

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

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]	[1,2,3,7,8,9]
2	[0, 0, -z]	[4,5,6,10,11,12]

 Table 3: Wyckoff site: 3b, site symmetry: $m2'm$

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

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

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

 Table 5: Wyckoff site: 6d, site symmetry: $m..$

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

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	$[x, y, -z]$	[5]
5	$[-y, x - y, -z]$	[6]
6	$[-x + y, -x, -z]$	[4]
7	$[y, x, -z]$	[11]
8	$[x - y, -y, -z]$	[10]
9	$[-x, -x + y, -z]$	[12]
10	$[y, x, z]$	[9]
11	$[x - y, -y, z]$	[8]
12	$[-x, -x + y, z]$	[7]