

Table 1: Wyckoff site: **3a**, site symmetry: $\bar{3}21'$

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

Table 2: Wyckoff site: **3b**, site symmetry: $\bar{3}21'$

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

Table 3: Wyckoff site: **6c**, site symmetry: $11'$

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