

Table 1: Wyckoff site:  $1o$ , site symmetry:  $-31m1'$ 

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:  $3.m$ 

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	$[x, -x, 0]$	$[1, 4, 13, 16]$
2	$[x, 2x, 0]$	$[2, 6, 14, 18]$
3	$[-2x, -x, 0]$	$[3, 5, 15, 17]$
4	$[-x, x, 0]$	$[7, 10, 19, 22]$
5	$[-x, -2x, 0]$	$[8, 12, 20, 24]$
6	$[2x, x, 0]$	$[9, 11, 21, 23]$

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

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

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	$[-y, -x, -z]$	$[4, 16]$
5	$[-x + y, y, -z]$	$[5, 17]$
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	$[y, x, z]$	$[10, 22]$
11	$[x - y, -y, z]$	$[11, 23]$
12	$[-x, -x + y, z]$	$[12, 24]$