

Table 1: Wyckoff site: 1o, site symmetry: 622

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: 6.

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

Table 3: Wyckoff site: 6b, site symmetry: .2.

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

Table 4: Wyckoff site: 6c, site symmetry: .2

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

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

No.	position	mapping
1	[x, y, z]	[1]
2	[-y, x - y, z]	[3]
3	[-x + y, -x, z]	[5]

continued ...

Table 5

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