MSG No. 167.103 $R\bar{3}c$ [Type I, trigonal]

Table 1: Wyckoff site: 6a, site symmetry: 32.

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

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

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

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

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

Table 4: Wyckoff site: `18d`, site symmetry: `-1`

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

Table 5: Wyckoff site: `18e`, site symmetry: `.2.`

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

Table 6: Wyckoff site: `36f`, site symmetry: `1`

No.	position	mapping
1	$[x,\, y,\, z]$	[1]
2	$[-y,\, x-y,\, z]$	[2]
3	$[-x+y,\, -x,\, z]$	[3]
4	$\left[x-y,\, -y,\, \frac{1}{2}-z\right]$	[4]
5	$\left[y,\, x,\, \frac{1}{2}-z\right]$	[5]
6	$\left[-x,\, -x+y,\, \frac{1}{2}-z\right]$	[6]
7	$[-x,\, -y,\, -z]$	[7]
8	$[y,\, -x+y,\, -z]$	[8]
9	$[x-y,\, x,\, -z]$	[9]
10	$\left[-x+y,\, y,\, z+\frac{1}{2}\right]$	[10]
11	$\left[-y,\, -x,\, z+\frac{1}{2}\right]$	[11]
12	$\left[x,\, x-y,\, z+\frac{1}{2}\right]$	[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	$\left[x-y+\frac{2}{3},\, \frac{1}{3}-y,\, \frac{5}{6}-z\right]$	[16]
17	$\left[y+\frac{2}{3},\, x+\frac{1}{3},\, \frac{5}{6}-z\right]$	[17]
18	$\left[\frac{2}{3}-x,\, -x+y+\frac{1}{3},\, \frac{5}{6}-z\right]$	[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	$\left[-x+y+\frac{2}{3},\, y+\frac{1}{3},\, z+\frac{5}{6}\right]$	[22]
23	$\left[\frac{2}{3}-y,\, \frac{1}{3}-x,\, z+\frac{5}{6}\right]$	[23]
24	$\left[x+\frac{2}{3},\, x-y+\frac{1}{3},\, z+\frac{5}{6}\right]$	[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	$\left[x-y+\frac{1}{3},\, \frac{2}{3}-y,\, \frac{1}{6}-z\right]$	[28]
29	$\left[y+\frac{1}{3},\, x+\frac{2}{3},\, \frac{1}{6}-z\right]$	[29]
30	$\left[\frac{1}{3}-x,\, -x+y+\frac{2}{3},\, \frac{1}{6}-z\right]$	[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	$\left[-x+y+\frac{1}{3},\, y+\frac{2}{3},\, z+\frac{1}{6}\right]$	[34]
35	$\left[\frac{1}{3}-y,\, \frac{2}{3}-x,\, z+\frac{1}{6}\right]$	[35]
36	$\left[x+\frac{1}{3},\, x-y+\frac{2}{3},\, z+\frac{1}{6}\right]$	[36]