MSG No. 167.104 $R\bar{3}c1'$ [Type II, trigonal]

Table 1: Wyckoff site: 6a, site symmetry: 32.1'

No.	position	mapping
1	$\left[0,\ 0,\ \frac{1}{4}\right]$	[1,2,3,4,5,6,37,38,39,40,41,42]
2	$\left[0,\ 0,\ \frac{3}{4}\right]$	[7,8,9,10,11,12,43,44,45,46,47,48]
3	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{7}{12}\right]$	[13,14,15,16,17,18,49,50,51,52,53,54]
4	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{12}\right]$	[19,20,21,22,23,24,55,56,57,58,59,60]
5	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{11}{12}\right]$	[25,26,27,28,29,30,61,62,63,64,65,66]
6	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{5}{12}\right]$	[31,32,33,34,35,36,67,68,69,70,71,72]

Table 2: Wyckoff site: 6b, site symmetry: -3..1'

No.	position	mapping
1	$[0,\ 0,\ 0]$	[1,2,3,7,8,9,37,38,39,43,44,45]
2	$\left[0,\ 0,\ \frac{1}{2}\right]$	[4,5,6,10,11,12,40,41,42,46,47,48]
3	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{3}\right]$	[13,14,15,19,20,21,49,50,51,55,56,57]
4	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{5}{6}\right]$	[16,17,18,22,23,24,52,53,54,58,59,60]
5	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{2}{3}\right]$	[25,26,27,31,32,33,61,62,63,67,68,69]
6	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{6}\right]$	[28,29,30,34,35,36,64,65,66,70,71,72]

Table 3: Wyckoff site: 12c, site symmetry: 3..1'

No.	position	mapping
1	$[0,\ 0,\ z]$	[1,2,3,37,38,39]
2	$\left[0,\ 0,\ \frac{1}{2}-z\right]$	[4,5,6,40,41,42]
3	$[0,\ 0,\ -z]$	[7,8,9,43,44,45]
4	$\left[0,\ 0,\ z+\frac{1}{2}\right]$	[10,11,12,46,47,48]
5	$\left[\frac{2}{3},\ \frac{1}{3},\ z+\frac{1}{3}\right]$	[13,14,15,49,50,51]
6	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{5}{6}-z\right]$	[16,17,18,52,53,54]
7	$\left[\frac{2}{3},\ \frac{1}{3},\ \frac{1}{3}-z\right]$	[19,20,21,55,56,57]
8	$\left[\frac{2}{3},\ \frac{1}{3},\ z+\frac{5}{6}\right]$	[22,23,24,58,59,60]
9	$\left[\frac{1}{3},\ \frac{2}{3},\ z+\frac{2}{3}\right]$	[25,26,27,61,62,63]
10	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{1}{6}-z\right]$	[28,29,30,64,65,66]
11	$\left[\frac{1}{3},\ \frac{2}{3},\ \frac{2}{3}-z\right]$	[31,32,33,67,68,69]
12	$\left[\frac{1}{3},\ \frac{2}{3},\ z+\frac{1}{6}\right]$	[34,35,36,70,71,72]

