

# A (Very) Brief Introduction to Geometric Group Theory

Gregory McColm

Department of Mathematics & Statistics

University of South Florida

Tampa, FL USA



# This is a hot area

There have been fourteen Abel prize winners since Jean Paul Serre won the prize for just about everything (including geometric group theory), and since then ...

... for their work in geometric group theory and allied areas:

Jacques Tits (2008)

Mikhail Gromov (2009)

# A (Very) Brief Introduction to Geometric Group Theory

Geometric Group Theory uses the algebraic machinery of geometry and topology to understand groups.

# A (Very) Brief Introduction to Geometric Group Theory

Geometric Group Theory uses the algebraic machinery of geometry and topology to understand groups.

Crystallographers may not be so interested in groups in themselves, but they are interested in geometric and topological objects that represent crystal structures.

# A (Very) Brief Introduction to Geometric Group Theory

Geometric Group Theory uses the algebraic machinery of geometry and topology to understand groups.

Crystallographers may not be so interested in groups in themselves, but they are interested in geometric and topological objects that represent crystal structures.

We can turn the agenda of geometric group theory on its head to work on representations of crystal structures.

# A (Very) Brief Introduction to Geometric Group Theory

Today...

# A (Very) Brief Introduction to Geometric Group Theory

Today...

- Graphs were the original (combinatorial!) representations in the theory. But “digraphs” are more readily used...

# A (Very) Brief Introduction to Geometric Group Theory

Today...

- Graphs were the original (combinatorial!) representations in the theory. But “digraphs” are more readily used...
- Using a group to navigate a graph.



# A (Very) Brief Introduction to Geometric Group Theory

Today...

- Graphs were the original (combinatorial!) representations in the theory. But “digraphs” are more readily used...
- Using a group to navigate a graph.
- What might this be good for?

# About Graphs

...

If you believe in bonds between atoms

– at least as a useful metaphor –

– or if you are making a polymer out of molecular  
building blocks –

then you can represent nano-structures with graphs.

# Graphs

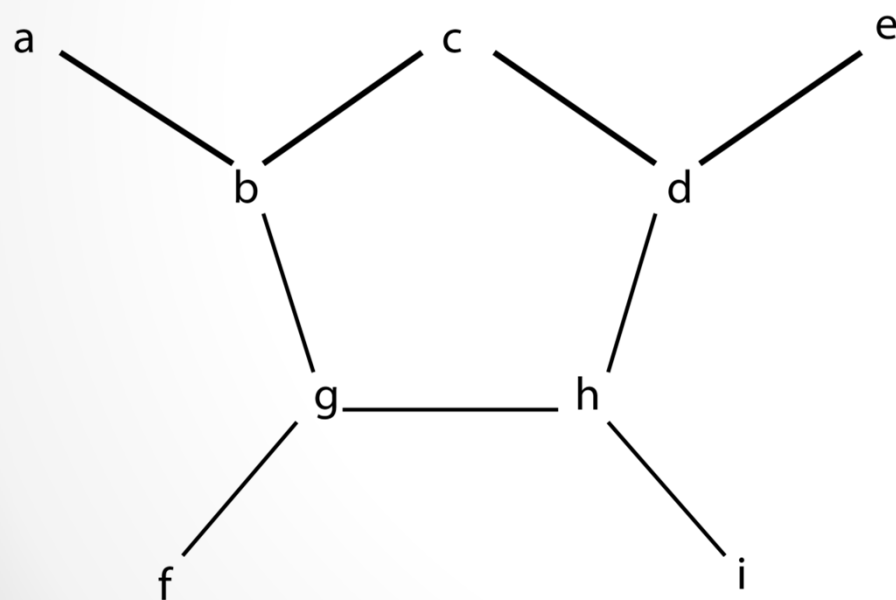
A combinatorist would say that a **graph** is an ordered pair  $(V, E)$  where  $V$  is a set of **vertices** and  $E$  is a set of **edges**. Usually there is at most one edge for each pair of vertices.

# Graphs

A combinatorist would say that a **graph** is an ordered pair  $(V, E)$  where  $V$  is a set of **vertices** and  $E$  is a set of **edges**. Usually there is at most one edge for each pair of vertices.

(A topologist would have a quite different definition. Let's not go into that right now.)

# Graphs



This graph has nine vertices

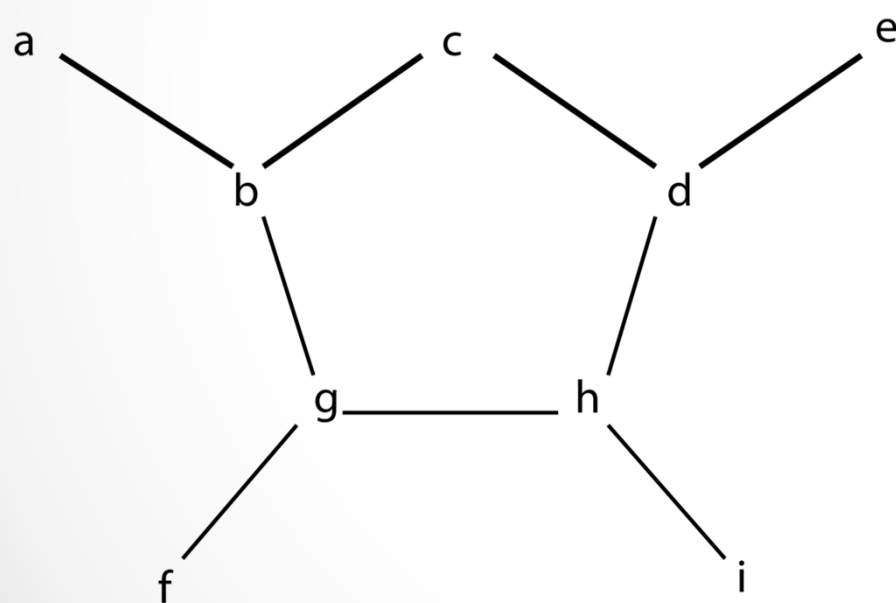
$V = \{a, b, c, d, e, f, g, h, i\}$   
and nine edges

