MSG No. 70.532 $F_S ddd$ [Type IV, orthorhombic]

Table 1: Wyckoff site: 16a, site symmetry: 222

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

Table 2: Wyckoff site: 16b, site symmetry: 22'2'

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

Table 3: Wyckoff site: `16c`, site symmetry: `2'2'2`

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

Table 4: Wyckoff site: `16d`, site symmetry: `2'22'`

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

Table 5: Wyckoff site: `32e`, site symmetry: `-1`

No.	position	mapping
1	[0, 0, 0]	`[1,5]`

continued ...

Table 5

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

Table 6: Wyckoff site: 32f, site symmetry: -1'

No.	position	mapping
1	$\left[\frac{3}{4},\ \frac{3}{4},\ \frac{3}{4}\right]$	[1,61]
2	$\left[\frac{3}{4},\ 0,\ 0\right]$	[2,54]
3	$\left[0,\ \frac{3}{4},\ 0\right]$	[3,47]
4	$\left[0,\ 0,\ \frac{3}{4}\right]$	[4,40]
5	$\left[\frac{1}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	[5,57]
6	$\left[\frac{1}{4},\ 0,\ 0\right]$	[6,50]
7	$\left[0,\ \frac{1}{4},\ 0\right]$	[7,43]
8	$\left[0,\ 0,\ \frac{1}{4}\right]$	[8,36]
9	$\left[\frac{3}{4},\ \frac{1}{4},\ \frac{1}{4}\right]$	[9,53]

continued ...

Table 6

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

Table 7: Wyckoff site: 32g, site symmetry: 2..

No.	position	mapping
1	$\left[x, \frac{7}{8}, \frac{7}{8}\right]$	[1,2]
2	$\left[\frac{3}{4} - x, \frac{7}{8}, \frac{7}{8}\right]$	[3,4]
3	$\left[-x, \frac{1}{8}, \frac{1}{8}\right]$	[5,6]
4	$\left[x + \frac{1}{4}, \frac{1}{8}, \frac{1}{8}\right]$	[7,8]
5	$\left[x, \frac{3}{8}, \frac{3}{8}\right]$	[9,10]
6	$\left[\frac{3}{4} - x, \frac{3}{8}, \frac{3}{8}\right]$	[11,12]
7	$\left[-x, \frac{5}{8}, \frac{5}{8}\right]$	[13,14]
8	$\left[x + \frac{1}{4}, \frac{5}{8}, \frac{5}{8}\right]$	[15,16]
9	$\left[x + \frac{1}{2}, \frac{7}{8}, \frac{3}{8}\right]$	[17,18]
10	$\left[\frac{1}{4} - x, \frac{7}{8}, \frac{3}{8}\right]$	[19,20]
11	$\left[\frac{1}{2} - x, \frac{1}{8}, \frac{5}{8}\right]$	[21,22]
12	$\left[x + \frac{3}{4}, \frac{1}{8}, \frac{5}{8}\right]$	[23,24]
13	$\left[x + \frac{1}{2}, \frac{3}{8}, \frac{7}{8}\right]$	[25,26]
14	$\left[\frac{1}{4} - x, \frac{3}{8}, \frac{7}{8}\right]$	[27,28]
15	$\left[\frac{1}{2} - x, \frac{5}{8}, \frac{1}{8}\right]$	[29,30]
16	$\left[x + \frac{3}{4}, \frac{5}{8}, \frac{1}{8}\right]$	[31,32]
17	$\left[x, \frac{7}{8}, \frac{3}{8}\right]$	[33,34]

continued ...

Table 7

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

Table 8: Wyckoff site: 32h, site symmetry: 2’..

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

continued ...

