

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

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

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

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

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

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