

Table 1: Wyckoff site: 2a, site symmetry: $6'22'$

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

Table 2: Wyckoff site: 2b, site symmetry: $6'/m..$

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

Table 3: Wyckoff site: 4c, site symmetry: $3.2'$

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

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

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

Table 5: Wyckoff site: 4e, site symmetry: $6'..$

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

Table 6: Wyckoff site: $6\mathbf{f}$, site symmetry: $2'22'$

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

Table 7: Wyckoff site: $6\mathbf{g}$, site symmetry: $2'/m..$

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

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	$[\frac{2}{3}, \frac{1}{3}, \frac{1}{2} - z]$	[4, 5, 6]
3	$[\frac{1}{3}, \frac{2}{3}, -z]$	[7, 8, 9]
4	$[\frac{2}{3}, \frac{1}{3}, z + \frac{1}{2}]$	[10, 11, 12]
5	$[\frac{2}{3}, \frac{1}{3}, z]$	[13, 14, 15]
6	$[\frac{1}{3}, \frac{2}{3}, \frac{1}{2} - z]$	[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: $12\mathbf{i}$, site symmetry: $2'..$

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	[1, 14]
2	$[0, \frac{1}{2}, z]$	[2, 15]
3	$[\frac{1}{2}, \frac{1}{2}, z]$	[3, 13]
4	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[4, 17]
5	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[5, 18]
6	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[6, 16]
7	$[\frac{1}{2}, \frac{1}{2}, -z]$	[7, 21]

continued ...

Table 9

No.	position	mapping
8	$[\frac{1}{2}, 0, -z]$	[8,19]
9	$[0, \frac{1}{2}, -z]$	[9,20]
10	$[\frac{1}{2}, \frac{1}{2}, z + \frac{1}{2}]$	[10,24]
11	$[\frac{1}{2}, 0, z + \frac{1}{2}]$	[11,22]
12	$[0, \frac{1}{2}, z + \frac{1}{2}]$	[12,23]

Table 10: Wyckoff site: 12j, site symmetry: .2.

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

Table 11: Wyckoff site: 12k, site symmetry: . . 2'

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

Table 12: Wyckoff site: 12l, site symmetry: m .

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

Table 13: Wyckoff site: 24m, 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	$[-x + y, -x, -z]$	[7]
8	$[x, y, -z]$	[8]
9	$[-y, x - y, -z]$	[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	$[x - y, x, z]$	[13]
14	$[-x, -y, z]$	[14]
15	$[y, -x + y, z]$	[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	$[y, -x + y, -z]$	[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]