

Table 1: Wyckoff site: 2a, site symmetry: 23 .

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

Table 2: Wyckoff site: 4b, site symmetry: $.32$

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

Table 3: Wyckoff site: 4c, site symmetry: $.32$

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

Table 4: Wyckoff site: 6d, site symmetry: $222..$

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

Table 5: Wyckoff site: 6e, site symmetry: 2.22

No.	position	mapping
1	$[\frac{1}{4}, 0, \frac{1}{2}]$	$[1, 8, 13, 14]$
2	$[\frac{3}{4}, 0, \frac{1}{2}]$	$[2, 3, 9, 10]$

continued ...

Table 5

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

Table 6: Wyckoff site: 6f, site symmetry: 2.22

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

Table 7: Wyckoff site: 8g, site symmetry: .3.

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

Table 8: Wyckoff site: 12h, site symmetry: 2..

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

continued ...

Table 8

No.	position	mapping
10	$[0, 0, x]$	$[18, 21]$
11	$[0, 0, -x]$	$[19, 23]$
12	$[0, -x, 0]$	$[20, 22]$

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

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

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

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

Table 11: Wyckoff site: 12k, site symmetry: $\dots 2$

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

Table 12: Wyckoff site: 12l, site symmetry: $\dots 2$

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

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

No.	position	mapping
1	$[x, y, z]$	[1]
2	$[x + \frac{1}{2}, \frac{1}{2} - z, y + \frac{1}{2}]$	[2]
3	$[x + \frac{1}{2}, z + \frac{1}{2}, \frac{1}{2} - y]$	[3]
4	$[z + \frac{1}{2}, y + \frac{1}{2}, \frac{1}{2} - x]$	[4]
5	$[\frac{1}{2} - z, y + \frac{1}{2}, x + \frac{1}{2}]$	[5]
6	$[\frac{1}{2} - y, x + \frac{1}{2}, z + \frac{1}{2}]$	[6]
7	$[y + \frac{1}{2}, \frac{1}{2} - x, z + \frac{1}{2}]$	[7]
8	$[x, -y, -z]$	[8]
9	$[-x, y, -z]$	[9]

continued ...

Table 13

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