$E = \{\{a, b\}, \{b, c\}, \{c, d\},$   
 $\{d, e\}, \{b, g\}, \{g, f\},$   
 $\{g, h\}, \{h, d\}, \{h, i\}\}.$

# Graphs

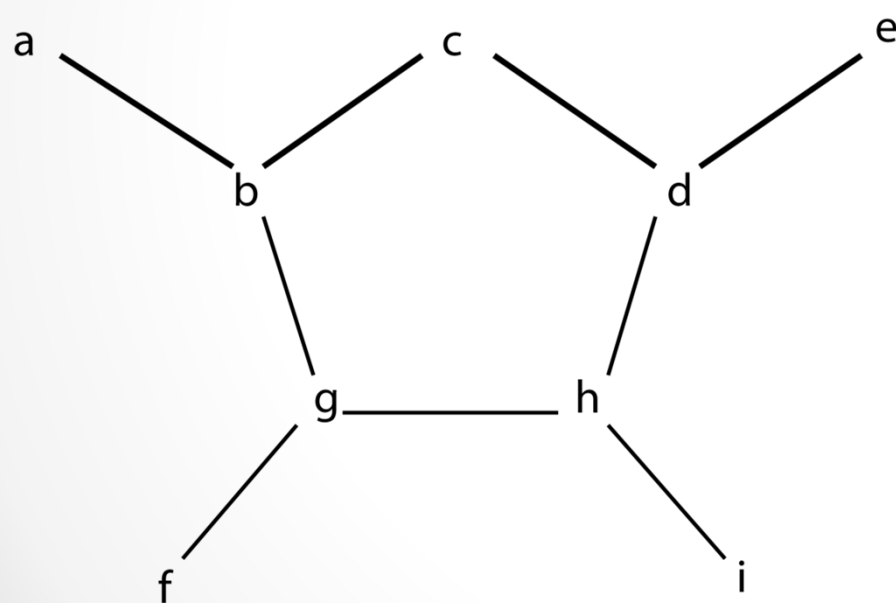
An ***automorphism*** on a graph is a one-to-one function sending vertices to vertices and edges to edges so that *edge-vertex incidence is preserved*.

# Graphs



This graph has two automorphisms:

# Graphs

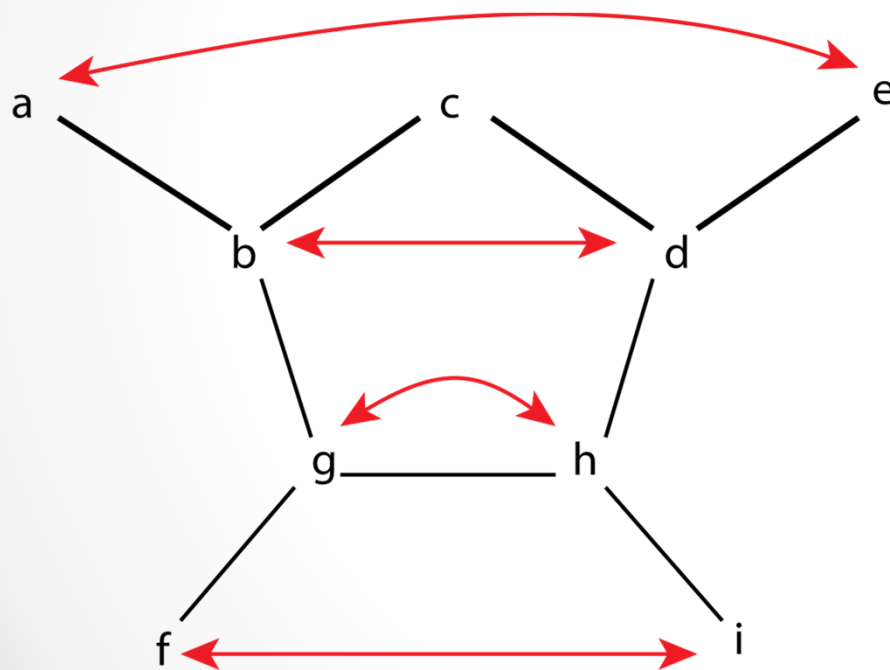


This graph has two automorphisms:

- The identity, that sends each vertex to itself and each edge to itself, and



# Graphs

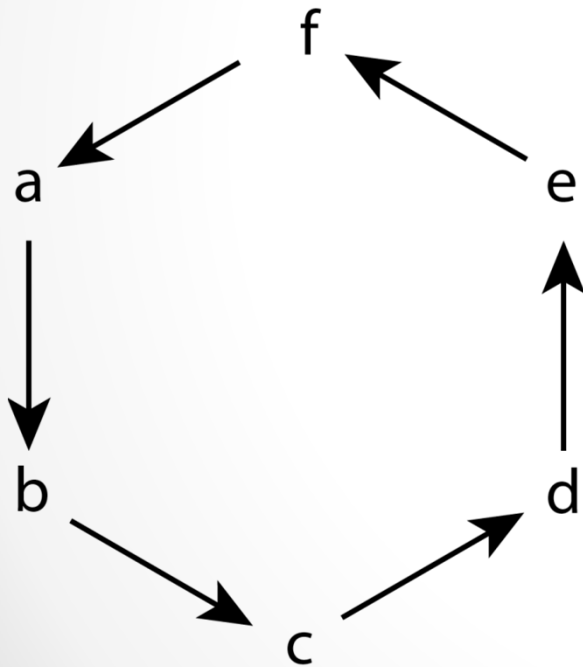


This graph has two automorphisms:

- The identity, that sends each vertex to itself and each edge to itself, and
- The “reflection” at left, switching vertices along red arrows.

