

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

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: $6\mathbf{a}$, site symmetry: $2\mathbf{mm}$.

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

Table 3: Wyckoff site: $8\mathbf{b}$, site symmetry: $\bar{3}$.

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	$[-x, -x, -x]$	$[13, 17, 21, 37, 41, 45]$
6	$[x, x, -x]$	$[16, 20, 24, 40, 44, 48]$
7	$[x, -x, x]$	$[15, 19, 23, 39, 43, 47]$
8	$[-x, x, x]$	$[14, 18, 22, 38, 42, 46]$

Table 4: Wyckoff site: $12\mathbf{c}$, site symmetry: $\mathbf{m}\bar{3}$.

No.	position	mapping
1	$[0, y, z]$	$[1, 14, 25, 38]$
2	$[0, -y, z]$	$[4, 15, 28, 39]$
3	$[0, y, -z]$	$[3, 16, 27, 40]$
4	$[0, -y, -z]$	$[2, 13, 26, 37]$
5	$[z, 0, y]$	$[9, 23, 33, 47]$
6	$[z, 0, -y]$	$[10, 24, 34, 48]$
7	$[-z, 0, y]$	$[12, 22, 36, 46]$
8	$[-z, 0, -y]$	$[11, 21, 35, 45]$
9	$[y, z, 0]$	$[5, 20, 29, 44]$

continued ...

Table 4

No.	position	mapping
10	$[-y, z, 0]$	$[7, 18, 31, 42]$
11	$[y, -z, 0]$	$[6, 19, 30, 43]$
12	$[-y, -z, 0]$	$[8, 17, 32, 41]$

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	$[-x, -y, -z]$	$[13, 37]$
14	$[x, y, -z]$	$[16, 40]$
15	$[x, -y, z]$	$[15, 39]$
16	$[-x, y, z]$	$[14, 38]$
17	$[-z, -x, -y]$	$[21, 45]$
18	$[-z, x, y]$	$[22, 46]$
19	$[z, x, -y]$	$[24, 48]$
20	$[z, -x, y]$	$[23, 47]$
21	$[-y, -z, -x]$	$[17, 41]$
22	$[y, -z, x]$	$[19, 43]$
23	$[-y, z, x]$	$[18, 42]$
24	$[y, z, -x]$	$[20, 44]$