MSG No. 141.560 I_c4_1/amd [Type IV, tetragonal]

Table 1: Wyckoff site: `8a`, site symmetry: `-4m2`

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

Table 2: Wyckoff site: `8b`, site symmetry: `-4'm2'`

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

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

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

continued ...

Table 3

No.	position	mapping
16	$\left[\frac{3}{4}, \frac{1}{2}, \frac{7}{8}\right]$	`[16,25,46,63]`

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

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

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

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

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

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

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

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

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	$\left[\frac{3}{4},\ 0,\ -z\right]$	[4,53]
5	$\left[\frac{1}{4},\ \frac{1}{2},\ -z\right]$	[5,52]
6	$\left[\frac{1}{4},\ \frac{1}{2},\ z\right]$	[6,49]
7	$\left[\frac{3}{4},\ 0,\ \frac{3}{4}-z\right]$	[7,56]
8	$\left[\frac{1}{4},\ \frac{1}{2},\ \frac{3}{4}-z\right]$	[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	$\left[\frac{1}{4},\ 0,\ z\right]$	[12,61]
13	$\left[\frac{3}{4},\ \frac{1}{2},\ z\right]$	[13,60]
14	$\left[\frac{3}{4},\ \frac{1}{2},\ -z\right]$	[14,57]
15	$\left[\frac{1}{4},\ 0,\ z+\frac{1}{4}\right]$	[15,64]
16	$\left[\frac{3}{4},\ \frac{1}{2},\ z+\frac{1}{4}\right]$	[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	$\left[\frac{1}{4},\ \frac{1}{2},\ \frac{1}{2}-z\right]$	[20,37]
21	$\left[\frac{3}{4},\ 0,\ \frac{1}{2}-z\right]$	[21,36]
22	$\left[\frac{3}{4},\ 0,\ z+\frac{1}{2}\right]$	[22,33]
23	$\left[\frac{1}{4},\ \frac{1}{2},\ \frac{1}{4}-z\right]$	[23,40]
24	$\left[\frac{3}{4},\ 0,\ \frac{1}{4}-z\right]$	[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	$\left[\frac{3}{4},\ \frac{1}{2},\ z+\frac{1}{2}\right]$	[28,45]
29	$\left[\frac{1}{4},\ 0,\ z+\frac{1}{2}\right]$	[29,44]
30	$\left[\frac{1}{4},\ 0,\ \frac{1}{2}-z\right]$	[30,41]
31	$\left[\frac{3}{4},\ \frac{1}{2},\ z+\frac{3}{4}\right]$	[31,48]
32	$\left[\frac{1}{4},\ 0,\ z+\frac{3}{4}\right]$	[32,47]

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

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

continued ...

Table 9

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

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

No.	position	mapping
1	$\left[x,\, x+\frac{1}{4},\, \frac{5}{8}\right]$	[1,39]
2	$\left[-x,\, x+\frac{3}{4},\, \frac{7}{8}\right]$	[2,37]
3	$\left[x,\, \frac{3}{4}-x,\, \frac{7}{8}\right]$	[3,36]
4	$\left[x,\, \frac{3}{4}-x,\, \frac{3}{8}\right]$	[4,35]
5	$\left[-x,\, x+\frac{3}{4},\, \frac{3}{8}\right]$	[5,34]
6	$\left[-x,\, \frac{1}{4}-x,\, \frac{5}{8}\right]$	[6,40]
7	$\left[x,\, x+\frac{1}{4},\, \frac{1}{8}\right]$	[7,33]
8	$\left[-x,\, \frac{1}{4}-x,\, \frac{1}{8}\right]$	[8,38]
9	$\left[-x,\, \frac{3}{4}-x,\, \frac{3}{8}\right]$	[9,47]
10	$\left[x,\, \frac{1}{4}-x,\, \frac{1}{8}\right]$	[10,45]
11	$\left[-x,\, x+\frac{1}{4},\, \frac{1}{8}\right]$	[11,44]
12	$\left[-x,\, x+\frac{1}{4},\, \frac{5}{8}\right]$	[12,43]
13	$\left[x,\, \frac{1}{4}-x,\, \frac{5}{8}\right]$	[13,42]
14	$\left[x,\, x+\frac{3}{4},\, \frac{3}{8}\right]$	[14,48]
15	$\left[-x,\, \frac{3}{4}-x,\, \frac{7}{8}\right]$	[15,41]
16	$\left[x,\, x+\frac{3}{4},\, \frac{7}{8}\right]$	[16,46]
17	$\left[x+\frac{1}{2},\, x+\frac{3}{4},\, \frac{1}{8}\right]$	[17,55]

continued ...

