

Table 1: Wyckoff site: 1o, site symmetry: 23

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

Table 2: Wyckoff site: 4a, site symmetry: .3.

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

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

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

Table 4: Wyckoff site: 12c, 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]
5	[z, x, y]	[9]
6	[z, -x, -y]	[10]
7	[-z, -x, y]	[12]
8	[-z, x, -y]	[11]
9	[y, z, x]	[5]
10	[-y, z, -x]	[7]
11	[y, -z, -x]	[6]
12	[-y, -z, x]	[8]