

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	$[x + \frac{1}{3}, x - y + \frac{2}{3}, z + \frac{1}{6}]$	$[18]$