

Table 1: Wyckoff site: 2a, site symmetry: 622

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

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

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

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

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

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

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

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

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

Table 6: Wyckoff site: **6f**, site symmetry: 222

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	$[1, 4]$
2	$[\frac{1}{2}, \frac{1}{2}, z]$	$[2, 5]$
3	$[0, \frac{1}{2}, z]$	$[3, 6]$
4	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	$[7, 11]$
5	$[0, \frac{1}{2}, \frac{1}{2} - z]$	$[8, 12]$
6	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	$[9, 10]$
7	$[\frac{1}{2}, 0, -z]$	$[13, 16]$

continued ...

Table 9

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

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

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

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

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

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

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

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

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