

Table 1: Wyckoff site: 2a, site symmetry:  $-6'm'2$

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

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

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

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

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

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

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

Table 5: Wyckoff site: 2e, site symmetry:  $-6'm'2$

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

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

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

Table 7: Wyckoff site: 4g, site symmetry:  $3m'$ .

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

Table 8: Wyckoff site: 4h, site symmetry:  $3m'$ .

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

Table 9: Wyckoff site: 4i, site symmetry:  $3m'$ .

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

Table 10: Wyckoff site: 6j, site symmetry:  $m'm'2$ 

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

Table 11: Wyckoff site: 6k, site symmetry:  $mm'2'$ 

No.	position	mapping
1	$[x, -x, \frac{1}{4}]$	$[1, 8, 18, 23]$
2	$[x, 2x, \frac{1}{4}]$	$[2, 9, 16, 24]$

*continued ...*

Table 11

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

Table 12: Wyckoff site: 121, 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	$[x, x - y, 0]$	[4,24]
5	$[-x + y, y, 0]$	[5,22]
6	$[-y, -x, 0]$	[6,23]
7	$[-x + y, -x, \frac{1}{2}]$	[7,15]
8	$[x, y, \frac{1}{2}]$	[8,13]
9	$[-y, x - y, \frac{1}{2}]$	[9,14]
10	$[-x + y, y, \frac{1}{2}]$	[10,17]
11	$[-y, -x, \frac{1}{2}]$	[11,18]
12	$[x, x - y, \frac{1}{2}]$	[12,16]

Table 13: Wyckoff site: 12m, site symmetry:  $m..$ 

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

Table 14: Wyckoff site: 12n, site symmetry:  $.m'$ .

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

Table 15: Wyckoff site: 24o, site symmetry: 1

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