MSG No. 166.100 $R\bar{3}'m'$ [Type III, trigonal]

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

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: -3'm'.

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]

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]