

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

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

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

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

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

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