

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry:  $-6'..$

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

Table 4: Wyckoff site: 4d, site symmetry:  $3.2'$

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

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

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

Table 6: Wyckoff site: 6f, site symmetry:  $\dots 2'/m'$ 

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

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

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

Table 8: Wyckoff site: 8h, site symmetry:  $3..$ 

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

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

No.	position	mapping
1	$[x, 2x, 0]$	[1, 17]
2	$[-2x, -x, 0]$	[2, 18]
3	$[x, -x, 0]$	[3, 16]
4	$[-x, -2x, \frac{1}{2}]$	[4, 14]
5	$[2x, x, \frac{1}{2}]$	[5, 15]
6	$[-x, x, \frac{1}{2}]$	[6, 13]
7	$[-x, -2x, 0]$	[7, 23]

*continued ...*

Table 9

No.	position	mapping
8	$[2x, x, 0]$	[8,24]
9	$[-x, x, 0]$	[9,22]
10	$[x, 2x, \frac{1}{2}]$	[10,20]
11	$[-2x, -x, \frac{1}{2}]$	[11,21]
12	$[x, -x, \frac{1}{2}]$	[12,19]

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

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

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

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

Table 12: Wyckoff site: 241, site symmetry: 1

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