

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

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

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

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

Table 3: Wyckoff site: 4c, site symmetry:  $3.2$ 

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

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

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

Table 5: Wyckoff site: 4e, site symmetry:  $6'..$ 

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

Table 6: Wyckoff site: **6f**, site symmetry:  $2'2'2$ 

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	[1, 14]
2	$[0, \frac{1}{2}, z]$	[2, 15]
3	$[\frac{1}{2}, \frac{1}{2}, z]$	[3, 13]
4	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[4, 18]
5	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[5, 16]
6	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[6, 17]
7	$[\frac{1}{2}, 0, -z]$	[7, 20]

*continued ...*

Table 9

No.	position	mapping
8	$[0, \frac{1}{2}, -z]$	[8,21]
9	$[\frac{1}{2}, \frac{1}{2}, -z]$	[9,19]
10	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[10,24]
11	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[11,22]
12	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[12,23]

Table 10: Wyckoff site: 12j, site symmetry:  $.2'$ .

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

Table 11: Wyckoff site: 12k, site symmetry:  $..2$ 

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

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

Table 13: Wyckoff site: 24m, site symmetry: 1

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