

Table 1: Wyckoff site: **6a**, site symmetry: $3..$

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

 Table 2: Wyckoff site: **18b**, site symmetry: 1

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