

Table 1: Wyckoff site: 2a, site symmetry: 622

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

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

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

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

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

Table 6: Wyckoff site: 6f, site symmetry: 222

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

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

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

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

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

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

No.	position	mapping
1	$[\frac{1}{2}, 0, z]$	[1,4]
2	$[\frac{1}{2}, \frac{1}{2}, z]$	[2,5]
3	$[0, \frac{1}{2}, z]$	[3,6]
4	$[\frac{1}{2}, 0, \frac{1}{2} - z]$	[7,11]
5	$[0, \frac{1}{2}, \frac{1}{2} - z]$	[8,12]
6	$[\frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z]$	[9,10]
7	$[\frac{1}{2}, 0, -z]$	[13,16]

*continued ...*

Table 9

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

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

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

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

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

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

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

Table 13: Wyckoff site: 24m, site symmetry: 1

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