

Table 1: Wyckoff site: 2a, site symmetry: $62'2'$

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	$[0, 0, 0]$	$[1, 2, 3, 4, 5, 6, 19, 20, 21, 22, 23, 24]$
2	$[0, 0, \frac{1}{2}]$	$[7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18]$

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

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

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

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

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

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

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

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

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

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

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

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	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[7,11]
5	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[8,12]
6	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[9,10]
7	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[13,17]

continued ...

Table 9

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

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

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

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

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

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

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

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	$[-x + y, y, z + \frac{1}{2}]$	$[7]$
8	$[-y, -x, z + \frac{1}{2}]$	$[8]$
9	$[x, x - y, z + \frac{1}{2}]$	$[9]$
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	$[x - y, -y, \frac{1}{2} - z]$	$[13]$
14	$[y, x, \frac{1}{2} - z]$	$[14]$
15	$[-x, -x + y, \frac{1}{2} - z]$	$[15]$
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	$[-x + y, -x, -z]$	$[20]$
21	$[y, -x + y, -z]$	$[21]$
22	$[x, y, -z]$	$[22]$
23	$[x - y, x, -z]$	$[23]$
24	$[-y, x - y, -z]$	$[24]$