

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

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: $m'2'm$

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

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, $-z$]	[4, 11]
5	[0, x , $-z$]	[5, 12]
6	[$-x$, $-x$, $-z$]	[6, 10]

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

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

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