MSG No. 142.562 $I4_1/acd1'$ [Type II, tetragonal]

Table 1: Wyckoff site: 8a, site symmetry: -4..1'

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

Table 2: Wyckoff site: 8b, site symmetry: 2.221'

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

Table 3: Wyckoff site: 16c, site symmetry: -11'

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

continued ...

Table 3

No.	position	mapping
16	$\left[\frac{3}{4}, \frac{3}{4}, \frac{3}{4}\right]$	[24,32,56,64]

Table 4: Wyckoff site: 16d, site symmetry: 2..1'

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

Table 5: Wyckoff site: 16e, site symmetry: .2.1'

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

Table 6: Wyckoff site: `16f`, site symmetry: `..21'`

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

Table 7: Wyckoff site: `32g`, site symmetry: `11'`

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

continued ...

Table 7

No.	position	mapping
24	$\left[\frac{3}{4}-y,\ \frac{3}{4}-x,\ \frac{3}{4}-z\right]$	[24,56]
25	$\left[\frac{1}{2}-x,\ \frac{1}{2}-y,\ \frac{1}{2}-z\right]$	[25,57]
26	$\left[y+\frac{1}{4},\ \frac{3}{4}-x,\ \frac{1}{4}-z\right]$	[26,58]
27	$\left[\frac{3}{4}-y,\ x+\frac{3}{4},\ \frac{1}{4}-z\right]$	[27,59]
28	$\left[\frac{1}{2}-x,\ y+\frac{1}{2},\ z\right]$	[28,60]
29	$\left[x+\frac{1}{2},\ -y,\ z\right]$	[29,61]
30	$\left[x+\frac{1}{2},\ y,\ \frac{1}{2}-z\right]$	[30,62]
31	$\left[\frac{1}{4}-y,\ \frac{3}{4}-x,\ z+\frac{3}{4}\right]$	[31,63]
32	$\left[y+\frac{3}{4},\ x+\frac{3}{4},\ z+\frac{3}{4}\right]$	[32,64]