

MSG No. 160.65 *R*3*m* [Type I, trigonal]

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

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: .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: 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]