

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

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

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

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

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

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

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

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

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	$[0, 0, -z]$	$[7, 9, 11, 16, 17, 18]$
4	$[0, 0, \frac{1}{2} - z]$	$[8, 10, 12, 13, 14, 15]$

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

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

Table 7: Wyckoff site: **6g**, site symmetry:  $m2'm'$ 

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

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

No.	position	mapping
1	$[\frac{1}{3}, \frac{2}{3}, z]$	$[1, 3, 5]$
2	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	$[2, 4, 6]$
3	$[\frac{2}{3}, \frac{1}{3}, -z]$	$[7, 9, 11]$
4	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	$[8, 10, 12]$
5	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$	$[13, 14, 15]$
6	$[\frac{1}{3}, \frac{2}{3}, -z]$	$[16, 17, 18]$
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: **12i**, site symmetry:  $\dots 2'$ 

No.	position	mapping
1	$[x, 2x, 0]$	$[1, 17]$
2	$[-x, x, \frac{1}{2}]$	$[2, 15]$
3	$[-2x, -x, 0]$	$[3, 18]$
4	$[-x, -2x, \frac{1}{2}]$	$[4, 13]$
5	$[x, -x, 0]$	$[5, 16]$
6	$[2x, x, \frac{1}{2}]$	$[6, 14]$
7	$[-x, -2x, 0]$	$[7, 23]$

*continued ...*

Table 9

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

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

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

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	$[-x, 0, -z]$	[7,17]
8	$[-x, -x, \frac{1}{2} - z]$	[8,15]
9	$[0, -x, -z]$	[9,18]
10	$[x, 0, \frac{1}{2} - z]$	[10,13]
11	$[x, x, -z]$	[11,16]
12	$[0, x, \frac{1}{2} - z]$	[12,14]

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	$[-x, -y, -z]$	[7]
8	$[-x + y, -x, \frac{1}{2} - z]$	[8]
9	$[y, -x + y, -z]$	[9]
10	$[x, y, \frac{1}{2} - z]$	[10]
11	$[x - y, x, -z]$	[11]
12	$[-y, x - y, \frac{1}{2} - z]$	[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	$[x, x - y, -z]$	[16]
17	$[-x + y, y, -z]$	[17]
18	$[-y, -x, -z]$	[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]