

Table 1: Wyckoff site: 1o, site symmetry: $\bar{3}1m'$

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: $3.m'$

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: 6b, site symmetry: $. . 2$

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

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

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

Table 5: Wyckoff site: 12d, site symmetry: 1

No.	position	mapping
1	[x, y, z]	[1]
2	[-y, x - y, z]	[2]
3	[-x + y, -x, z]	[3]

continued ...

Table 5

No.	position	mapping
4	$[-y, -x, -z]$	[7]
5	$[-x + y, y, -z]$	[8]
6	$[x, x - y, -z]$	[9]
7	$[-x, -y, -z]$	[4]
8	$[y, -x + y, -z]$	[5]
9	$[x - y, x, -z]$	[6]
10	$[y, x, z]$	[10]
11	$[x - y, -y, z]$	[11]
12	$[-x, -x + y, z]$	[12]