

Table 1: Wyckoff site: 3a, site symmetry:  $2'..$

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

Table 2: Wyckoff site: 3b, site symmetry:  $2'..$

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

Table 3: Wyckoff site: 6c, site symmetry: 1

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