

Table 1: Wyckoff site:  $1o$ , site symmetry:  $-6m21'$ 

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:  $3b$ , site symmetry:  $mm2$ 

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

 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	$[x, -x, -z]$	$[6, 8, 18, 20]$
5	$[x, 2x, -z]$	$[4, 9, 16, 21]$
6	$[-2x, -x, -z]$	$[5, 7, 17, 19]$

 Table 5: Wyckoff site:  $6d$ , site symmetry:  $m.$ 

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

Table 6: Wyckoff site: 12e, site symmetry: 1

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