Table 4: Wyckoff site: `18d`, site symmetry: `-11'`

No.	position	mapping
1	$\left[\frac{1}{2}, 0, 0\right]$	`[1,7,37,43]`
2	$\left[0, \frac{1}{2}, 0\right]$	`[2,8,38,44]`
3	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[3,9,39,45]`
4	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[4,10,40,46]`
5	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[5,11,41,47]`
6	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[6,12,42,48]`
7	$\left[\frac{1}{6}, \frac{1}{3}, \frac{1}{3}\right]$	`[13,19,49,55]`
8	$\left[\frac{2}{3}, \frac{5}{6}, \frac{1}{3}\right]$	`[14,20,50,56]`
9	$\left[\frac{1}{6}, \frac{5}{6}, \frac{1}{3}\right]$	`[15,21,51,57]`
10	$\left[\frac{1}{6}, \frac{1}{3}, \frac{5}{6}\right]$	`[16,22,52,58]`
11	$\left[\frac{2}{3}, \frac{5}{6}, \frac{5}{6}\right]$	`[17,23,53,59]`
12	$\left[\frac{1}{6}, \frac{5}{6}, \frac{5}{6}\right]$	`[18,24,54,60]`
13	$\left[\frac{5}{6}, \frac{2}{3}, \frac{2}{3}\right]$	`[25,31,61,67]`
14	$\left[\frac{1}{3}, \frac{1}{6}, \frac{2}{3}\right]$	`[26,32,62,68]`
15	$\left[\frac{5}{6}, \frac{1}{6}, \frac{2}{3}\right]$	`[27,33,63,69]`
16	$\left[\frac{5}{6}, \frac{2}{3}, \frac{1}{6}\right]$	`[28,34,64,70]`
17	$\left[\frac{1}{3}, \frac{1}{6}, \frac{1}{6}\right]$	`[29,35,65,71]`
18	$\left[\frac{5}{6}, \frac{1}{6}, \frac{1}{6}\right]$	`[30,36,66,72]`

Table 5: Wyckoff site: `18e`, site symmetry: `.2.1'`

No.	position	mapping
1	$\left[x, 0, \frac{1}{4}\right]$	`[1,4,37,40]`
2	$\left[0, x, \frac{1}{4}\right]$	`[2,5,38,41]`
3	$\left[-x, -x, \frac{1}{4}\right]$	`[3,6,39,42]`
4	$\left[-x, 0, \frac{3}{4}\right]$	`[7,10,43,46]`
5	$\left[0, -x, \frac{3}{4}\right]$	`[8,11,44,47]`
6	$\left[x, x, \frac{3}{4}\right]$	`[9,12,45,48]`
7	$\left[x+\frac{2}{3}, \frac{1}{3}, \frac{7}{12}\right]$	`[13,16,49,52]`
8	$\left[\frac{2}{3}, x+\frac{1}{3}, \frac{7}{12}\right]$	`[14,17,50,53]`
9	$\left[\frac{2}{3}-x, \frac{1}{3}-x, \frac{7}{12}\right]$	`[15,18,51,54]`
10	$\left[\frac{2}{3}-x, \frac{1}{3}, \frac{1}{12}\right]$	`[19,22,55,58]`
11	$\left[\frac{2}{3}, \frac{1}{3}-x, \frac{1}{12}\right]$	`[20,23,56,59]`
12	$\left[x+\frac{2}{3}, x+\frac{1}{3}, \frac{1}{12}\right]$	`[21,24,57,60]`
13	$\left[x+\frac{1}{3}, \frac{2}{3}, \frac{11}{12}\right]$	`[25,28,61,64]`
14	$\left[\frac{1}{3}, x+\frac{2}{3}, \frac{11}{12}\right]$	`[26,29,62,65]`
15	$\left[\frac{1}{3}-x, \frac{2}{3}-x, \frac{11}{12}\right]$	`[27,30,63,66]`
16	$\left[\frac{1}{3}-x, \frac{2}{3}, \frac{5}{12}\right]$	`[31,34,67,70]`
17	$\left[\frac{1}{3}, \frac{2}{3}-x, \frac{5}{12}\right]$	`[32,35,68,71]`
18	$\left[x+\frac{1}{3}, x+\frac{2}{3}, \frac{5}{12}\right]$	`[33,36,69,72]`

