

Table 1: Wyckoff site: 1o, site symmetry:  $\bar{6}m21'$ 

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	$[x, x - y, -z]$	$[4, 16]$