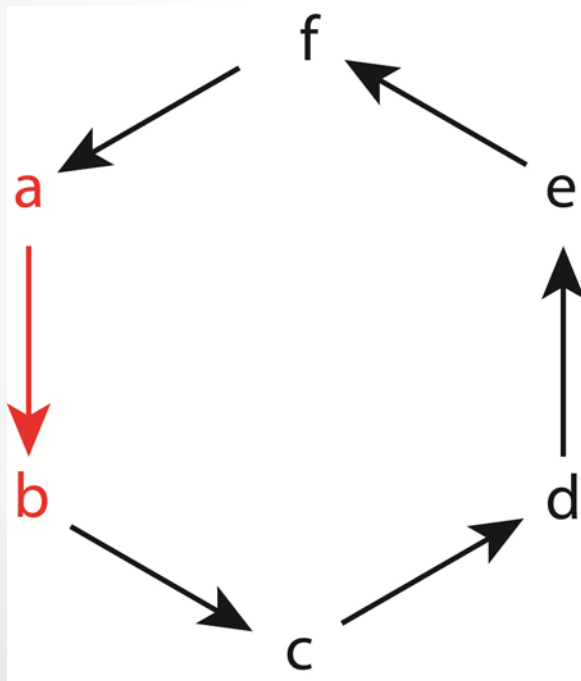
# Digraphs

It is not controversial to say that a **directed graph** or **digraph** is a pair  $(N, A)$ , where  $N$  is a set of **nodes** and  $A$  is a set of **arcs**, each of which points from a **source** vertex to a **target**.



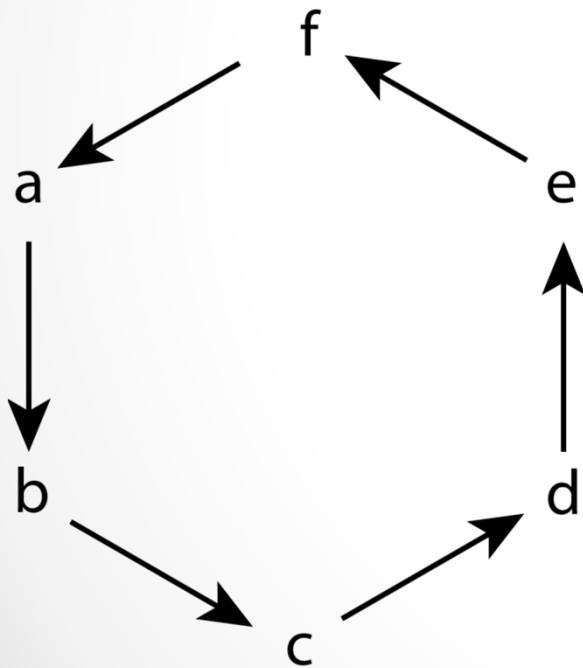
# Digraphs

It is not controversial to say that a **directed graph** or **digraph** is a pair  $(N, A)$ , where  $N$  is a set of **nodes** and  $A$  is a set of **arcs**, each of which points from a **source** vertex to a **target**.



Notice in  $(a, b)$ ,  $a$  is the source and  $b$  the target, but in  $(b, a)$ , it's the other way around.

# Digraphs



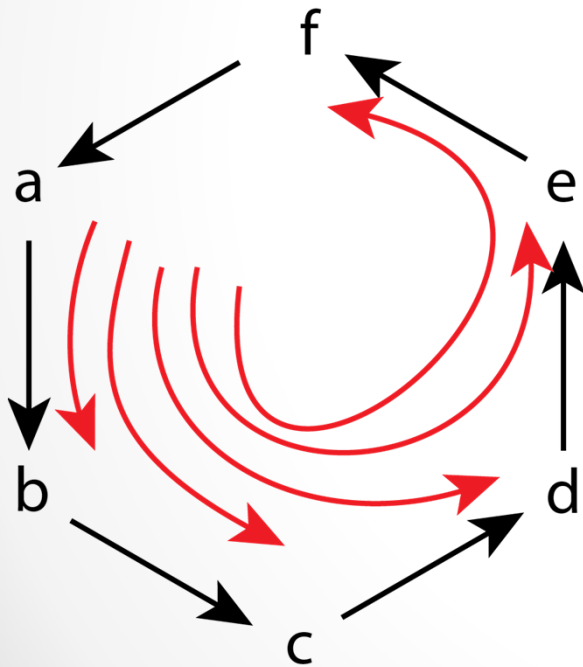
This digraph has six nodes

$N = \{a, b, c, d, e, f\}$ ,  
and six arcs

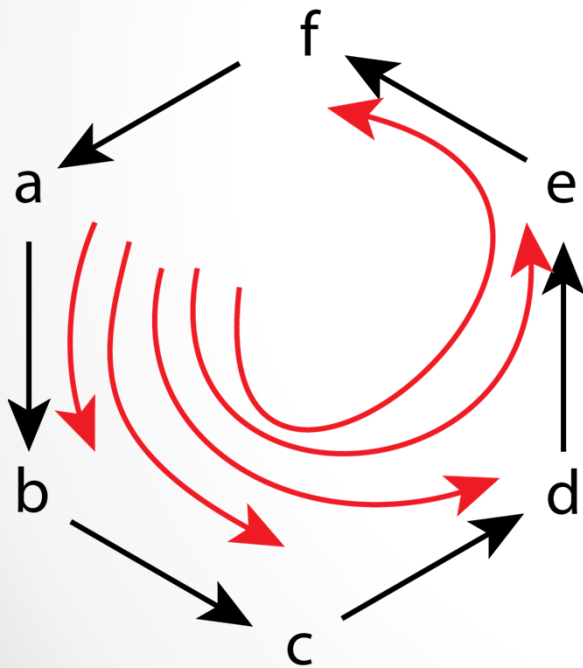
$A = \{(a, b), (b, c), (c, d), (d, e), (e, f), (f, a)\}$ .

