

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:  $6'm'm$

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:  $m'2'm$

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:  $m'm'2$

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:  $.m'$ .

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:  $m'..$ 

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]