

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3]$
2	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{3}]$	$[4, 5, 6]$
3	$[\frac{1}{3}, \frac{2}{3}, z + \frac{2}{3}]$	$[7, 8, 9]$

Table 2: Wyckoff site:  $9b$ , site symmetry:  $1$ 

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x - y, z]$	$[2]$
3	$[-x + y, -x, z]$	$[3]$
4	$[x + \frac{2}{3}, y + \frac{1}{3}, z + \frac{1}{3}]$	$[4]$
5	$[\frac{2}{3} - y, x - y + \frac{1}{3}, z + \frac{1}{3}]$	$[5]$
6	$[-x + y + \frac{2}{3}, \frac{1}{3} - x, z + \frac{1}{3}]$	$[6]$
7	$[x + \frac{1}{3}, y + \frac{2}{3}, z + \frac{2}{3}]$	$[7]$
8	$[\frac{1}{3} - y, x - y + \frac{2}{3}, z + \frac{2}{3}]$	$[8]$
9	$[-x + y + \frac{1}{3}, \frac{2}{3} - x, z + \frac{2}{3}]$	$[9]$