# Digraphs

An ***automorphism*** of a digraph sends nodes to nodes and arcs to arcs, preserving node-arc incidence.



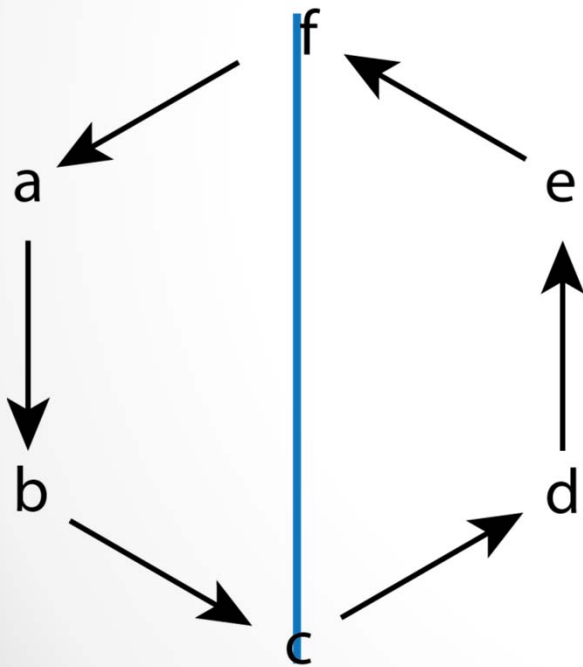
# Digraphs



This digraph has six automorphisms:

The identity and then counterclockwise rotations by  $60^\circ$ ,  $120^\circ$ ,  $180^\circ$ ,  $240^\circ$ , and  $300^\circ$ .

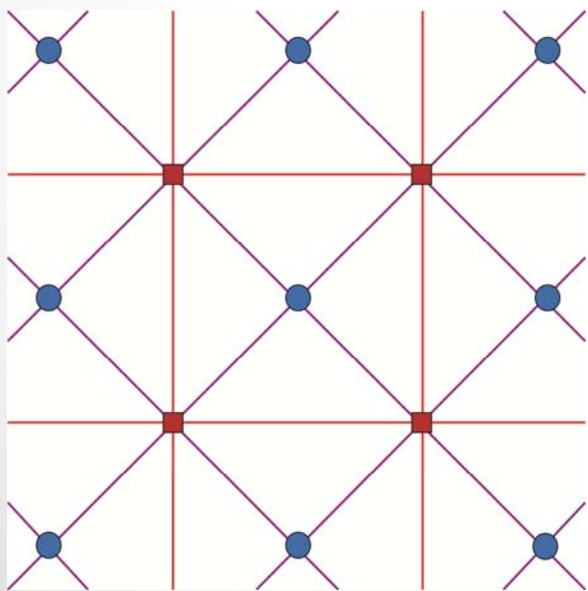
# Digraphs



Reflection across the vertical line is not an automorphism as that would reverse arrows.

# Digraphs

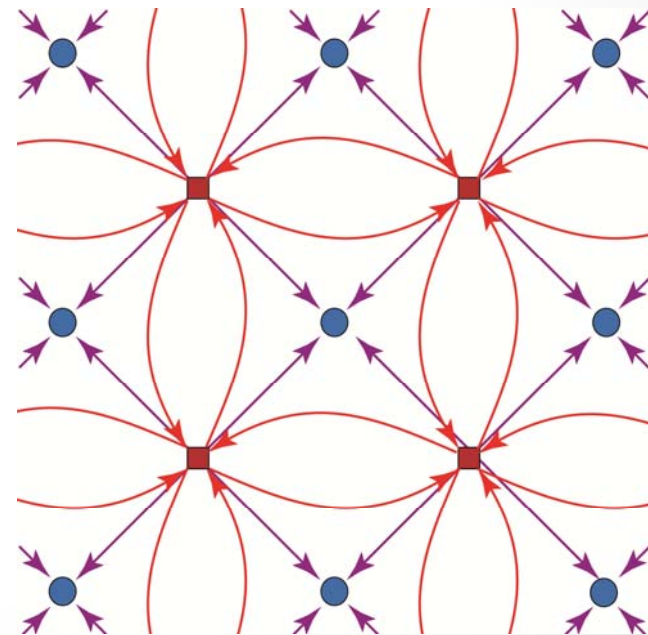
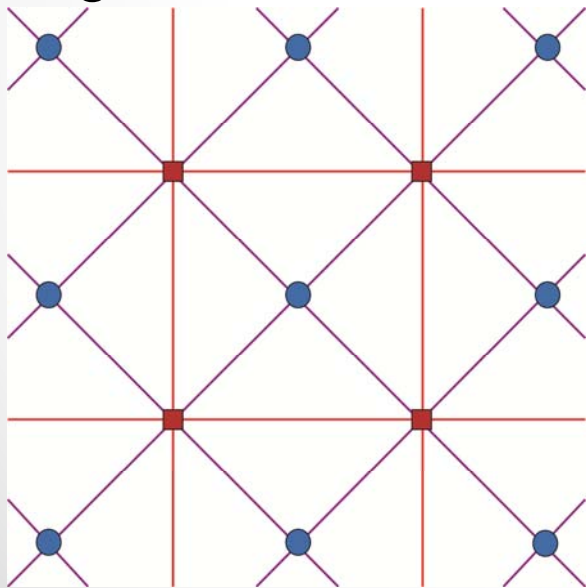
Combinatorial group theory typically works with digraphs, not graphs. But that may suit our purpose: in many molecules and crystal structures, there are bonds or linkers connecting two atoms or MBBs that are not from the same orbit – or at least, cannot be switched by any symmetry of the structure.





