

Table 1: Wyckoff site: 1o, site symmetry: 222

No.	position	mapping
1	$[0, 0, 0]$	$[1, 2, 3, 4]$

Table 2: Wyckoff site: 2a, site symmetry: 2. .

No.	position	mapping
1	$[x, 0, 0]$	$[1, 2]$
2	$[-x, 0, 0]$	$[3, 4]$

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

No.	position	mapping
1	$[0, y, 0]$	$[1, 3]$
2	$[0, -y, 0]$	$[2, 4]$

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

No.	position	mapping
1	$[0, 0, z]$	$[1, 4]$
2	$[0, 0, -z]$	$[2, 3]$

Table 5: Wyckoff site: 4d, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	$[1]$
2	$[-x, -y, z]$	$[4]$
3	$[-x, y, -z]$	$[3]$
4	$[x, -y, -z]$	$[2]$