

Table 1: Wyckoff site: 1o, site symmetry:  $-62'm'$ 

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

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

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

Table 3: Wyckoff site: 3b, site symmetry:  $m2'm$ 

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

Table 4: Wyckoff site: 6c, site symmetry:  $.m$ 

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

Table 5: Wyckoff site: 6d, site symmetry:  $m.$ 

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

Table 6: Wyckoff site:  $12e$ , site symmetry:  $1$ 

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