

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

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

Table 2: Wyckoff site: 2b, site symmetry:  $-3.m$

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

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

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

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

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

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

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

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

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

Table 7: Wyckoff site:  $6\mathbf{g}$ , site symmetry:  $m2m$ 

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

Table 8: Wyckoff site:  $8\mathbf{h}$ , site symmetry:  $3..$ 

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

Table 9: Wyckoff site:  $12\mathbf{i}$ , site symmetry:  $\dots 2$ 

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

*continued ...*

Table 9

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

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

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

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

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

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

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