

Table 1: Wyckoff site: $1o$, site symmetry: $6'/m'mm'$

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: $2a$, site symmetry: $6'mm'$

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

Table 3: Wyckoff site: $6b$, site symmetry: $m'2m$

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

Table 4: Wyckoff site: $6c$, site symmetry: $m'm2$

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

Table 5: Wyckoff site: $12d$, site symmetry: $. . m$

No.	position	mapping
1	$[x, 0, z]$	$[1, 23]$
2	$[0, x, z]$	$[2, 24]$
3	$[-x, -x, z]$	$[3, 22]$

continued ...

Table 5

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

Table 6: Wyckoff site: $12e$, site symmetry: $\bar{6}m$.

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

Table 7: Wyckoff site: $12f$, site symmetry: $m\bar{3}m$.

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

Table 8: Wyckoff site: $24g$, site symmetry: 1

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