

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

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

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

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

Table 3: Wyckoff site: 6c, site symmetry: $11'$

No.	position	mapping
1	$[x, y, z]$	$[1, 7]$
2	$[x - y, x, z + \frac{2}{3}]$	$[2, 8]$
3	$[-y, x - y, z + \frac{1}{3}]$	$[3, 9]$
4	$[-x, -y, z]$	$[4, 10]$
5	$[-x + y, -x, z + \frac{2}{3}]$	$[5, 11]$
6	$[y, -x + y, z + \frac{1}{3}]$	$[6, 12]$