

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

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: $-3' .m$

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

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

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

Table 4: Wyckoff site: 4d, site symmetry: $3.2'$

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

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

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

Table 6: Wyckoff site: **6f**, site symmetry: $\dots 2'/m$

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

Table 7: Wyckoff site: **6g**, site symmetry: $m2m$

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

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

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

Table 9: Wyckoff site: **12i**, site symmetry: $\dots 2'$

No.	position	mapping
1	$[x, 2x, 0]$	$[1, 17]$
2	$[-2x, -x, 0]$	$[2, 18]$
3	$[x, -x, 0]$	$[3, 16]$
4	$[-x, -2x, \frac{1}{2}]$	$[4, 14]$
5	$[2x, x, \frac{1}{2}]$	$[5, 15]$
6	$[-x, x, \frac{1}{2}]$	$[6, 13]$
7	$[x, -x, \frac{1}{2}]$	$[7, 24]$

continued ...

Table 9

No.	position	mapping
8	$[x, 2x, \frac{1}{2}]$	[8,22]
9	$[-2x, -x, \frac{1}{2}]$	[9,23]
10	$[-x, x, 0]$	[10,21]
11	$[-x, -2x, 0]$	[11,19]
12	$[2x, x, 0]$	[12,20]

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

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

Table 11: Wyckoff site: 12k, 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	$[x, 0, \frac{1}{2} - z]$	[4,8]
5	$[0, x, \frac{1}{2} - z]$	[5,9]
6	$[-x, -x, \frac{1}{2} - z]$	[6,7]
7	$[x, x, z + \frac{1}{2}]$	[13,24]
8	$[-x, 0, z + \frac{1}{2}]$	[14,22]
9	$[0, -x, z + \frac{1}{2}]$	[15,23]
10	$[x, x, -z]$	[16,21]
11	$[-x, 0, -z]$	[17,19]
12	$[0, -x, -z]$	[18,20]

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