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

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

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

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

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

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

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

No.	position	mapping
1	$\left[x,\ \frac{1}{4},\ \frac{1}{4}\right]$	`[1,10,40,47]`

continued ...

Table 12

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

Table 13: Wyckoff site: 16m, site symmetry: m2m

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

Table 14: Wyckoff site: 16n, site symmetry: m2'm'

No.	position	mapping
1	$\left[0,\ y,\ \frac{1}{4}\right]$	[1,6,35,40]
2	$\left[0,\ -y,\ \frac{3}{4}\right]$	[2,5,36,39]
3	$\left[0,\ y,\ \frac{3}{4}\right]$	[3,8,33,38]

continued ...

Table 14

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

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

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

Table 16: Wyckoff site: 16p, site symmetry: m'2m'

No.	position	mapping
1	$\left[\frac{1}{4},\ y,\ \frac{1}{4}\right]$	[1,19,40,54]
2	$\left[\frac{1}{4},\ -y,\ \frac{3}{4}\right]$	[2,20,39,53]
3	$\left[\frac{3}{4},\ y,\ \frac{3}{4}\right]$	[3,17,38,56]
4	$\left[\frac{3}{4},\ -y,\ \frac{1}{4}\right]$	[4,18,37,55]
5	$\left[\frac{3}{4},\ -y,\ \frac{3}{4}\right]$	[5,23,36,50]

continued ...

Table 16

No.	position	mapping
6	$\left[\frac{3}{4}, y, \frac{1}{4}\right]$	[6,24,35,49]
7	$\left[\frac{1}{4}, -y, \frac{1}{4}\right]$	[7,21,34,52]
8	$\left[\frac{1}{4}, y, \frac{3}{4}\right]$	[8,22,33,51]
9	$\left[\frac{1}{4}, y+\frac{1}{2}, \frac{3}{4}\right]$	[9,27,48,62]
10	$\left[\frac{1}{4}, \frac{1}{2}-y, \frac{1}{4}\right]$	[10,28,47,61]
11	$\left[\frac{3}{4}, y+\frac{1}{2}, \frac{1}{4}\right]$	[11,25,46,64]
12	$\left[\frac{3}{4}, \frac{1}{2}-y, \frac{3}{4}\right]$	[12,26,45,63]
13	$\left[\frac{3}{4}, \frac{1}{2}-y, \frac{1}{4}\right]$	[13,31,44,58]
14	$\left[\frac{3}{4}, y+\frac{1}{2}, \frac{3}{4}\right]$	[14,32,43,57]
15	$\left[\frac{1}{4}, \frac{1}{2}-y, \frac{3}{4}\right]$	[15,29,42,60]
16	$\left[\frac{1}{4}, y+\frac{1}{2}, \frac{1}{4}\right]$	[16,30,41,59]

Table 17: Wyckoff site: 16q, site symmetry: mm2

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

Table 18: Wyckoff site: 16r, site symmetry: mm'2'

No.	position	mapping
1	$\left[0, \frac{1}{4}, z\right]$	[1,6,44,47]
2	$\left[0, \frac{3}{4}, -z\right]$	[2,5,43,48]
3	$\left[0, \frac{1}{4}, -z\right]$	[3,8,42,45]
4	$\left[0, \frac{3}{4}, z\right]$	[4,7,41,46]
5	$\left[0, \frac{3}{4}, z+\frac{1}{2}\right]$	[9,14,36,39]
6	$\left[0, \frac{1}{4}, \frac{1}{2}-z\right]$	[10,13,35,40]
7	$\left[0, \frac{3}{4}, \frac{1}{2}-z\right]$	[11,16,34,37]

continued ...

Table 18

No.	position	mapping
8	$\left[0,\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[12,15,33,38]
9	$\left[\frac{1}{2},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[17,22,60,63]
10	$\left[\frac{1}{2},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[18,21,59,64]
11	$\left[\frac{1}{2},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	[19,24,58,61]
12	$\left[\frac{1}{2},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[20,23,57,62]
13	$\left[\frac{1}{2},\ \frac{3}{4},\ z\right]$	[25,30,52,55]
14	$\left[\frac{1}{2},\ \frac{1}{4},\ -z\right]$	[26,29,51,56]
15	$\left[\frac{1}{2},\ \frac{3}{4},\ -z\right]$	[27,32,50,53]
16	$\left[\frac{1}{2},\ \frac{1}{4},\ z\right]$	[28,31,49,54]

Table 19: Wyckoff site: 16s, site symmetry: m'm2'

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

Table 20: Wyckoff site: 16t, site symmetry: m'm'2

No.	position	mapping
1	$\left[\frac{1}{4},\ \frac{1}{4},\ z\right]$	[1,28,47,54]
2	$\left[\frac{1}{4},\ \frac{3}{4},\ -z\right]$	[2,27,48,53]
3	$\left[\frac{3}{4},\ \frac{1}{4},\ -z\right]$	[3,26,45,56]
4	$\left[\frac{3}{4},\ \frac{3}{4},\ z\right]$	[4,25,46,55]
5	$\left[\frac{3}{4},\ \frac{3}{4},\ -z\right]$	[5,32,43,50]
6	$\left[\frac{3}{4},\ \frac{1}{4},\ z\right]$	[6,31,44,49]
7	$\left[\frac{1}{4},\ \frac{3}{4},\ z\right]$	[7,30,41,52]
8	$\left[\frac{1}{4},\ \frac{1}{4},\ -z\right]$	[8,29,42,51]
9	$\left[\frac{1}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[9,20,39,62]

continued ...

