

Table 1: Wyckoff site: 1o, site symmetry: 312'

No.	position	mapping
1	[0, 0, 0]	[1,2,3,4,5,6]

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

No.	position	mapping
1	[0, 0, z]	[1,2,3]
2	[0, 0, -z]	[4,5,6]

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

No.	position	mapping
1	[x, -x, 0]	[1,4]
2	[x, 2x, 0]	[2,6]
3	[-2x, -x, 0]	[3,5]

Table 4: Wyckoff site: 6c, site symmetry: 1

No.	position	mapping
1	[x, y, z]	[1]
2	[-y, x - y, z]	[2]
3	[-x + y, -x, z]	[3]
4	[-y, -x, -z]	[4]
5	[-x + y, y, -z]	[5]
6	[x, x - y, -z]	[6]