

Table 1: Wyckoff site: 1o, site symmetry: $-6m2$

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

Table 2: Wyckoff site: 2a, site symmetry: $3m.$

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: 3b, site symmetry: $mm2$

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: 6c, site symmetry: $.m.$

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: 6d, site symmetry: $m. .$

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]