MSG No. 166.101 $R\bar{3}m'$ [Type III, trigonal]

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

No.	position	mapping
1	$[0, 0, 0]$	`[1,2,3,4,5,6,7,8,9,10,11,12]`
2	$\left[\frac{2}{3}, \frac{1}{3}, \frac{1}{3}\right]$	`[13,14,15,16,17,18,19,20,21,22,23,24]`
3	$\left[\frac{1}{3}, \frac{2}{3}, \frac{2}{3}\right]$	`[25,26,27,28,29,30,31,32,33,34,35,36]`

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

No.	position	mapping
1	$\left[0, 0, \frac{1}{2}\right]$	`[1,2,3,4,5,6,7,8,9,10,11,12]`
2	$\left[\frac{2}{3}, \frac{1}{3}, \frac{5}{6}\right]$	`[13,14,15,16,17,18,19,20,21,22,23,24]`
3	$\left[\frac{1}{3}, \frac{2}{3}, \frac{1}{6}\right]$	`[25,26,27,28,29,30,31,32,33,34,35,36]`

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

No.	position	mapping
1	$[0, 0, z]$	`[1,2,3,10,11,12]`
2	$[0, 0, -z]$	`[4,5,6,7,8,9]`
3	$\left[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{3}\right]$	`[13,14,15,22,23,24]`
4	$\left[\frac{2}{3}, \frac{1}{3}, \frac{1}{3} - z\right]$	`[16,17,18,19,20,21]`
5	$\left[\frac{1}{3}, \frac{2}{3}, z + \frac{2}{3}\right]$	`[25,26,27,34,35,36]`
6	$\left[\frac{1}{3}, \frac{2}{3}, \frac{2}{3} - z\right]$	`[28,29,30,31,32,33]`

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

No.	position	mapping
1	$\left[\frac{1}{2}, 0, \frac{1}{2}\right]$	`[1,4,7,10]`
2	$\left[0, \frac{1}{2}, \frac{1}{2}\right]$	`[2,5,8,11]`
3	$\left[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right]$	`[3,6,9,12]`
4	$\left[\frac{1}{6}, \frac{1}{3}, \frac{5}{6}\right]$	`[13,16,19,22]`
5	$\left[\frac{2}{3}, \frac{5}{6}, \frac{5}{6}\right]$	`[14,17,20,23]`
6	$\left[\frac{1}{6}, \frac{5}{6}, \frac{5}{6}\right]$	`[15,18,21,24]`
7	$\left[\frac{5}{6}, \frac{2}{3}, \frac{1}{6}\right]$	`[25,28,31,34]`
8	$\left[\frac{1}{3}, \frac{1}{6}, \frac{1}{6}\right]$	`[26,29,32,35]`
9	$\left[\frac{5}{6}, \frac{1}{6}, \frac{1}{6}\right]$	`[27,30,33,36]`

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

No.	position	mapping
1	$\left[\frac{1}{2}, 0, 0\right]$	`[1,4,7,10]`
2	$\left[0, \frac{1}{2}, 0\right]$	`[2,5,8,11]`
3	$\left[\frac{1}{2}, \frac{1}{2}, 0\right]$	`[3,6,9,12]`
4	$\left[\frac{1}{6}, \frac{1}{3}, \frac{1}{3}\right]$	`[13,16,19,22]`
5	$\left[\frac{2}{3}, \frac{5}{6}, \frac{1}{3}\right]$	`[14,17,20,23]`
6	$\left[\frac{1}{6}, \frac{5}{6}, \frac{1}{3}\right]$	`[15,18,21,24]`
7	$\left[\frac{5}{6}, \frac{2}{3}, \frac{2}{3}\right]$	`[25,28,31,34]`
8	$\left[\frac{1}{3}, \frac{1}{6}, \frac{2}{3}\right]$	`[26,29,32,35]`
9	$\left[\frac{5}{6}, \frac{1}{6}, \frac{2}{3}\right]$	`[27,30,33,36]`

Table 6: Wyckoff site: `18f`, site symmetry: `.2'`.

