

MSG No. 148.19 $R\bar{3}'$ [Type III, trigonal]

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

No.	position	mapping
1	[0, 0, 0]	[1,2,3,4,5,6]
2	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{3}]$	[7,8,9,10,11,12]
3	$[\frac{1}{3}, \frac{2}{3}, \frac{2}{3}]$	[13,14,15,16,17,18]

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

No.	position	mapping
1	$[0, 0, \frac{1}{2}]$	[1,2,3,4,5,6]
2	$[\frac{2}{3}, \frac{1}{3}, \frac{5}{6}]$	[7,8,9,10,11,12]
3	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{6}]$	[13,14,15,16,17,18]

Table 3: Wyckoff site: 6c, site symmetry: 3..

No.	position	mapping
1	$[0, 0, z]$	[1,2,3]
2	$[0, 0, -z]$	[4,5,6]
3	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{3}]$	[7,8,9]
4	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{3} - z]$	[10,11,12]
5	$[\frac{1}{3}, \frac{2}{3}, z + \frac{2}{3}]$	[13,14,15]
6	$[\frac{1}{3}, \frac{2}{3}, \frac{2}{3} - z]$	[16,17,18]

Table 4: Wyckoff site: 9d, site symmetry: -1'

No.	position	mapping
1	$[\frac{1}{2}, 0, \frac{1}{2}]$	[1,4]
2	$[0, \frac{1}{2}, \frac{1}{2}]$	[2,5]
3	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2}]$	[3,6]
4	$[\frac{1}{6}, \frac{1}{3}, \frac{5}{6}]$	[7,10]
5	$[\frac{2}{3}, \frac{5}{6}, \frac{5}{6}]$	[8,11]
6	$[\frac{1}{6}, \frac{5}{6}, \frac{5}{6}]$	[9,12]
7	$[\frac{5}{6}, \frac{2}{3}, \frac{1}{6}]$	[13,16]
8	$[\frac{1}{3}, \frac{1}{6}, \frac{1}{6}]$	[14,17]
9	$[\frac{5}{6}, \frac{1}{6}, \frac{1}{6}]$	[15,18]

Table 5: Wyckoff site: 9e, site symmetry: -1'

No.	position	mapping
1	$[\frac{1}{2}, 0, 0]$	[1,4]
2	$[0, \frac{1}{2}, 0]$	[2,5]
3	$[\frac{1}{2}, \frac{1}{2}, 0]$	[3,6]
4	$[\frac{1}{6}, \frac{1}{3}, \frac{1}{3}]$	[7,10]
5	$[\frac{2}{3}, \frac{5}{6}, \frac{1}{3}]$	[8,11]
6	$[\frac{1}{6}, \frac{5}{6}, \frac{1}{3}]$	[9,12]
7	$[\frac{5}{6}, \frac{2}{3}, \frac{2}{3}]$	[13,16]
8	$[\frac{1}{3}, \frac{1}{6}, \frac{2}{3}]$	[14,17]
9	$[\frac{5}{6}, \frac{1}{6}, \frac{2}{3}]$	[15,18]

Table 6: Wyckoff site: 18f, 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]
5	$[y, -x + y, -z]$	[5]
6	$[x - y, x, -z]$	[6]
7	$[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$	[7]
8	$[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{1}{3}]$	[8]
9	$[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{1}{3}]$	[9]
10	$[\frac{2}{3} - x, \frac{1}{3} - y, \frac{1}{3} - z]$	[10]
11	$[y + \frac{2}{3}, -x + y + \frac{1}{3}, \frac{1}{3} - z]$	[11]
12	$[x - y + \frac{2}{3}, x + \frac{1}{3}, \frac{1}{3} - z]$	[12]
13	$[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$	[13]
14	$[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{2}{3}]$	[14]
15	$[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{2}{3}]$	[15]
16	$[\frac{1}{3} - x, \frac{2}{3} - y, \frac{2}{3} - z]$	[16]
17	$[y + \frac{1}{3}, -x + y + \frac{2}{3}, \frac{2}{3} - z]$	[17]
18	$[x - y + \frac{1}{3}, x + \frac{2}{3}, \frac{2}{3} - z]$	[18]