

Table 1: Wyckoff site: 2a, site symmetry:  $-62m$

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

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

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

Table 3: Wyckoff site: 4c, site symmetry:  $-6..$

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

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

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

Table 5: Wyckoff site: 4e, site symmetry:  $3.m$

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

Table 6: Wyckoff site: **6f**, site symmetry: **m2m**

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

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

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

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

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

Table 9: Wyckoff site: **12i**, site symmetry: **..m**

No.	position	mapping
1	$[x, 0, z]$	$[1, 11]$
2	$[0, x, z]$	$[2, 12]$
3	$[-x, -x, z]$	$[3, 10]$
4	$[x, 0, -z]$	$[4, 8]$
5	$[0, x, -z]$	$[5, 9]$
6	$[-x, -x, -z]$	$[6, 7]$
7	$[x, 0, z + \frac{1}{2}]$	$[13, 23]$

*continued ...*

Table 9

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

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

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

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

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

Table 12: Wyckoff site: 241, site symmetry: 1

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