

Table 1: Wyckoff site: 1a, site symmetry:  $6..1'$

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

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

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

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

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

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

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