No.	position	mapping
1	$[x, 0, 0]$	`[1,7]`
2	$[0, x, 0]$	`[2,8]`
3	$[-x, -x, 0]$	`[3,9]`
4	$[-x, 0, 0]$	`[4,10]`
5	$[0, -x, 0]$	`[5,11]`
6	$[x, x, 0]$	`[6,12]`
7	$\left[x + \frac{2}{3}, \frac{1}{3}, \frac{1}{3}\right]$	`[13,19]`
8	$\left[\frac{2}{3}, x + \frac{1}{3}, \frac{1}{3}\right]$	`[14,20]`
9	$\left[\frac{2}{3} - x, \frac{1}{3} - x, \frac{1}{3}\right]$	`[15,21]`
10	$\left[\frac{2}{3} - x, \frac{1}{3}, \frac{1}{3}\right]$	`[16,22]`
11	$\left[\frac{2}{3}, \frac{1}{3} - x, \frac{1}{3}\right]$	`[17,23]`
12	$\left[x + \frac{2}{3}, x + \frac{1}{3}, \frac{1}{3}\right]$	`[18,24]`
13	$\left[x + \frac{1}{3}, \frac{2}{3}, \frac{2}{3}\right]$	`[25,31]`
14	$\left[\frac{1}{3}, x + \frac{2}{3}, \frac{2}{3}\right]$	`[26,32]`
15	$\left[\frac{1}{3} - x, \frac{2}{3} - x, \frac{2}{3}\right]$	`[27,33]`
16	$\left[\frac{1}{3} - x, \frac{2}{3}, \frac{2}{3}\right]$	`[28,34]`
17	$\left[\frac{1}{3}, \frac{2}{3} - x, \frac{2}{3}\right]$	`[29,35]`
18	$\left[x + \frac{1}{3}, x + \frac{2}{3}, \frac{2}{3}\right]$	`[30,36]`

Table 7: Wyckoff site: `18g`, site symmetry: `.2'`.

No.	position	mapping
1	$\left[x, 0, \frac{1}{2}\right]$	`[1,7]`
2	$\left[0, x, \frac{1}{2}\right]$	`[2,8]`
3	$\left[-x, -x, \frac{1}{2}\right]$	`[3,9]`
4	$\left[-x, 0, \frac{1}{2}\right]$	`[4,10]`
5	$\left[0, -x, \frac{1}{2}\right]$	`[5,11]`
6	$\left[x, x, \frac{1}{2}\right]$	`[6,12]`

continued ...

Table 7

No.	position	mapping
7	$\left[x+\frac{2}{3},\ \frac{1}{3},\ \frac{5}{6}\right]$	[13,19]
8	$\left[\frac{2}{3},\ x+\frac{1}{3},\ \frac{5}{6}\right]$	[14,20]
9	$\left[\frac{2}{3}-x,\ \frac{1}{3}-x,\ \frac{5}{6}\right]$	[15,21]
10	$\left[\frac{2}{3}-x,\ \frac{1}{3},\ \frac{5}{6}\right]$	[16,22]
11	$\left[\frac{2}{3},\ \frac{1}{3}-x,\ \frac{5}{6}\right]$	[17,23]
12	$\left[x+\frac{2}{3},\ x+\frac{1}{3},\ \frac{5}{6}\right]$	[18,24]
13	$\left[x+\frac{1}{3},\ \frac{2}{3},\ \frac{1}{6}\right]$	[25,31]
14	$\left[\frac{1}{3},\ x+\frac{2}{3},\ \frac{1}{6}\right]$	[26,32]
15	$\left[\frac{1}{3}-x,\ \frac{2}{3}-x,\ \frac{1}{6}\right]$	[27,33]
16	$\left[\frac{1}{3}-x,\ \frac{2}{3},\ \frac{1}{6}\right]$	[28,34]
17	$\left[\frac{1}{3},\ \frac{2}{3}-x,\ \frac{1}{6}\right]$	[29,35]
18	$\left[x+\frac{1}{3},\ x+\frac{2}{3},\ \frac{1}{6}\right]$	[30,36]

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

No.	position	mapping
1	$[x,\ -x,\ z]$	[1,11]
2	$[x,\ 2x,\ z]$	[2,12]
3	$[-2x,\ -x,\ z]$	[3,10]
4	$[-x,\ x,\ -z]$	[4,8]
5	$[-x,\ -2x,\ -z]$	[5,9]
6	$[2x,\ x,\ -z]$	[6,7]
7	$\left[x+\frac{2}{3},\ \frac{1}{3}-x,\ z+\frac{1}{3}\right]$	[13,23]
8	$\left[x+\frac{2}{3},\ 2x+\frac{1}{3},\ z+\frac{1}{3}\right]$	[14,24]
9	$\left[\frac{2}{3}-2x,\ \frac{1}{3}-x,\ z+\frac{1}{3}\right]$	[15,22]
10	$\left[\frac{2}{3}-x,\ x+\frac{1}{3},\ \frac{1}{3}-z\right]$	[16,20]
11	$\left[\frac{2}{3}-x,\ \frac{1}{3}-2x,\ \frac{1}{3}-z\right]$	[17,21]
12	$\left[2x+\frac{2}{3},\ x+\frac{1}{3},\ \frac{1}{3}-z\right]$	[18,19]
13	$\left[x+\frac{1}{3},\ \frac{2}{3}-x,\ z+\frac{2}{3}\right]$	[25,35]
14	$\left[x+\frac{1}{3},\ 2x+\frac{2}{3},\ z+\frac{2}{3}\right]$	[26,36]
15	$\left[\frac{1}{3}-2x,\ \frac{2}{3}-x,\ z+\frac{2}{3}\right]$	[27,34]
16	$\left[\frac{1}{3}-x,\ x+\frac{2}{3},\ \frac{2}{3}-z\right]$	[28,32]
17	$\left[\frac{1}{3}-x,\ \frac{2}{3}-2x,\ \frac{2}{3}-z\right]$	[29,33]
18	$\left[2x+\frac{1}{3},\ x+\frac{2}{3},\ \frac{2}{3}-z\right]$	[30,31]

