

Table 1: Wyckoff site: 1o, site symmetry: 4321'

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, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48]

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

No.	position	mapping
1	[x, 0, 0]	[1, 2, 19, 20, 25, 26, 43, 44]
2	[-x, 0, 0]	[3, 4, 17, 18, 27, 28, 41, 42]
3	[0, x, 0]	[9, 11, 14, 16, 33, 35, 38, 40]
4	[0, -x, 0]	[10, 12, 13, 15, 34, 36, 37, 39]
5	[0, 0, x]	[5, 8, 22, 23, 29, 32, 46, 47]
6	[0, 0, -x]	[6, 7, 21, 24, 30, 31, 45, 48]

Table 3: Wyckoff site: 8b, site symmetry: .3.

No.	position	mapping
1	[x, x, x]	[1, 5, 9, 25, 29, 33]
2	[-x, -x, x]	[4, 8, 12, 28, 32, 36]
3	[-x, x, -x]	[3, 7, 11, 27, 31, 35]
4	[x, -x, -x]	[2, 6, 10, 26, 30, 34]
5	[x, x, -x]	[16, 20, 24, 40, 44, 48]
6	[-x, -x, -x]	[13, 17, 21, 37, 41, 45]
7	[x, -x, x]	[15, 19, 23, 39, 43, 47]
8	[-x, x, x]	[14, 18, 22, 38, 42, 46]

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

No.	position	mapping
1	[0, y, y]	[1, 18, 25, 42]
2	[0, -y, y]	[4, 19, 28, 43]
3	[0, y, -y]	[3, 20, 27, 44]
4	[0, -y, -y]	[2, 17, 26, 41]
5	[y, 0, y]	[9, 15, 33, 39]
6	[y, 0, -y]	[10, 16, 34, 40]
7	[-y, 0, y]	[12, 14, 36, 38]
8	[-y, 0, -y]	[11, 13, 35, 37]
9	[y, y, 0]	[5, 24, 29, 48]

*continued ...*

Table 4

No.	position	mapping
10	$[-y, y, 0]$	$[7, 22, 31, 46]$
11	$[y, -y, 0]$	$[6, 23, 30, 47]$
12	$[-y, -y, 0]$	$[8, 21, 32, 45]$

Table 5: Wyckoff site: 24d, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	$[1, 25]$
2	$[-x, -y, z]$	$[4, 28]$
3	$[-x, y, -z]$	$[3, 27]$
4	$[x, -y, -z]$	$[2, 26]$
5	$[z, x, y]$	$[9, 33]$
6	$[z, -x, -y]$	$[10, 34]$
7	$[-z, -x, y]$	$[12, 36]$
8	$[-z, x, -y]$	$[11, 35]$
9	$[y, z, x]$	$[5, 29]$
10	$[-y, z, -x]$	$[7, 31]$
11	$[y, -z, -x]$	$[6, 30]$
12	$[-y, -z, x]$	$[8, 32]$
13	$[y, x, -z]$	$[16, 40]$
14	$[-y, -x, -z]$	$[13, 37]$
15	$[y, -x, z]$	$[15, 39]$
16	$[-y, x, z]$	$[14, 38]$
17	$[x, z, -y]$	$[20, 44]$
18	$[-x, z, y]$	$[18, 42]$
19	$[-x, -z, -y]$	$[17, 41]$
20	$[x, -z, y]$	$[19, 43]$
21	$[z, y, -x]$	$[24, 48]$
22	$[z, -y, x]$	$[23, 47]$
23	$[-z, y, x]$	$[22, 46]$
24	$[-z, -y, -x]$	$[21, 45]$