Table 20

No.	position	mapping
10	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	[10,19,40,61]
11	$\left[\frac{3}{4},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[11,18,37,64]
12	$\left[\frac{3}{4},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[12,17,38,63]
13	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	[13,24,35,58]
14	$\left[\frac{3}{4},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[14,23,36,57]
15	$\left[\frac{1}{4},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[15,22,33,60]
16	$\left[\frac{1}{4},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[16,21,34,59]

Table 21: Wyckoff site: 32u, site symmetry: m..

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

Table 22: Wyckoff site: 32v, site symmetry: m'..

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

Table 23: Wyckoff site: 32w, site symmetry: .m.

No.	position	mapping
1	$[x,\, 0,\, z]$	[1,7]
2	$[x,\, 0,\, -z]$	[2,8]
3	$[-x,\, 0,\, -z]$	[3,5]
4	$[-x,\, 0,\, z]$	[4,6]
5	$\left[x,\, \frac{1}{2},\, z+\frac{1}{2}\right]$	[9,15]
6	$\left[x,\, \frac{1}{2},\, \frac{1}{2}-z\right]$	[10,16]
7	$\left[-x,\, \frac{1}{2},\, \frac{1}{2}-z\right]$	[11,13]

continued ...

Table 23

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

Table 24: Wyckoff site: 32x, site symmetry: .m'.

No.	position	mapping
1	$\left[x,\ \frac{1}{4},\ z\right]$	[1,47]
2	$\left[x,\ \frac{3}{4},\ -z\right]$	[2,48]
3	$\left[-x,\ \frac{1}{4},\ -z\right]$	[3,45]
4	$\left[-x,\ \frac{3}{4},\ z\right]$	[4,46]
5	$\left[-x,\ \frac{3}{4},\ -z\right]$	[5,43]
6	$\left[-x,\ \frac{1}{4},\ z\right]$	[6,44]
7	$\left[x,\ \frac{3}{4},\ z\right]$	[7,41]
8	$\left[x,\ \frac{1}{4},\ -z\right]$	[8,42]
9	$\left[x,\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[9,39]
10	$\left[x,\ \frac{1}{4},\ \frac{1}{2}-z\right]$	[10,40]
11	$\left[-x,\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[11,37]
12	$\left[-x,\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[12,38]
13	$\left[-x,\ \frac{1}{4},\ \frac{1}{2}-z\right]$	[13,35]
14	$\left[-x,\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[14,36]
15	$\left[x,\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[15,33]

continued ...

Table 24

No.	position	mapping
16	$\left[x,\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[16,34]
17	$\left[x+\frac{1}{2},\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[17,63]
18	$\left[x+\frac{1}{2},\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[18,64]
19	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ \frac{1}{2}-z\right]$	[19,61]
20	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[20,62]
21	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ \frac{1}{2}-z\right]$	[21,59]
22	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ z+\frac{1}{2}\right]$	[22,60]
23	$\left[x+\frac{1}{2},\ \frac{3}{4},\ z+\frac{1}{2}\right]$	[23,57]
24	$\left[x+\frac{1}{2},\ \frac{1}{4},\ \frac{1}{2}-z\right]$	[24,58]
25	$\left[x+\frac{1}{2},\ \frac{3}{4},\ z\right]$	[25,55]
26	$\left[x+\frac{1}{2},\ \frac{1}{4},\ -z\right]$	[26,56]
27	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ -z\right]$	[27,53]
28	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ z\right]$	[28,54]
29	$\left[\frac{1}{2}-x,\ \frac{1}{4},\ -z\right]$	[29,51]
30	$\left[\frac{1}{2}-x,\ \frac{3}{4},\ z\right]$	[30,52]
31	$\left[x+\frac{1}{2},\ \frac{1}{4},\ z\right]$	[31,49]
32	$\left[x+\frac{1}{2},\ \frac{3}{4},\ -z\right]$	[32,50]

Table 25: Wyckoff site: 32y, site symmetry: ..m

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

continued ...

Table 25

No.	position	mapping
24	$\left[-x,\ \frac{1}{2}-y,\ 0\right]$	[44,45]
25	$\left[x+\frac{1}{2},\ y,\ 0\right]$	[49,56]
26	$\left[x+\frac{1}{2},\ -y,\ 0\right]$	[50,55]
27	$\left[\frac{1}{2}-x,\ y,\ 0\right]$	[51,54]
28	$\left[\frac{1}{2}-x,\ -y,\ 0\right]$	[52,53]
29	$\left[x+\frac{1}{2},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[57,64]
30	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[58,63]
31	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[59,62]
32	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}\right]$	[60,61]

Table 26: Wyckoff site: 32z, site symmetry: ..m'

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

continued ...

