

Table 1: Wyckoff site: 2a, site symmetry: $-6'2m'$

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

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

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

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

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

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

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

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

Table 6: Wyckoff site: $6\mathbf{f}$, site symmetry: $m'2m'$

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

Table 7: Wyckoff site: $6\mathbf{g}$, site symmetry: $m2'm'$

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

Table 8: Wyckoff site: $8\mathbf{h}$, 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	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	$[7, 8, 9]$
4	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	$[10, 11, 12]$
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	$[\frac{1}{3}, \frac{2}{3}, -z]$	$[19, 20, 21]$
8	$[\frac{2}{3}, \frac{1}{3}, z]$	$[22, 23, 24]$

Table 9: Wyckoff site: $12\mathbf{i}$, site symmetry: $..m'$

No.	position	mapping
1	$[x, 0, z]$	$[1, 23]$
2	$[0, x, z]$	$[2, 24]$
3	$[-x, -x, z]$	$[3, 22]$
4	$[x, 0, -z]$	$[4, 20]$
5	$[0, x, -z]$	$[5, 21]$
6	$[-x, -x, -z]$	$[6, 19]$
7	$[-x, -x, \frac{1}{2} - z]$	$[7, 18]$

continued ...

Table 9

No.	position	mapping
8	$[x, 0, \frac{1}{2} - z]$	[8,16]
9	$[0, x, \frac{1}{2} - z]$	[9,17]
10	$[-x, -x, z + \frac{1}{2}]$	[10,15]
11	$[x, 0, z + \frac{1}{2}]$	[11,13]
12	$[0, x, z + \frac{1}{2}]$	[12,14]

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

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

Table 11: Wyckoff site: 12k, 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	$[x - y, -y, \frac{3}{4}]$	[4,11]
5	$[y, x, \frac{3}{4}]$	[5,12]
6	$[-x, -x + y, \frac{3}{4}]$	[6,10]
7	$[x, y, \frac{3}{4}]$	[13,20]
8	$[-y, x - y, \frac{3}{4}]$	[14,21]
9	$[-x + y, -x, \frac{3}{4}]$	[15,19]
10	$[x - y, -y, \frac{1}{4}]$	[16,23]
11	$[y, x, \frac{1}{4}]$	[17,24]
12	$[-x, -x + y, \frac{1}{4}]$	[18,22]

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	$[-x + y, -x, \frac{1}{2} - z]$	[7]
8	$[x, y, \frac{1}{2} - z]$	[8]
9	$[-y, x - y, \frac{1}{2} - z]$	[9]
10	$[-x, -x + y, z + \frac{1}{2}]$	[10]
11	$[x - y, -y, z + \frac{1}{2}]$	[11]
12	$[y, x, z + \frac{1}{2}]$	[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	$[-x + y, -x, -z]$	[19]
20	$[x, y, -z]$	[20]
21	$[-y, x - y, -z]$	[21]
22	$[-x, -x + y, z]$	[22]
23	$[x - y, -y, z]$	[23]
24	$[y, x, z]$	[24]