

Table 1: Wyckoff site: 1o, site symmetry: $-31m1'$

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

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

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

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

Table 5: Wyckoff site: 12d, 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]

continued ...

Table 5

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