

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

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

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: 6b, site symmetry:  $m'2m$ 

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

 Table 4: Wyckoff site: 6c, site symmetry:  $m'm'2$ 

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: 12d, site symmetry:  $. . m$ 

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	$[0, x, -z]$	[9,18]
8	$[x, 0, -z]$	[7,16]
9	$[-x, -x, -z]$	[11,14]
10	$[0, -x, -z]$	[12,15]
11	$[-x, 0, -z]$	[10,13]
12	$[x, x, -z]$	[8,17]

Table 6: Wyckoff site: 12e, 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: 12f, site symmetry:  $m'..$ 

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

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	$[y, x, -z]$	[9]
8	$[x - y, -y, -z]$	[7]
9	$[-x, -x + y, -z]$	[11]
10	$[-y, -x, -z]$	[12]
11	$[-x + y, y, -z]$	[10]
12	$[x, x - y, -z]$	[8]
13	$[-x, -y, -z]$	[13]
14	$[y, -x + y, -z]$	[15]
15	$[x - y, x, -z]$	[17]
16	$[x, y, -z]$	[16]
17	$[-y, x - y, -z]$	[18]
18	$[-x + y, -x, -z]$	[14]
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]