

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

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

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

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

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

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

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

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

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

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

Table 6: Wyckoff site:  $6f$ , site symmetry:  $2'22'$ 

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

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

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

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

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

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

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

*continued ...*

Table 9

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

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

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

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

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

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

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

Table 13: Wyckoff site: 12m, site symmetry:  $\dots 2$ 

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

Table 14: Wyckoff site: 24n, site symmetry: 1

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x - y, x, z + \frac{1}{2}]$	[2]
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	$[x - y, -y, -z]$	[7]
8	$[y, x, -z]$	[8]
9	$[-x, -x + y, -z]$	[9]

*continued ...*

Table 14

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