

Table 1: Wyckoff site: 1o, site symmetry: 321

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, 0, 0]	[1,4]
2	[0, x, 0]	[2,5]
3	[-x, -x, 0]	[3,6]

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]	[5]
5	[x - y, -y, -z]	[4]
6	[-x, -x + y, -z]	[6]