

Table 1: Wyckoff site:  $1\mathbf{o}$ , site symmetry:  $6/\bar{m}\bar{m}'m'$ 

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:  $2\mathbf{a}$ , site symmetry:  $6\bar{m}'m'$ 

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

Table 3: Wyckoff site:  $6\mathbf{b}$ , site symmetry:  $\bar{m}2'm$ 

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

Table 4: Wyckoff site:  $6\mathbf{c}$ , site symmetry:  $\bar{m}m'2$ 

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

Table 5: Wyckoff site:  $12\mathbf{d}$ , site symmetry:  $\bar{6}m$ 

No.	position	mapping
1	$[x, 0, z]$	$[1, 22]$
2	$[0, x, z]$	$[3, 24]$
3	$[-x, -x, z]$	$[5, 20]$

*continued ...*

Table 5

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

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

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

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

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

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

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