Table 10

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

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

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

continued ...

Table 11

No.	position	mapping
26	$\left[y+\frac{1}{4},\ 0,\ \frac{3}{4}\right]$	[26,64]
27	$\left[\frac{3}{4}-y,\ \frac{1}{2},\ \frac{3}{4}\right]$	[27,63]
28	$\left[\frac{3}{4},\ y+\frac{1}{2},\ 0\right]$	[28,46]
29	$\left[\frac{1}{4},\ -y,\ 0\right]$	[29,41]
30	$\left[\frac{1}{4},\ y,\ 0\right]$	[30,44]
31	$\left[\frac{3}{4}-y,\ \frac{1}{2},\ \frac{1}{4}\right]$	[31,59]
32	$\left[y+\frac{1}{4},\ 0,\ \frac{1}{4}\right]$	[32,58]

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

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

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

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

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	$[x,\ -y,\ -z]$	`[4]`
5	$\left[-x,\ y+\frac{1}{2},\ -z\right]$	`[5]`
6	$\left[-x,\ \frac{1}{2}-y,\ z\right]$	`[6]`
7	$\left[y+\frac{3}{4},\ x+\frac{1}{4},\ \frac{3}{4}-z\right]$	`[7]`

continued ...

Table 14

No.	position	mapping
8	$\left[\frac{1}{4}-y,\ \frac{1}{4}-x,\ \frac{3}{4}-z\right]$	[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	$[-x,\ y,\ z]$	[12]
13	$\left[x,\ \frac{1}{2}-y,\ z\right]$	[13]
14	$\left[x,\ y+\frac{1}{2},\ -z\right]$	[14]
15	$\left[\frac{1}{4}-y,\ \frac{3}{4}-x,\ z+\frac{1}{4}\right]$	[15]
16	$\left[y+\frac{3}{4},\ x+\frac{3}{4},\ z+\frac{1}{4}\right]$	[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	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[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	$\left[y+\frac{1}{4},\ x+\frac{3}{4},\ \frac{1}{4}-z\right]$	[23]
24	$\left[\frac{3}{4}-y,\ \frac{3}{4}-x,\ \frac{1}{4}-z\right]$	[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	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z+\frac{1}{2}\right]$	[28]
29	$\left[x+\frac{1}{2},\ -y,\ z+\frac{1}{2}\right]$	[29]
30	$\left[x+\frac{1}{2},\ y,\ \frac{1}{2}-z\right]$	[30]
31	$\left[\frac{3}{4}-y,\ \frac{1}{4}-x,\ z+\frac{3}{4}\right]$	[31]
32	$\left[y+\frac{1}{4},\ x+\frac{1}{4},\ z+\frac{3}{4}\right]$	[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	$\left[x,\ -y,\ \frac{1}{2}-z\right]$	[36]
37	$\left[-x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[37]
38	$\left[-x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[38]
39	$\left[y+\frac{3}{4},\ x+\frac{1}{4},\ \frac{1}{4}-z\right]$	[39]
40	$\left[\frac{1}{4}-y,\ \frac{1}{4}-x,\ \frac{1}{4}-z\right]$	[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	$\left[-x,\ y,\ z+\frac{1}{2}\right]$	[44]
45	$\left[x,\ \frac{1}{2}-y,\ z+\frac{1}{2}\right]$	[45]
46	$\left[x,\ y+\frac{1}{2},\ \frac{1}{2}-z\right]$	[46]
47	$\left[\frac{1}{4}-y,\ \frac{3}{4}-x,\ z+\frac{3}{4}\right]$	[47]
48	$\left[y+\frac{3}{4},\ x+\frac{3}{4},\ z+\frac{3}{4}\right]$	[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	$\left[x+\frac{1}{2},\ \frac{1}{2}-y,\ -z\right]$	[52]
53	$\left[\frac{1}{2}-x,\ y,\ -z\right]$	[53]
54	$\left[\frac{1}{2}-x,\ -y,\ z\right]$	[54]

continued ...

Table 14

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