

Table 1: Wyckoff site:  $1o$ , site symmetry:  $-6m'2'$

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:  $3m'$ .

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

Table 3: Wyckoff site:  $3b$ , site symmetry:  $mm2$

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

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

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

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]