

Table 1: Wyckoff site: $1o$, site symmetry: $-3'm1$

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]	[1,2,3,4,5,6]
2	[0, 0, $-z$]	[7,8,9,10,11,12]

 Table 3: Wyckoff site: $6b$, site symmetry: $.2'$.

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

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

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

 Table 5: Wyckoff site: $12d$, site symmetry: 1

No.	position	mapping
1	[x , y , z]	[1]
2	[$-y$, $x - y$, z]	[2]
3	[$-x + y$, $-x$, z]	[3]

continued ...

Table 5

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