

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

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

Table 3: Wyckoff site: $3b$, site symmetry: $m'2m$

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

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

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

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]