

Table 1: Wyckoff site: 2a, site symmetry:  $6'22'$ 

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	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{4}]$	$[1, 2, 3, 16, 17, 18]$
2	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{4}]$	$[4, 5, 6, 13, 14, 15]$
3	$[\frac{1}{3}, \frac{2}{3}, \frac{3}{4}]$	$[7, 8, 9, 22, 23, 24]$
4	$[\frac{2}{3}, \frac{1}{3}, \frac{3}{4}]$	$[10, 11, 12, 19, 20, 21]$

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

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

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:  $2'22'$ 

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

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

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

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	$[\frac{1}{3}, \frac{2}{3}, -z]$	[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	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[16,17,18]
7	$[\frac{2}{3}, \frac{1}{3}, -z]$	[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	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[4,17]
5	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[5,18]
6	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[6,16]
7	$[\frac{1}{2}, \frac{1}{2}, -z]$	[7,21]

*continued ...*

Table 9

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

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

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

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

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

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	$[x - y, -y, \frac{1}{2} - z]$	[4]
5	$[y, x, \frac{1}{2} - z]$	[5]
6	$[-x, -x + y, \frac{1}{2} - z]$	[6]
7	$[-x + y, -x, -z]$	[7]
8	$[x, y, -z]$	[8]
9	$[-y, x - y, -z]$	[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	$[x, x - y, \frac{1}{2} - z]$	[16]
17	$[-x + y, y, \frac{1}{2} - z]$	[17]
18	$[-y, -x, \frac{1}{2} - z]$	[18]
19	$[-x, -y, -z]$	[19]
20	$[y, -x + y, -z]$	[20]
21	$[x - y, x, -z]$	[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]