

Table 1: Wyckoff site: 2a, site symmetry: $-3'm$.

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

Table 2: Wyckoff site: 2b, site symmetry: $-6'm2'$

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

Table 3: Wyckoff site: 2c, site symmetry: $-6'm2'$

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

Table 4: Wyckoff site: 2d, site symmetry: $-6'm2'$

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

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

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

Table 6: Wyckoff site: **4f**, site symmetry: **3m**.

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

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

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

Table 8: Wyckoff site: **6h**, site symmetry: **m'm2'**

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

Table 9: Wyckoff site: **12i**, site symmetry: **.2'**.

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

continued ...

Table 9

No.	position	mapping
12	$[0, x, \frac{1}{2}]$	[12,24]

Table 10: Wyckoff site: 12j, site symmetry: $m'\bar{1}$

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

Table 11: Wyckoff site: 12k, site symmetry: $\bar{1}m$

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

Table 12: Wyckoff site: 24l, site symmetry: $\bar{1}$

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x - y, x, z + \frac{1}{2}]$	[2]

continued ...

Table 12

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