MSG No. 142.570 I_c4_1/acd [Type IV, tetragonal]

Table 1: Wyckoff site: `8a`, site symmetry: `-4m'2'`

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

Table 2: Wyckoff site: `8b`, site symmetry: `-4'm'2`

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

Table 3: Wyckoff site: `16c`, site symmetry: `2.22`

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

continued ...

Table 3

No.	position	mapping
16	$\left[\frac{3}{4}, \frac{1}{2}, \frac{5}{8}\right]$	`[27,28,42,45]`

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

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

Table 5: Wyckoff site: `16e`, site symmetry: `.2'/m'.`

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

Table 6: Wyckoff site: `16f`, site symmetry: `.2/m'.`

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

Table 7: Wyckoff site: `16g`, site symmetry: `2m'm'.`

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

Table 8: Wyckoff site: `32h`, site symmetry: `2'..`

No.	position	mapping
1	$\left[\frac{3}{4}, 0, z\right]$	`[1,54]`

continued ...

Table 8

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

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

No.	position	mapping
1	$\left[x, x+\frac{1}{4}, \frac{7}{8}\right]$	[1,39]
2	$\left[-x, x+\frac{3}{4}, \frac{1}{8}\right]$	[2,53]
3	$\left[x, \frac{3}{4}-x, \frac{1}{8}\right]$	[3,52]
4	$\left[x+\frac{1}{2}, \frac{1}{4}-x, \frac{1}{8}\right]$	[4,51]
5	$\left[\frac{1}{2}-x, x+\frac{1}{4}, \frac{1}{8}\right]$	[5,50]
6	$\left[-x, \frac{1}{4}-x, \frac{7}{8}\right]$	[6,40]
7	$\left[x, x+\frac{1}{4}, \frac{3}{8}\right]$	[7,33]
8	$\left[-x, \frac{1}{4}-x, \frac{3}{8}\right]$	[8,38]
9	$\left[-x, \frac{3}{4}-x, \frac{1}{8}\right]$	[9,63]

continued ...

Table 9

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

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

No.	position	mapping
1	$\left[x,\ x+\frac{1}{4},\ \frac{5}{8}\right]$	[1,7]
2	$\left[-x,\ x+\frac{3}{4},\ \frac{7}{8}\right]$	[2,21]
3	$\left[x,\ \frac{3}{4}-x,\ \frac{7}{8}\right]$	[3,20]
4	$\left[x+\frac{1}{2},\ \frac{1}{4}-x,\ \frac{3}{8}\right]$	[4,19]
5	$\left[\frac{1}{2}-x,\ x+\frac{1}{4},\ \frac{3}{8}\right]$	[5,18]
6	$\left[-x,\ \frac{1}{4}-x,\ \frac{5}{8}\right]$	[6,8]
7	$\left[-x,\ \frac{3}{4}-x,\ \frac{3}{8}\right]$	[9,31]
8	$\left[x,\ \frac{1}{4}-x,\ \frac{1}{8}\right]$	[10,13]
9	$\left[-x,\ x+\frac{1}{4},\ \frac{1}{8}\right]$	[11,12]
10	$\left[x,\ x+\frac{3}{4},\ \frac{3}{8}\right]$	[14,32]
11	$\left[\frac{1}{2}-x,\ \frac{1}{4}-x,\ \frac{7}{8}\right]$	[15,25]
12	$\left[x+\frac{1}{2},\ x+\frac{1}{4},\ \frac{7}{8}\right]$	[16,30]
13	$\left[x+\frac{1}{2},\ x+\frac{3}{4},\ \frac{1}{8}\right]$	[17,23]
14	$\left[\frac{1}{2}-x,\ \frac{3}{4}-x,\ \frac{1}{8}\right]$	[22,24]
15	$\left[x+\frac{1}{2},\ \frac{3}{4}-x,\ \frac{5}{8}\right]$	[26,29]
16	$\left[\frac{1}{2}-x,\ x+\frac{3}{4},\ \frac{5}{8}\right]$	[27,28]
17	$\left[x,\ x+\frac{1}{4},\ \frac{1}{8}\right]$	[33,39]

continued ...

Table 10

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

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

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

continued ...

Table 11

No.	position	mapping
26	$\left[\frac{3}{4},\ y+\frac{1}{2},\ 0\right]$	[46,60]
27	$\left[\frac{3}{4}-y,\ \frac{1}{2},\ \frac{1}{4}\right]$	[47,59]
28	$\left[y+\frac{1}{4},\ 0,\ \frac{1}{4}\right]$	[48,58]
29	$\left[\frac{1}{4},\ y+\frac{1}{2},\ \frac{1}{2}\right]$	[49,53]
30	$\left[\frac{3}{4}-y,\ 0,\ \frac{3}{4}\right]$	[50,56]
31	$\left[y+\frac{1}{4},\ \frac{1}{2},\ \frac{3}{4}\right]$	[51,55]
32	$\left[\frac{3}{4},\ -y,\ \frac{1}{2}\right]$	[52,54]

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

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

Table 13: Wyckoff site: 32m, site symmetry: .m'.

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

Table 14: Wyckoff site: 64n, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$\left[\frac{1}{4}-y,\ x+\frac{3}{4},\ z+\frac{1}{4}\right]$	[2]
3	$\left[y+\frac{3}{4},\ \frac{3}{4}-x,\ z+\frac{1}{4}\right]$	[3]
4	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[4]
5	$\left[\frac{1}{2}-x,\ y,\ -z\right]$	[5]
6	$\left[-x,\ \frac{1}{2}-y,\ z\right]$	[6]
7	$\left[y+\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{4}-z\right]$	[7]

continued ...

Table 14

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

continued ...

Table 14

No.	position	mapping
55	$\left[y+\frac{1}{4},\, x+\frac{3}{4},\, \frac{1}{4}-z\right]$	[55]
56	$\left[\frac{3}{4}-y,\, \frac{3}{4}-x,\, \frac{1}{4}-z\right]$	[56]
57	$\left[\frac{1}{2}-x,\, \frac{1}{2}-y,\, -z\right]$	[57]
58	$\left[y+\frac{1}{4},\, \frac{3}{4}-x,\, \frac{3}{4}-z\right]$	[58]
59	$\left[\frac{3}{4}-y,\, x+\frac{3}{4},\, \frac{3}{4}-z\right]$	[59]
60	$\left[\frac{1}{2}-x,\, y+\frac{1}{2},\, z+\frac{1}{2}\right]$	[60]
61	$\left[x+\frac{1}{2},\, -y,\, z+\frac{1}{2}\right]$	[61]
62	$\left[x+\frac{1}{2},\, y,\, -z\right]$	[62]
63	$\left[\frac{1}{4}-y,\, \frac{3}{4}-x,\, z+\frac{1}{4}\right]$	[63]
64	$\left[y+\frac{3}{4},\, x+\frac{3}{4},\, z+\frac{1}{4}\right]$	[64]