

Table 1: Wyckoff site: $1\mathbf{o}$, site symmetry: $\mathbf{m}'\bar{3}'$

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: $2\mathbf{mm}$.

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

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	$[-x, -x, -x]$	$[13, 17, 21]$
6	$[x, x, -x]$	$[16, 20, 24]$
7	$[x, -x, x]$	$[15, 19, 23]$
8	$[-x, x, x]$	$[14, 18, 22]$

Table 4: Wyckoff site: $12\mathbf{c}$, site symmetry: $\mathbf{m}'..$

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

continued ...

Table 4

No.	position	mapping
11	$[y, -z, 0]$	[6, 19]
12	$[-y, -z, 0]$	[8, 17]

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	$[-x, -y, -z]$	[13]
14	$[x, y, -z]$	[16]
15	$[x, -y, z]$	[15]
16	$[-x, y, z]$	[14]
17	$[-z, -x, -y]$	[21]
18	$[-z, x, y]$	[22]
19	$[z, x, -y]$	[24]
20	$[z, -x, y]$	[23]
21	$[-y, -z, -x]$	[17]
22	$[y, -z, x]$	[19]
23	$[-y, z, x]$	[18]
24	$[y, z, -x]$	[20]