

Table 1: Wyckoff site: 1o, site symmetry: 2221'

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

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

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

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

No.	position	mapping
1	[0, y, 0]	[1,3,5,7]
2	[0, -y, 0]	[2,4,6,8]

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

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

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

No.	position	mapping
1	[x, y, z]	[1,5]
2	[-x, -y, z]	[4,8]
3	[-x, y, -z]	[3,7]
4	[x, -y, -z]	[2,6]