

Table 1: Wyckoff site: 1o, site symmetry: $\bar{3}m$.

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: $3m$.

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: 6b, site symmetry: $.2$.

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

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

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

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