

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

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

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

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

Table 3: Wyckoff site: **6c**, site symmetry:  $2'22'$

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

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

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

Table 5: Wyckoff site: **12e**, site symmetry:  $2'..$ 

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

Table 6: Wyckoff site: **12f**, site symmetry:  $2'..$ 

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

Table 7: Wyckoff site: **12g**, site symmetry:  $.2.$ 

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

*continued ...*

Table 7

No.	position	mapping
10	$[-x, 0, 0]$	$[16, 23]$
11	$[-x, -x, \frac{1}{6}]$	$[17, 21]$
12	$[0, -x, \frac{1}{3}]$	$[18, 24]$

Table 8: Wyckoff site: 12h, site symmetry:  $.2'$ .

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

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

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

Table 10: Wyckoff site: 12j, site symmetry:  $\dots 2$ 

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

Table 11: Wyckoff site: 24k, site symmetry: 1

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