

Table 1: Wyckoff site: 6a, site symmetry:  $\dots 2$

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

Table 2: Wyckoff site: 6b, site symmetry:  $\dots 2'$

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