

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

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:  $m2'm$ 

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

Table 4: Wyckoff site:  $6c$ , site symmetry:  $mm2$ 

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

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	$[0, x, -z]$	$[9, 17]$
8	$[x, 0, -z]$	$[8, 16]$
9	$[-x, -x, -z]$	$[7, 18]$
10	$[0, -x, -z]$	$[6, 20]$
11	$[-x, 0, -z]$	$[5, 19]$
12	$[x, x, -z]$	$[4, 21]$

Table 6: Wyckoff site:  $12\mathbf{e}$ , 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	$[2x, x, -z]$	$[17, 20]$
8	$[-x, -2x, -z]$	$[16, 19]$
9	$[-x, x, -z]$	$[18, 21]$
10	$[-2x, -x, -z]$	$[6, 9]$
11	$[x, 2x, -z]$	$[5, 8]$
12	$[x, -x, -z]$	$[4, 7]$

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

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

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	$[y, x, -z]$	[17]
8	$[x - y, -y, -z]$	[16]
9	$[-x, -x + y, -z]$	[18]
10	$[-y, -x, -z]$	[6]
11	$[-x + y, y, -z]$	[5]
12	$[x, x - y, -z]$	[4]
13	$[-x, -y, -z]$	[19]
14	$[y, -x + y, -z]$	[20]
15	$[x - y, x, -z]$	[21]
16	$[x, y, -z]$	[8]
17	$[-y, x - y, -z]$	[9]
18	$[-x + y, -x, -z]$	[7]
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]