

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

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]$

Table 2: Wyckoff site: $2a$, site symmetry: $3m$.

No.	position	mapping
1	$[0, 0, z]$	$[1, 2, 3, 10, 11, 12, 13, 14, 15, 22, 23, 24]$
2	$[0, 0, -z]$	$[4, 5, 6, 7, 8, 9, 16, 17, 18, 19, 20, 21]$

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

No.	position	mapping
1	$[x, 0, 0]$	$[1, 4, 13, 16]$
2	$[0, x, 0]$	$[2, 5, 14, 17]$
3	$[-x, -x, 0]$	$[3, 6, 15, 18]$
4	$[-x, 0, 0]$	$[7, 10, 19, 22]$
5	$[0, -x, 0]$	$[8, 11, 20, 23]$
6	$[x, x, 0]$	$[9, 12, 21, 24]$

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

No.	position	mapping
1	$[x, -x, z]$	$[1, 11, 13, 23]$
2	$[x, 2x, z]$	$[2, 12, 14, 24]$
3	$[-2x, -x, z]$	$[3, 10, 15, 22]$
4	$[-x, x, -z]$	$[5, 7, 17, 19]$
5	$[2x, x, -z]$	$[4, 9, 16, 21]$
6	$[-x, -2x, -z]$	$[6, 8, 18, 20]$

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

No.	position	mapping
1	$[x, y, z]$	$[1, 13]$
2	$[-y, x - y, z]$	$[2, 14]$
3	$[-x + y, -x, z]$	$[3, 15]$

continued ...

Table 5

No.	position	mapping
4	$[y, x, -z]$	$[5, 17]$
5	$[x - y, -y, -z]$	$[4, 16]$
6	$[-x, -x + y, -z]$	$[6, 18]$
7	$[-x, -y, -z]$	$[7, 19]$
8	$[y, -x + y, -z]$	$[8, 20]$
9	$[x - y, x, -z]$	$[9, 21]$
10	$[-y, -x, z]$	$[11, 23]$
11	$[-x + y, y, z]$	$[10, 22]$
12	$[x, x - y, z]$	$[12, 24]$