

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

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

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

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

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	$[x - y, -y, \frac{2}{3} - z]$	[4]
5	$[y, x, -z]$	[5]
6	$[-x, -x + y, \frac{1}{3} - z]$	[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	$[x - y, -y, \frac{1}{6} - z]$	[10]
11	$[y, x, \frac{1}{2} - z]$	[11]
12	$[-x, -x + y, \frac{5}{6} - z]$	[12]