

Table 1: Wyckoff site: $1\mathbf{o}$, site symmetry: $4'32'$

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: $6\mathbf{a}$, 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: $8\mathbf{b}$, 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: $12\mathbf{c}$, 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	$[-z, -y, -x]$	$[21]$