Table 26

No.	position	mapping
32	$\left[x+\frac{1}{2}, y+\frac{1}{2}, \frac{3}{4}\right]$	[32,57]

Table 27: Wyckoff site: 64A, 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	$[-x, -y, -z]$	[5]
6	$[-x, y, z]$	[6]
7	$[x, -y, z]$	[7]
8	$[x, y, -z]$	[8]
9	$\left[x, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[9]
10	$\left[x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[10]
11	$\left[-x, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[11]
12	$\left[-x, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[12]
13	$\left[-x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[13]
14	$\left[-x, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[14]
15	$\left[x, \frac{1}{2}-y, z+\frac{1}{2}\right]$	[15]
16	$\left[x, y+\frac{1}{2}, \frac{1}{2}-z\right]$	[16]
17	$\left[x+\frac{1}{2}, y, z+\frac{1}{2}\right]$	[17]
18	$\left[x+\frac{1}{2}, -y, \frac{1}{2}-z\right]$	[18]
19	$\left[\frac{1}{2}-x, y, \frac{1}{2}-z\right]$	[19]
20	$\left[\frac{1}{2}-x, -y, z+\frac{1}{2}\right]$	[20]
21	$\left[\frac{1}{2}-x, -y, \frac{1}{2}-z\right]$	[21]
22	$\left[\frac{1}{2}-x, y, z+\frac{1}{2}\right]$	[22]
23	$\left[x+\frac{1}{2}, -y, z+\frac{1}{2}\right]$	[23]
24	$\left[x+\frac{1}{2}, y, \frac{1}{2}-z\right]$	[24]
25	$\left[x+\frac{1}{2}, y+\frac{1}{2}, z\right]$	[25]
26	$\left[x+\frac{1}{2}, \frac{1}{2}-y, -z\right]$	[26]
27	$\left[\frac{1}{2}-x, y+\frac{1}{2}, -z\right]$	[27]
28	$\left[\frac{1}{2}-x, \frac{1}{2}-y, z\right]$	[28]
29	$\left[\frac{1}{2}-x, \frac{1}{2}-y, -z\right]$	[29]
30	$\left[\frac{1}{2}-x, y+\frac{1}{2}, z\right]$	[30]
31	$\left[x+\frac{1}{2}, \frac{1}{2}-y, z\right]$	[31]
32	$\left[x+\frac{1}{2}, y+\frac{1}{2}, -z\right]$	[32]
33	$\left[x, y, z+\frac{1}{2}\right]$	[33]
34	$\left[x, -y, \frac{1}{2}-z\right]$	[34]
35	$\left[-x, y, \frac{1}{2}-z\right]$	[35]
36	$\left[-x, -y, z+\frac{1}{2}\right]$	[36]
37	$\left[-x, -y, \frac{1}{2}-z\right]$	[37]
38	$\left[-x, y, z+\frac{1}{2}\right]$	[38]
39	$\left[x, -y, z+\frac{1}{2}\right]$	[39]

continued ...

Table 27

No.	position	mapping
40	$\left[x,\, y,\, \frac{1}{2}-z\right]$	[40]
41	$\left[x,\, y+\frac{1}{2},\, z\right]$	[41]
42	$\left[x,\, \frac{1}{2}-y,\, -z\right]$	[42]
43	$\left[-x,\, y+\frac{1}{2},\, -z\right]$	[43]
44	$\left[-x,\, \frac{1}{2}-y,\, z\right]$	[44]
45	$\left[-x,\, \frac{1}{2}-y,\, -z\right]$	[45]
46	$\left[-x,\, y+\frac{1}{2},\, z\right]$	[46]
47	$\left[x,\, \frac{1}{2}-y,\, z\right]$	[47]
48	$\left[x,\, y+\frac{1}{2},\, -z\right]$	[48]
49	$\left[x+\frac{1}{2},\, y,\, z\right]$	[49]
50	$\left[x+\frac{1}{2},\, -y,\, -z\right]$	[50]
51	$\left[\frac{1}{2}-x,\, y,\, -z\right]$	[51]
52	$\left[\frac{1}{2}-x,\, -y,\, z\right]$	[52]
53	$\left[\frac{1}{2}-x,\, -y,\, -z\right]$	[53]
54	$\left[\frac{1}{2}-x,\, y,\, z\right]$	[54]
55	$\left[x+\frac{1}{2},\, -y,\, z\right]$	[55]
56	$\left[x+\frac{1}{2},\, y,\, -z\right]$	[56]
57	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[57]
58	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[58]
59	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[59]
60	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[60]
61	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, \frac{1}{2}-z\right]$	[61]
62	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[62]
63	$\left[x+\frac{1}{2},\, \frac{1}{2}-y,\, z+\frac{1}{2}\right]$	[63]
64	$\left[x+\frac{1}{2},\, y+\frac{1}{2},\, \frac{1}{2}-z\right]$	[64]