# Digraphs

Given a graph representing a crystal structure, we can represent that structure with a digraph, where each “symmetric” edge (viz., an edge whose vertices are switched by an automorphism) is represented by a pair of arcs, while each “asymmetric” edge is represented by a single arc.



# Graphs and Groups

For any graph  $\Gamma$ , the set of automorphisms of  $\Gamma$  form a **group** under composition  $\circ$ . Let's not go into groups now, but there are two things you should know about groups before we go on:

# Graphs and Groups

1. In 1939, Robert Frucht proved that every finite group was equivalent to the automorphism group of some finite graph.

# Graphs and Groups

1. In 1939, Robert Frucht proved that every finite group was equivalent to the automorphism group of some finite graph.

*This meant that graphs (and digraphs) could be used to “represent” groups – which was helpful because groups are abstract and strange beasts.*

# Graphs and Groups

2. In 1882, Walther von Dyck observed that sequences of actions – like recipes or itineraries – could be represented by elements of a group.

# Graphs and Groups

2. In 1882, Walther von Dyck observed that sequences of actions – like recipes or itineraries – could be represented by elements of a group.

*Dyck's observation helped launch “combinatorial group theory”, of which geometric group theory is a generalization.*

# Navigation



One of the popular descriptive mechanisms in mathematics is to describe a structure by describing all the components of the structure.

# Navigation



One of the popular descriptive mechanisms in mathematics is to describe a structure by describing all the components of the structure.

Another is to describe a structure by describing how it can be traversed.



# Navigation



One of the popular descriptive mechanisms in mathematics is to describe a structure by describing all the components of the structure.

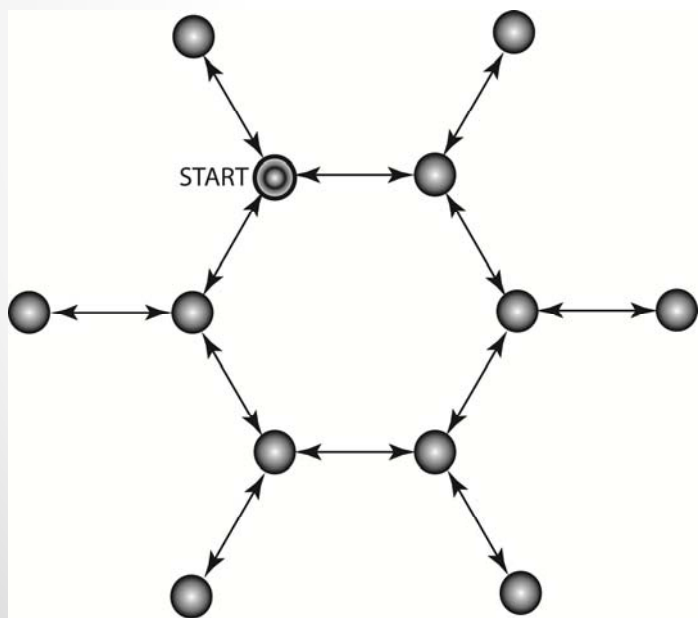
Another is to describe a structure by describing how it can be traversed.

These two mechanisms can be fused together ...

# Navigation

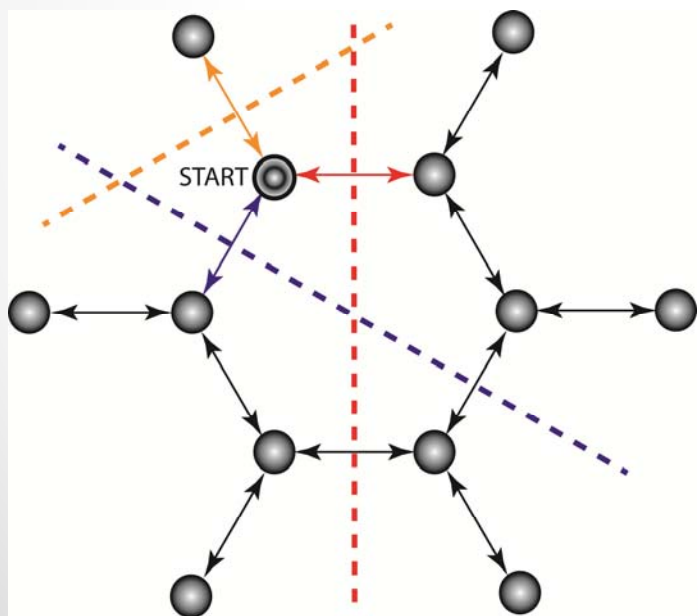
Suppose that you wanted to tour a foreign country by train. You had an itinerary that told you that on the first leg of your journey, you take the **blue** train. Then at the station, you take the **red** train. Then you take the **blue** train again. After these three hops, you are at your destination.