Table 6: Wyckoff site: `36f`, site symmetry: `11'`

No.	position	mapping
1	$[x,\ y,\ z]$	`[1,37]`
2	$[-y,\ x-y,\ z]$	`[2,38]`
3	$[-x+y,\ -x,\ z]$	`[3,39]`
4	$\left[x-y,\ -y,\ \frac{1}{2}-z\right]$	`[4,40]`
5	$\left[y,\ x,\ \frac{1}{2}-z\right]$	`[5,41]`
6	$\left[-x,\ -x+y,\ \frac{1}{2}-z\right]$	`[6,42]`
7	$[-x,\ -y,\ -z]$	`[7,43]`
8	$[y,\ -x+y,\ -z]$	`[8,44]`
9	$[x-y,\ x,\ -z]$	`[9,45]`
10	$\left[-x+y,\ y,\ z+\frac{1}{2}\right]$	`[10,46]`
11	$\left[-y,\ -x,\ z+\frac{1}{2}\right]$	`[11,47]`
12	$\left[x,\ x-y,\ z+\frac{1}{2}\right]$	`[12,48]`
13	$\left[x+\frac{2}{3},\ y+\frac{1}{3},\ z+\frac{1}{3}\right]$	`[13,49]`
14	$\left[\frac{2}{3}-y,\ x-y+\frac{1}{3},\ z+\frac{1}{3}\right]$	`[14,50]`
15	$\left[-x+y+\frac{2}{3},\ \frac{1}{3}-x,\ z+\frac{1}{3}\right]$	`[15,51]`
16	$\left[x-y+\frac{2}{3},\ \frac{1}{3}-y,\ \frac{5}{6}-z\right]$	`[16,52]`
17	$\left[y+\frac{2}{3},\ x+\frac{1}{3},\ \frac{5}{6}-z\right]$	`[17,53]`
18	$\left[\frac{2}{3}-x,\ -x+y+\frac{1}{3},\ \frac{5}{6}-z\right]$	`[18,54]`
19	$\left[\frac{2}{3}-x,\ \frac{1}{3}-y,\ \frac{1}{3}-z\right]$	`[19,55]`
20	$\left[y+\frac{2}{3},\ -x+y+\frac{1}{3},\ \frac{1}{3}-z\right]$	`[20,56]`
21	$\left[x-y+\frac{2}{3},\ x+\frac{1}{3},\ \frac{1}{3}-z\right]$	`[21,57]`
22	$\left[-x+y+\frac{2}{3},\ y+\frac{1}{3},\ z+\frac{5}{6}\right]$	`[22,58]`
23	$\left[\frac{2}{3}-y,\ \frac{1}{3}-x,\ z+\frac{5}{6}\right]$	`[23,59]`
24	$\left[x+\frac{2}{3},\ x-y+\frac{1}{3},\ z+\frac{5}{6}\right]$	`[24,60]`
25	$\left[x+\frac{1}{3},\ y+\frac{2}{3},\ z+\frac{2}{3}\right]$	`[25,61]`
26	$\left[\frac{1}{3}-y,\ x-y+\frac{2}{3},\ z+\frac{2}{3}\right]$	`[26,62]`
27	$\left[-x+y+\frac{1}{3},\ \frac{2}{3}-x,\ z+\frac{2}{3}\right]$	`[27,63]`
28	$\left[x-y+\frac{1}{3},\ \frac{2}{3}-y,\ \frac{1}{6}-z\right]$	`[28,64]`
29	$\left[y+\frac{1}{3},\ x+\frac{2}{3},\ \frac{1}{6}-z\right]$	`[29,65]`
30	$\left[\frac{1}{3}-x,\ -x+y+\frac{2}{3},\ \frac{1}{6}-z\right]$	`[30,66]`
31	$\left[\frac{1}{3}-x,\ \frac{2}{3}-y,\ \frac{2}{3}-z\right]$	`[31,67]`
32	$\left[y+\frac{1}{3},\ -x+y+\frac{2}{3},\ \frac{2}{3}-z\right]$	`[32,68]`
33	$\left[x-y+\frac{1}{3},\ x+\frac{2}{3},\ \frac{2}{3}-z\right]$	`[33,69]`
34	$\left[-x+y+\frac{1}{3},\ y+\frac{2}{3},\ z+\frac{1}{6}\right]$	`[34,70]`
35	$\left[\frac{1}{3}-y,\ \frac{2}{3}-x,\ z+\frac{1}{6}\right]$	`[35,71]`
36	$\left[x+\frac{1}{3},\ x-y+\frac{2}{3},\ z+\frac{1}{6}\right]$	`[36,72]`