

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

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: $m'm2$

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

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 , $-x$, $-z$]	[6,8]
5	[x , $2x$, $-z$]	[4,9]
6	[$-2x$, $-x$, $-z$]	[5,7]

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

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

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	$[x, y, -z]$	[8]
5	$[-y, x - y, -z]$	[9]
6	$[-x + y, -x, -z]$	[7]
7	$[-y, -x, z]$	[11]
8	$[-x + y, y, z]$	[10]
9	$[x, x - y, z]$	[12]
10	$[-y, -x, -z]$	[6]
11	$[-x + y, y, -z]$	[5]
12	$[x, x - y, -z]$	[4]