

Table 1: Wyckoff site: 6a, site symmetry: 2..

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

Table 2: Wyckoff site: 6b, site symmetry: 2..

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

Table 3: Wyckoff site: 12c, site symmetry: 1

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