

Table 1: Wyckoff site: 6a, site symmetry: 222

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

Table 2: Wyckoff site: 6b, site symmetry: 22'2'

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

Table 3: Wyckoff site: 6c, site symmetry: 222

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

Table 4: Wyckoff site: 6d, site symmetry: 22'2'

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

Table 5: Wyckoff site: 12e, site symmetry: 2. .

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

Table 6: Wyckoff site: 12f, site symmetry: 2. .

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

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

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

continued ...

Table 7

No.	position	mapping
10	$[-x, 0, \frac{1}{2}]$	[16,23]
11	$[-x, -x, \frac{1}{6}]$	[17,21]
12	$[0, -x, \frac{5}{6}]$	[18,24]

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

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

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

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

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

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

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

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