MSG No. 166.98 $R\bar{3}m1'$ [Type II, trigonal]

Table 1: Wyckoff site: `3a`, site symmetry: `-3m.1'`

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

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

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

Table 3: Wyckoff site: `6c`, site symmetry: `3m.1'`

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

Table 4: Wyckoff site: `9d`, site symmetry: `.2/m.1'`

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

Table 5: Wyckoff site: `9e`, site symmetry: `.2/m.1'`

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

Table 6: Wyckoff site: `18f`, site symmetry: `.2.1'`

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

Table 7: Wyckoff site: `18g`, site symmetry: `.2.1'`

No.	position	mapping
1	$\left[x, 0, \frac{1}{2}\right]$	`[1,4,37,40]`
2	$\left[0, x, \frac{1}{2}\right]$	`[2,5,38,41]`
3	$\left[-x, -x, \frac{1}{2}\right]$	`[3,6,39,42]`
4	$\left[-x, 0, \frac{1}{2}\right]$	`[7,10,43,46]`
5	$\left[0, -x, \frac{1}{2}\right]$	`[8,11,44,47]`
6	$\left[x, x, \frac{1}{2}\right]$	`[9,12,45,48]`

continued ...

Table 7

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

Table 8: Wyckoff site: 18h, site symmetry: .m.1'

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

Table 9: Wyckoff site: 36i, 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	$[x-y,\ -y,\ -z]$	[4,40]

continued ...

Table 9

No.	position	mapping
5	$[y,\, x,\, -z]$	[5,41]
6	$[-x,\, -x+y,\, -z]$	[6,42]
7	$[-x,\, -y,\, -z]$	[7,43]
8	$[y,\, -x+y,\, -z]$	[8,44]
9	$[x-y,\, x,\, -z]$	[9,45]
10	$[-x+y,\, y,\, z]$	[10,46]
11	$[-y,\, -x,\, z]$	[11,47]
12	$[x,\, x-y,\, z]$	[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	$\left[x-y+\frac{2}{3},\, \frac{1}{3}-y,\, \frac{1}{3}-z\right]$	[16,52]
17	$\left[y+\frac{2}{3},\, x+\frac{1}{3},\, \frac{1}{3}-z\right]$	[17,53]
18	$\left[\frac{2}{3}-x,\, -x+y+\frac{1}{3},\, \frac{1}{3}-z\right]$	[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	$\left[-x+y+\frac{2}{3},\, y+\frac{1}{3},\, z+\frac{1}{3}\right]$	[22,58]
23	$\left[\frac{2}{3}-y,\, \frac{1}{3}-x,\, z+\frac{1}{3}\right]$	[23,59]
24	$\left[x+\frac{2}{3},\, x-y+\frac{1}{3},\, z+\frac{1}{3}\right]$	[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	$\left[x-y+\frac{1}{3},\, \frac{2}{3}-y,\, \frac{2}{3}-z\right]$	[28,64]
29	$\left[y+\frac{1}{3},\, x+\frac{2}{3},\, \frac{2}{3}-z\right]$	[29,65]
30	$\left[\frac{1}{3}-x,\, -x+y+\frac{2}{3},\, \frac{2}{3}-z\right]$	[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	$\left[-x+y+\frac{1}{3},\, y+\frac{2}{3},\, z+\frac{2}{3}\right]$	[34,70]
35	$\left[\frac{1}{3}-y,\, \frac{2}{3}-x,\, z+\frac{2}{3}\right]$	[35,71]
36	$\left[x+\frac{1}{3},\, x-y+\frac{2}{3},\, z+\frac{2}{3}\right]$	[36,72]