MSG No. 166.97 $R\bar{3}m$ [Type I, 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	$[x, 0, 0]$	`[1,4]`
2	$[0, x, 0]$	`[2,5]`
3	$[-x, -x, 0]$	`[3,6]`
4	$[-x, 0, 0]$	`[7,10]`
5	$[0, -x, 0]$	`[8,11]`
6	$[x, x, 0]$	`[9,12]`
7	$\left[x + \frac{2}{3}, \frac{1}{3}, \frac{1}{3}\right]$	`[13,16]`
8	$\left[\frac{2}{3}, x + \frac{1}{3}, \frac{1}{3}\right]$	`[14,17]`
9	$\left[\frac{2}{3} - x, \frac{1}{3} - x, \frac{1}{3}\right]$	`[15,18]`
10	$\left[\frac{2}{3} - x, \frac{1}{3}, \frac{1}{3}\right]$	`[19,22]`
11	$\left[\frac{2}{3}, \frac{1}{3} - x, \frac{1}{3}\right]$	`[20,23]`
12	$\left[x + \frac{2}{3}, x + \frac{1}{3}, \frac{1}{3}\right]$	`[21,24]`
13	$\left[x + \frac{1}{3}, \frac{2}{3}, \frac{2}{3}\right]$	`[25,28]`
14	$\left[\frac{1}{3}, x + \frac{2}{3}, \frac{2}{3}\right]$	`[26,29]`
15	$\left[\frac{1}{3} - x, \frac{2}{3} - x, \frac{2}{3}\right]$	`[27,30]`
16	$\left[\frac{1}{3} - x, \frac{2}{3}, \frac{2}{3}\right]$	`[31,34]`
17	$\left[\frac{1}{3}, \frac{2}{3} - x, \frac{2}{3}\right]$	`[32,35]`
18	$\left[x + \frac{1}{3}, x + \frac{2}{3}, \frac{2}{3}\right]$	`[33,36]`

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

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

continued ...

Table 7

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

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	$[2x,\ x,\ -z]$	[4,9]
5	$[-x,\ x,\ -z]$	[5,7]
6	$[-x,\ -2x,\ -z]$	[6,8]
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	$\left[2x+\frac{2}{3},\ x+\frac{1}{3},\ \frac{1}{3}-z\right]$	[16,21]
11	$\left[\frac{2}{3}-x,\ x+\frac{1}{3},\ \frac{1}{3}-z\right]$	[17,19]
12	$\left[\frac{2}{3}-x,\ \frac{1}{3}-2x,\ \frac{1}{3}-z\right]$	[18,20]
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	$\left[2x+\frac{1}{3},\ x+\frac{2}{3},\ \frac{2}{3}-z\right]$	[28,33]
17	$\left[\frac{1}{3}-x,\ x+\frac{2}{3},\ \frac{2}{3}-z\right]$	[29,31]
18	$\left[\frac{1}{3}-x,\ \frac{2}{3}-2x,\ \frac{2}{3}-z\right]$	[30,32]

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	$[x-y,\ -y,\ -z]$	[4]

continued ...

Table 9

No.	position	mapping
5	$[y,\, x,\, -z]$	[5]
6	$[-x,\, -x+y,\, -z]$	[6]
7	$[-x,\, -y,\, -z]$	[7]
8	$[y,\, -x+y,\, -z]$	[8]
9	$[x-y,\, x,\, -z]$	[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	$\left[x-y+\frac{2}{3},\, \frac{1}{3}-y,\, \frac{1}{3}-z\right]$	[16]
17	$\left[y+\frac{2}{3},\, x+\frac{1}{3},\, \frac{1}{3}-z\right]$	[17]
18	$\left[\frac{2}{3}-x,\, -x+y+\frac{1}{3},\, \frac{1}{3}-z\right]$	[18]
19	$\left[\frac{2}{3}-x,\, \frac{1}{3}-y,\, \frac{1}{3}-z\right]$	[19]
20	$\left[y+\frac{2}{3},\, -x+y+\frac{1}{3},\, \frac{1}{3}-z\right]$	[20]
21	$\left[x-y+\frac{2}{3},\, x+\frac{1}{3},\, \frac{1}{3}-z\right]$	[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	$\left[x-y+\frac{1}{3},\, \frac{2}{3}-y,\, \frac{2}{3}-z\right]$	[28]
29	$\left[y+\frac{1}{3},\, x+\frac{2}{3},\, \frac{2}{3}-z\right]$	[29]
30	$\left[\frac{1}{3}-x,\, -x+y+\frac{2}{3},\, \frac{2}{3}-z\right]$	[30]
31	$\left[\frac{1}{3}-x,\, \frac{2}{3}-y,\, \frac{2}{3}-z\right]$	[31]
32	$\left[y+\frac{1}{3},\, -x+y+\frac{2}{3},\, \frac{2}{3}-z\right]$	[32]
33	$\left[x-y+\frac{1}{3},\, x+\frac{2}{3},\, \frac{2}{3}-z\right]$	[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]