

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3]$
2	$[0, 0, z + \frac{1}{2}]$	$[4, 5, 6]$

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

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	$[1, 2, 3]$
2	$[\frac{1}{3}, \frac{2}{3}, z + \frac{1}{2}]$	$[4, 5, 6]$

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

No.	position	mapping
1	$[\frac{2}{3}, \frac{1}{3}, z]$	$[1, 2, 3]$
2	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	$[4, 5, 6]$

Table 4: Wyckoff site: 6d, site symmetry:  $1$

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-y, x - y, z]$	$[2]$
3	$[-x + y, -x, z]$	$[3]$
4	$[-x + y, y, z + \frac{1}{2}]$	$[4]$
5	$[-y, -x, z + \frac{1}{2}]$	$[5]$
6	$[x, x - y, z + \frac{1}{2}]$	$[6]$