

Table 1: Wyckoff site: 2a, site symmetry:  $3..1'$

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

Table 2: Wyckoff site: 2b, site symmetry:  $3..1'$

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

Table 3: Wyckoff site: 2c, site symmetry:  $3..1'$

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

Table 4: Wyckoff site: 6d, site symmetry:  $11'$

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