

Table 1: Wyckoff site: $1\mathbf{o}$, site symmetry: $-6'm'2$

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

Table 2: Wyckoff site: $2\mathbf{a}$, site symmetry: $3\mathbf{m}'$.

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: $3\mathbf{b}$, site symmetry: $\mathbf{m}'m2$

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

Table 4: Wyckoff site: $6\mathbf{c}$, site symmetry: $\mathbf{.m.}$

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

Table 5: Wyckoff site: $6\mathbf{d}$, site symmetry: $\mathbf{m}'..$

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]