Table 8

No.	position	mapping
26	$\left[x+\frac{1}{2},\ \frac{3}{8},\ \frac{5}{8}\right]$	[26,57]
27	$\left[\frac{1}{4}-x,\ \frac{3}{8},\ \frac{5}{8}\right]$	[27,60]
28	$\left[\frac{1}{4}-x,\ \frac{3}{8},\ \frac{1}{8}\right]$	[28,59]
29	$\left[\frac{1}{2}-x,\ \frac{5}{8},\ \frac{7}{8}\right]$	[29,62]
30	$\left[\frac{1}{2}-x,\ \frac{5}{8},\ \frac{3}{8}\right]$	[30,61]
31	$\left[x+\frac{3}{4},\ \frac{5}{8},\ \frac{3}{8}\right]$	[31,64]
32	$\left[x+\frac{3}{4},\ \frac{5}{8},\ \frac{7}{8}\right]$	[32,63]

Table 9: Wyckoff site: 32i, site symmetry: .2.

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

Table 10: Wyckoff site: 32j, site symmetry: .2'.

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

Table 11: Wyckoff site: 32k, site symmetry: ..2

No.	position	mapping
1	$\left[\frac{7}{8},\ \frac{7}{8},\ z\right]$	[1,4]
2	$\left[\frac{7}{8},\ \frac{7}{8},\ \frac{3}{4}-z\right]$	[2,3]
3	$\left[\frac{1}{8},\ \frac{1}{8},\ -z\right]$	[5,8]
4	$\left[\frac{1}{8},\ \frac{1}{8},\ z+\frac{1}{4}\right]$	[6,7]
5	$\left[\frac{7}{8},\ \frac{3}{8},\ z+\frac{1}{2}\right]$	[9,12]
6	$\left[\frac{7}{8},\ \frac{3}{8},\ \frac{1}{4}-z\right]$	[10,11]
7	$\left[\frac{1}{8},\ \frac{5}{8},\ \frac{1}{2}-z\right]$	[13,16]

continued ...

Table 11

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

Table 12: Wyckoff site: 321, site symmetry: ..2'

No.	position	mapping
1	$\left[\frac{7}{8}, \frac{1}{8}, z\right]$	[1,44]
2	$\left[\frac{7}{8}, \frac{5}{8}, \frac{3}{4}-z\right]$	[2,43]
3	$\left[\frac{7}{8}, \frac{1}{8}, \frac{3}{4}-z\right]$	[3,42]
4	$\left[\frac{7}{8}, \frac{5}{8}, z\right]$	[4,41]
5	$\left[\frac{1}{8}, \frac{7}{8}, -z\right]$	[5,48]
6	$\left[\frac{1}{8}, \frac{3}{8}, z+\frac{1}{4}\right]$	[6,47]
7	$\left[\frac{1}{8}, \frac{7}{8}, z+\frac{1}{4}\right]$	[7,46]
8	$\left[\frac{1}{8}, \frac{3}{8}, -z\right]$	[8,45]
9	$\left[\frac{7}{8}, \frac{5}{8}, z+\frac{1}{2}\right]$	[9,36]
10	$\left[\frac{7}{8}, \frac{1}{8}, \frac{1}{4}-z\right]$	[10,35]
11	$\left[\frac{7}{8}, \frac{5}{8}, \frac{1}{4}-z\right]$	[11,34]
12	$\left[\frac{7}{8}, \frac{1}{8}, z+\frac{1}{2}\right]$	[12,33]
13	$\left[\frac{1}{8}, \frac{3}{8}, \frac{1}{2}-z\right]$	[13,40]
14	$\left[\frac{1}{8}, \frac{7}{8}, z+\frac{3}{4}\right]$	[14,39]
15	$\left[\frac{1}{8}, \frac{3}{8}, z+\frac{3}{4}\right]$	[15,38]

continued ...

Table 12

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

Table 13: Wyckoff site: 64m, site symmetry: 1

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

continued ...

