

Table 1: Wyckoff site: 1o, site symmetry: 432

No.	position	mapping
1	[0, 0, 0]	[1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24]

Table 2: Wyckoff site: 6a, site symmetry: 4..

No.	position	mapping
1	[x, 0, 0]	[1, 2, 19, 20]
2	[-x, 0, 0]	[3, 4, 17, 18]
3	[0, x, 0]	[9, 11, 14, 16]
4	[0, -x, 0]	[10, 12, 13, 15]
5	[0, 0, x]	[5, 8, 22, 23]
6	[0, 0, -x]	[6, 7, 21, 24]

Table 3: Wyckoff site: 8b, 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]
5	[x, x, -x]	[16, 20, 24]
6	[-x, -x, -x]	[13, 17, 21]
7	[x, -x, x]	[15, 19, 23]
8	[-x, x, x]	[14, 18, 22]

Table 4: Wyckoff site: 12c, site symmetry: ..2

No.	position	mapping
1	[0, y, y]	[1, 18]
2	[0, -y, y]	[4, 19]
3	[0, y, -y]	[3, 20]
4	[0, -y, -y]	[2, 17]
5	[y, 0, y]	[9, 15]
6	[y, 0, -y]	[10, 16]
7	[-y, 0, y]	[12, 14]
8	[-y, 0, -y]	[11, 13]
9	[y, y, 0]	[5, 24]
10	[-y, y, 0]	[7, 22]

continued ...

Table 4

No.	position	mapping
11	$[y, -y, 0]$	[6, 23]
12	$[-y, -y, 0]$	[8, 21]

Table 5: Wyckoff site: 24d, 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]
13	$[y, x, -z]$	[16]
14	$[-y, -x, -z]$	[13]
15	$[y, -x, z]$	[15]
16	$[-y, x, z]$	[14]
17	$[x, z, -y]$	[20]
18	$[-x, z, y]$	[18]
19	$[-x, -z, -y]$	[17]
20	$[x, -z, y]$	[19]
21	$[z, y, -x]$	[24]
22	$[z, -y, x]$	[23]
23	$[-z, y, x]$	[22]
24	$[-z, -y, -x]$	[21]