

Table 1: Wyckoff site: 1o, site symmetry: 3121'

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: 3..

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

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

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

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

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