

Table 1: Wyckoff site: 1o, site symmetry: 422

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

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

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

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

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

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

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

Table 5: Wyckoff site: 8d, site symmetry: 1

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

continued ...

Table 5

No.	position	mapping
8	$[-y, -x, -z]$	[5]