

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]