# Navigation



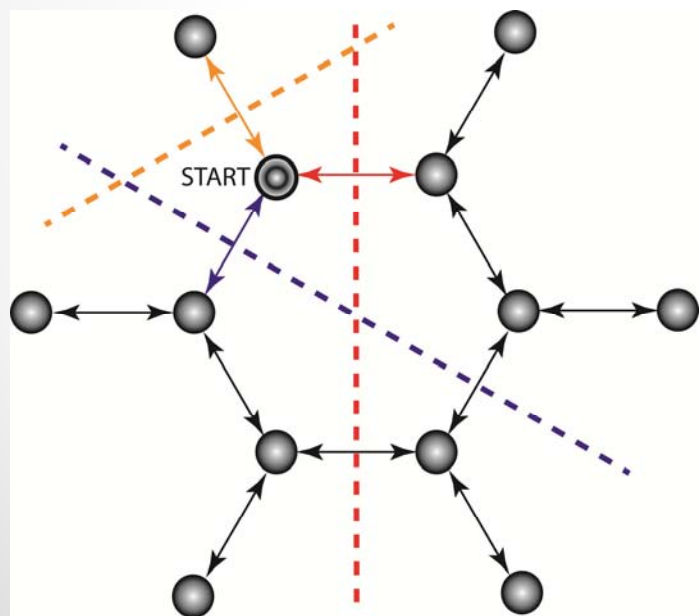
Suppose that you are at the ringed starting point and you wanted to take three steps counterclockwise around the benzene ring.

# Navigation



von Dyck says that each possible step involves reflecting across one of the three mirrors adjacent to the START node.

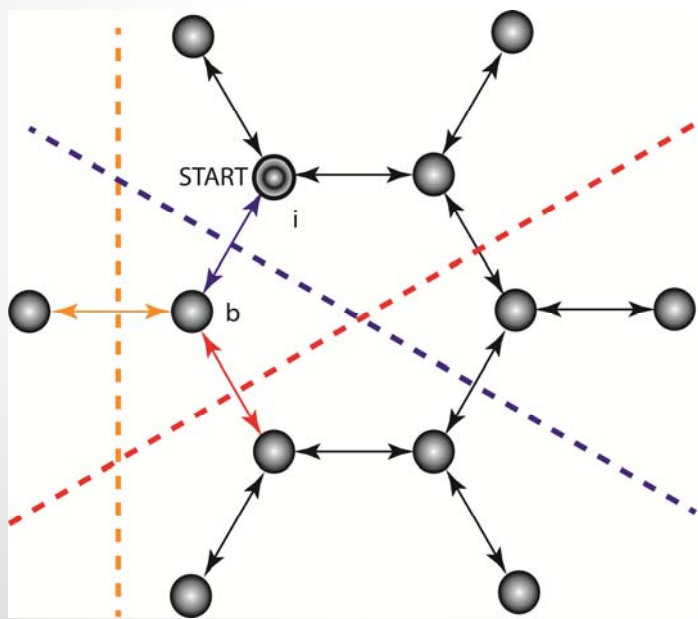
# Navigation



von Dyck says that each possible step involves reflecting across one of the three mirrors adjacent to the START node.

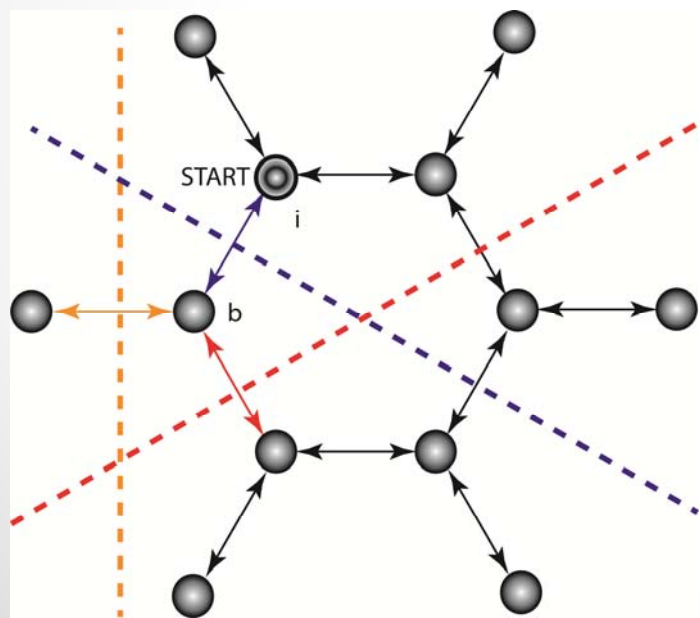
To start counterclockwise, reflect across the **blue mirror**.

# Navigation



Since we reached the next node by reflecting across the **blue mirror**, label that node with a “b”.

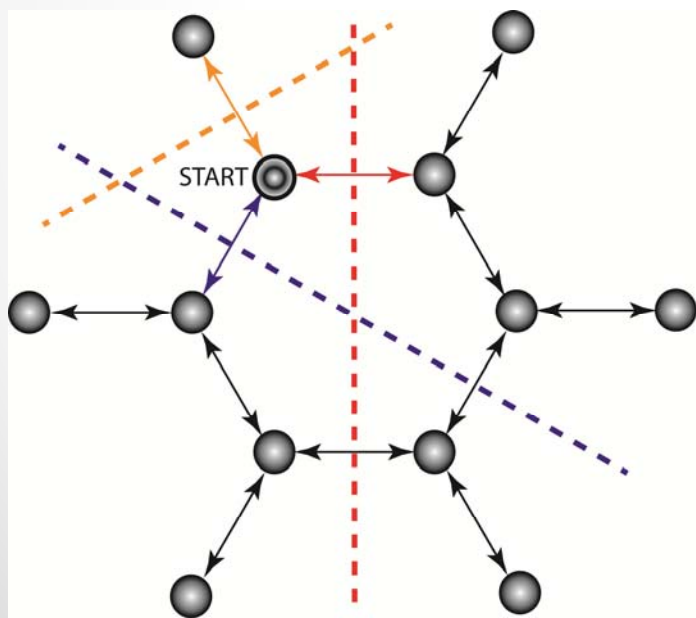
# Navigation



Since we reached the next node by reflecting across the **blue mirror**, label that node with a “b”.

