

MSG No. 160.67 $R\bar{3}m'$ [Type III, trigonal]

Table 1: Wyckoff site: **3a**, site symmetry: $\bar{3}m'$.

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

Table 2: Wyckoff site: **9b**, site symmetry: $\bar{6}m'$.

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

Table 3: Wyckoff site: **18c**, site symmetry: $\bar{1}$

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x - y, z]$	$[2]$
3	$[-x + y, -x, z]$	$[3]$
4	$[-x + y, y, z]$	$[4]$
5	$[-y, -x, z]$	$[5]$
6	$[x, x - y, z]$	$[6]$
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	$[-x + y + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$	$[10]$
11	$[\frac{2}{3} - y, \frac{1}{3} - x, z + \frac{1}{3}]$	$[11]$
12	$[x + \frac{2}{3}, x - y + \frac{1}{3}, z + \frac{1}{3}]$	$[12]$
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	$[-x + y + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$	$[16]$
17	$[\frac{1}{3} - y, \frac{2}{3} - x, z + \frac{2}{3}]$	$[17]$
18	$[x + \frac{1}{3}, x - y + \frac{2}{3}, z + \frac{2}{3}]$	$[18]$