Table 9: Wyckoff site: 36i, site symmetry: 1

No.	position	mapping
1	$[x,\ y,\ z]$	[1]
2	$[-y,\ x-y,\ z]$	[2]
3	$[-x+y,\ -x,\ z]$	[3]
4	$[-x,\ -y,\ -z]$	[4]

continued ...

Table 9

No.	position	mapping
5	$[y,\ -x+y,\ -z]$	[5]
6	$[x-y,\ x,\ -z]$	[6]
7	$[x-y,\ -y,\ -z]$	[7]
8	$[y,\ x,\ -z]$	[8]
9	$[-x,\ -x+y,\ -z]$	[9]
10	$[-x+y,\ y,\ z]$	[10]
11	$[-y,\ -x,\ z]$	[11]
12	$[x,\ x-y,\ z]$	[12]
13	$\left[x+\frac{2}{3},\ y+\frac{1}{3},\ z+\frac{1}{3}\right]$	[13]
14	$\left[\frac{2}{3}-y,\ x-y+\frac{1}{3},\ z+\frac{1}{3}\right]$	[14]
15	$\left[-x+y+\frac{2}{3},\ \frac{1}{3}-x,\ z+\frac{1}{3}\right]$	[15]
16	$\left[\frac{2}{3}-x,\ \frac{1}{3}-y,\ \frac{1}{3}-z\right]$	[16]
17	$\left[y+\frac{2}{3},\ -x+y+\frac{1}{3},\ \frac{1}{3}-z\right]$	[17]
18	$\left[x-y+\frac{2}{3},\ x+\frac{1}{3},\ \frac{1}{3}-z\right]$	[18]
19	$\left[x-y+\frac{2}{3},\ \frac{1}{3}-y,\ \frac{1}{3}-z\right]$	[19]
20	$\left[y+\frac{2}{3},\ x+\frac{1}{3},\ \frac{1}{3}-z\right]$	[20]
21	$\left[\frac{2}{3}-x,\ -x+y+\frac{1}{3},\ \frac{1}{3}-z\right]$	[21]
22	$\left[-x+y+\frac{2}{3},\ y+\frac{1}{3},\ z+\frac{1}{3}\right]$	[22]
23	$\left[\frac{2}{3}-y,\ \frac{1}{3}-x,\ z+\frac{1}{3}\right]$	[23]
24	$\left[x+\frac{2}{3},\ x-y+\frac{1}{3},\ z+\frac{1}{3}\right]$	[24]
25	$\left[x+\frac{1}{3},\ y+\frac{2}{3},\ z+\frac{2}{3}\right]$	[25]
26	$\left[\frac{1}{3}-y,\ x-y+\frac{2}{3},\ z+\frac{2}{3}\right]$	[26]
27	$\left[-x+y+\frac{1}{3},\ \frac{2}{3}-x,\ z+\frac{2}{3}\right]$	[27]
28	$\left[\frac{1}{3}-x,\ \frac{2}{3}-y,\ \frac{2}{3}-z\right]$	[28]
29	$\left[y+\frac{1}{3},\ -x+y+\frac{2}{3},\ \frac{2}{3}-z\right]$	[29]
30	$\left[x-y+\frac{1}{3},\ x+\frac{2}{3},\ \frac{2}{3}-z\right]$	[30]
31	$\left[x-y+\frac{1}{3},\ \frac{2}{3}-y,\ \frac{2}{3}-z\right]$	[31]
32	$\left[y+\frac{1}{3},\ x+\frac{2}{3},\ \frac{2}{3}-z\right]$	[32]
33	$\left[\frac{1}{3}-x,\ -x+y+\frac{2}{3},\ \frac{2}{3}-z\right]$	[33]
34	$\left[-x+y+\frac{1}{3},\ y+\frac{2}{3},\ z+\frac{2}{3}\right]$	[34]
35	$\left[\frac{1}{3}-y,\ \frac{2}{3}-x,\ z+\frac{2}{3}\right]$	[35]
36	$\left[x+\frac{1}{3},\ x-y+\frac{2}{3},\ z+\frac{2}{3}\right]$	[36]