Notice that I reflected the **yellow** and **red** mirrors across the **blue** mirror...

# Navigation

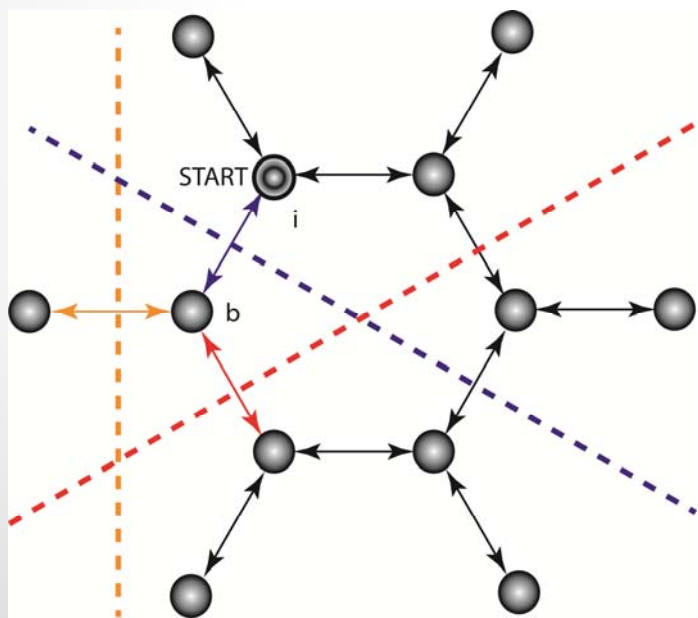


Since we reached the next node by reflecting across the **blue mirror**, label that node with a “b”.

Notice that I reflected the **yellow** and **red** mirrors across the **blue** mirror...



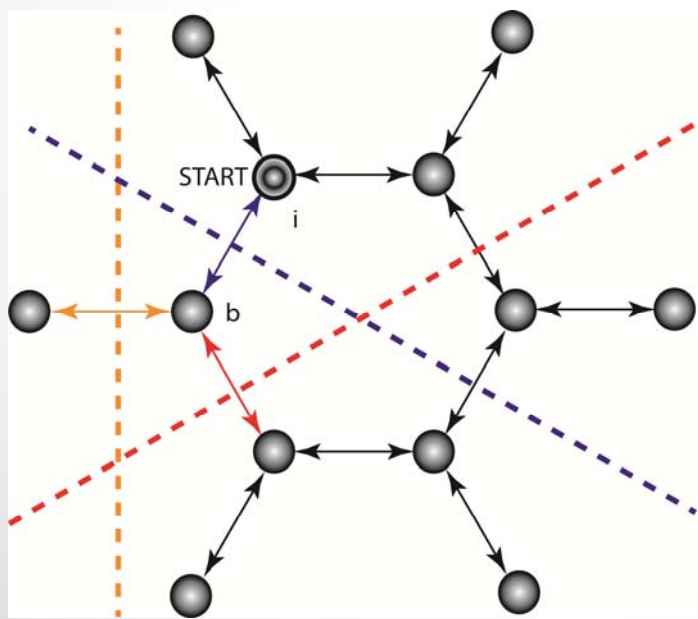
# Navigation



Since we reached the next node by reflecting across the **blue mirror**, label that node with a “b”.

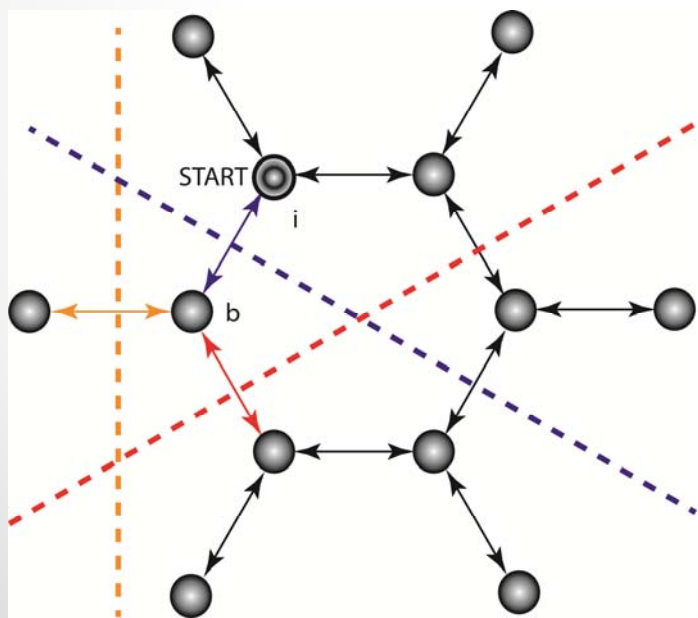
Notice that I reflected the **yellow** and **red** mirrors across the **blue** mirror...

