

Table 1: Wyckoff site: 2a, site symmetry:  $-3m'$ .

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

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

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

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

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

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

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

Table 5: Wyckoff site: 4e, site symmetry:  $3m'$ .

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

Table 6: Wyckoff site: 4f, site symmetry:  $3m'$ .

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

Table 7: Wyckoff site: 6g, site symmetry:  $.2'/m'$ .

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

Table 8: Wyckoff site: 6h, site symmetry:  $mm'2'$ .

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

Table 9: Wyckoff site: 12i, site symmetry:  $.2'$ .

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

*continued ...*

Table 9

No.	position	mapping
12	$[0, x, \frac{1}{2}]$	[12,24]

Table 10: Wyckoff site: 12j, site symmetry:  $m..$ 

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

Table 11: Wyckoff site: 12k, site symmetry:  $.m'$ 

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

Table 12: Wyckoff site: 24l, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x - y, x, z + \frac{1}{2}]$	[2]

*continued ...*

Table 12

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