Table 13

No.	position	mapping
24	$\left[x+\frac{3}{4}, y+\frac{1}{4}, \frac{1}{2}-z\right]$	[24]
25	$\left[x+\frac{1}{2}, y+\frac{1}{2}, z\right]$	[25]
26	$\left[x+\frac{1}{2}, \frac{1}{4}-y, \frac{3}{4}-z\right]$	[26]
27	$\left[\frac{1}{4}-x, y+\frac{1}{2}, \frac{3}{4}-z\right]$	[27]
28	$\left[\frac{1}{4}-x, \frac{1}{4}-y, z\right]$	[28]
29	$\left[\frac{1}{2}-x, \frac{1}{2}-y, -z\right]$	[29]
30	$\left[\frac{1}{2}-x, y+\frac{3}{4}, z+\frac{1}{4}\right]$	[30]
31	$\left[x+\frac{3}{4}, \frac{1}{2}-y, z+\frac{1}{4}\right]$	[31]
32	$\left[x+\frac{3}{4}, y+\frac{3}{4}, -z\right]$	[32]
33	$\left[x, y, z+\frac{1}{2}\right]$	[33]
34	$\left[x, \frac{3}{4}-y, \frac{1}{4}-z\right]$	[34]
35	$\left[\frac{3}{4}-x, y, \frac{1}{4}-z\right]$	[35]
36	$\left[\frac{3}{4}-x, \frac{3}{4}-y, z+\frac{1}{2}\right]$	[36]
37	$\left[-x, -y, \frac{1}{2}-z\right]$	[37]
38	$\left[-x, y+\frac{1}{4}, z+\frac{3}{4}\right]$	[38]
39	$\left[x+\frac{1}{4}, -y, z+\frac{3}{4}\right]$	[39]
40	$\left[x+\frac{1}{4}, y+\frac{1}{4}, \frac{1}{2}-z\right]$	[40]
41	$\left[x, y+\frac{1}{2}, z\right]$	[41]
42	$\left[x, \frac{1}{4}-y, \frac{3}{4}-z\right]$	[42]
43	$\left[\frac{3}{4}-x, y+\frac{1}{2}, \frac{3}{4}-z\right]$	[43]
44	$\left[\frac{3}{4}-x, \frac{1}{4}-y, z\right]$	[44]
45	$\left[-x, \frac{1}{2}-y, -z\right]$	[45]
46	$\left[-x, y+\frac{3}{4}, z+\frac{1}{4}\right]$	[46]
47	$\left[x+\frac{1}{4}, \frac{1}{2}-y, z+\frac{1}{4}\right]$	[47]
48	$\left[x+\frac{1}{4}, y+\frac{3}{4}, -z\right]$	[48]
49	$\left[x+\frac{1}{2}, y, z\right]$	[49]
50	$\left[x+\frac{1}{2}, \frac{3}{4}-y, \frac{3}{4}-z\right]$	[50]
51	$\left[\frac{1}{4}-x, y, \frac{3}{4}-z\right]$	[51]
52	$\left[\frac{1}{4}-x, \frac{3}{4}-y, z\right]$	[52]
53	$\left[\frac{1}{2}-x, -y, -z\right]$	[53]
54	$\left[\frac{1}{2}-x, y+\frac{1}{4}, z+\frac{1}{4}\right]$	[54]
55	$\left[x+\frac{3}{4}, -y, z+\frac{1}{4}\right]$	[55]
56	$\left[x+\frac{3}{4}, y+\frac{1}{4}, -z\right]$	[56]
57	$\left[x+\frac{1}{2}, y+\frac{1}{2}, z+\frac{1}{2}\right]$	[57]
58	$\left[x+\frac{1}{2}, \frac{1}{4}-y, \frac{1}{4}-z\right]$	[58]
59	$\left[\frac{1}{4}-x, y+\frac{1}{2}, \frac{1}{4}-z\right]$	[59]
60	$\left[\frac{1}{4}-x, \frac{1}{4}-y, z+\frac{1}{2}\right]$	[60]
61	$\left[\frac{1}{2}-x, \frac{1}{2}-y, \frac{1}{2}-z\right]$	[61]
62	$\left[\frac{1}{2}-x, y+\frac{3}{4}, z+\frac{3}{4}\right]$	[62]
63	$\left[x+\frac{3}{4}, \frac{1}{2}-y, z+\frac{3}{4}\right]$	[63]
64	$\left[x+\frac{3}{4}, y+\frac{3}{4}, \frac{1}{2}-z\right]$	[64]