

Table 1: Wyckoff site: 1o, site symmetry: $-62m1'$

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

Table 3: Wyckoff site: 3b, site symmetry: $m2m$

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

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

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

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