

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 19, 20, 21]$
2	$[0, 0, z + \frac{1}{2}]$	$[4, 5, 6, 22, 23, 24]$
3	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{3}]$	$[7, 8, 9, 25, 26, 27]$
4	$[\frac{2}{3}, \frac{1}{3}, z + \frac{5}{6}]$	$[10, 11, 12, 28, 29, 30]$
5	$[\frac{1}{3}, \frac{2}{3}, z + \frac{2}{3}]$	$[13, 14, 15, 31, 32, 33]$
6	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{6}]$	$[16, 17, 18, 34, 35, 36]$

 Table 2: Wyckoff site: 18b, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	$[1, 19]$
2	$[-y, x - y, z]$	$[2, 20]$
3	$[-x + y, -x, z]$	$[3, 21]$
4	$[-x + y, y, z + \frac{1}{2}]$	$[4, 22]$
5	$[-y, -x, z + \frac{1}{2}]$	$[5, 23]$
6	$[x, x - y, z + \frac{1}{2}]$	$[6, 24]$
7	$[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$	$[7, 25]$
8	$[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{1}{3}]$	$[8, 26]$
9	$[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{1}{3}]$	$[9, 27]$
10	$[-x + y + \frac{2}{3}, y + \frac{1}{3}, z + \frac{5}{6}]$	$[10, 28]$
11	$[\frac{2}{3} - y, \frac{1}{3} - x, z + \frac{5}{6}]$	$[11, 29]$
12	$[x + \frac{2}{3}, x - y + \frac{1}{3}, z + \frac{5}{6}]$	$[12, 30]$
13	$[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$	$[13, 31]$
14	$[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{2}{3}]$	$[14, 32]$
15	$[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{2}{3}]$	$[15, 33]$
16	$[-x + y + \frac{1}{3}, y + \frac{2}{3}, z + \frac{1}{6}]$	$[16, 34]$
17	$[\frac{1}{3} - y, \frac{2}{3} - x, z + \frac{1}{6}]$	$[17, 35]$
18	$[x + \frac{1}{3}, x - y + \frac{2}{3}, z + \frac{1}{6}]$	$[18, 36]$