

Table 1: Wyckoff site: **1a**, site symmetry:  $3m$ .

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

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

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

Table 3: Wyckoff site: **6c**, site symmetry:  $1$

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