# Navigation



We now face three mirrors.  
*These are the reflections of the original three mirrors, across the blue mirror.*

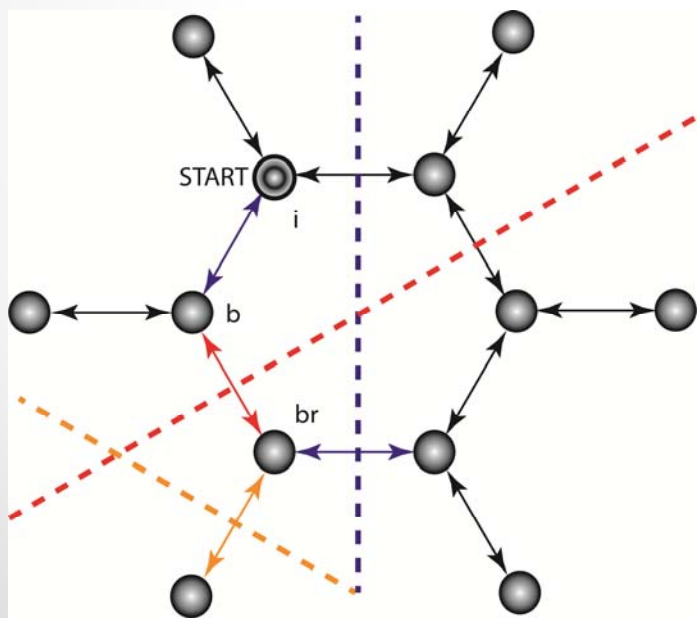
# Navigation



We now face three mirrors.  
*These are the reflections of the original three mirrors, across the blue mirror.*

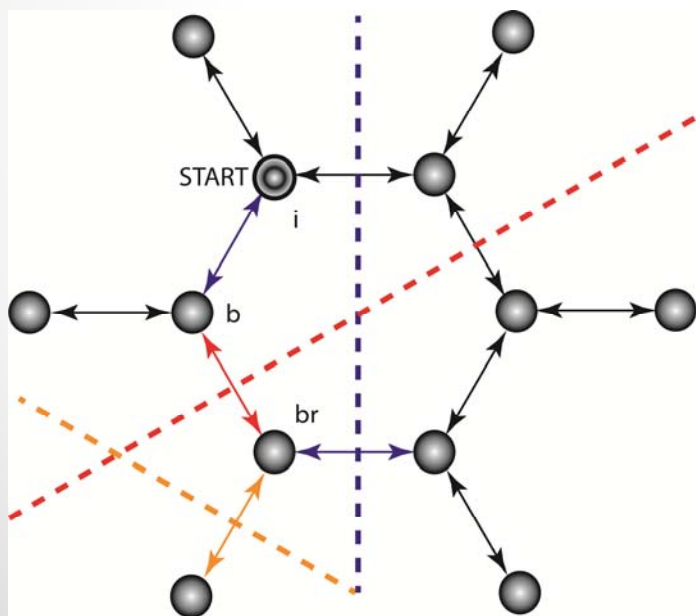
Going counterclockwise, our next step is to reflect across the red mirror.

# Navigation



Again, we label the next node with a “br” as we were at node “b” and we reflected across the red mirror to get to “br”.

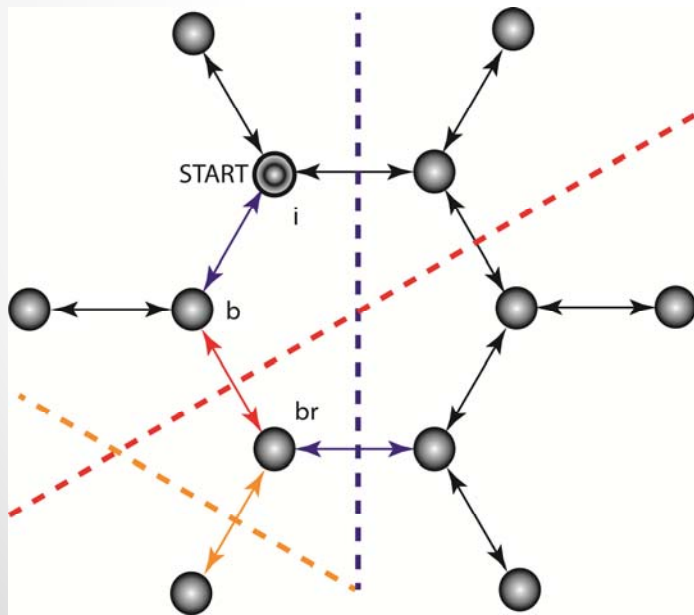
# Navigation



Again, we label the next node with a “br” as we were at node “b” and we reflected across the red mirror to get to “br”.

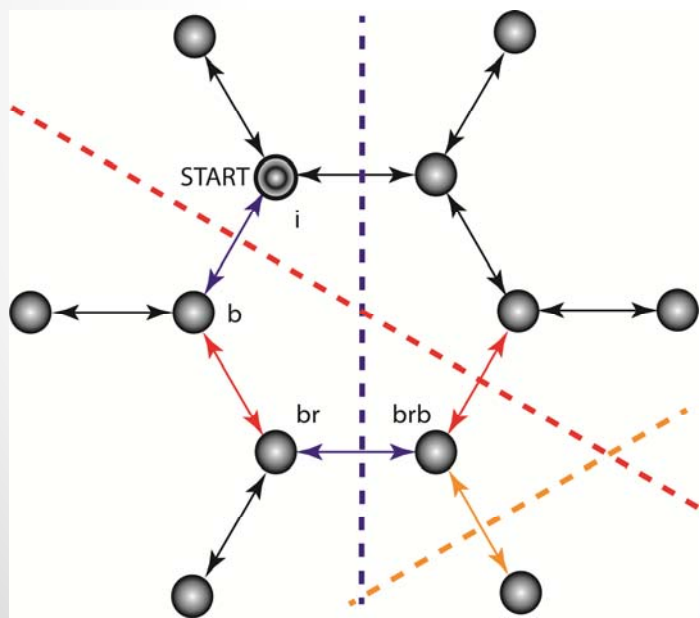
Again, we reflect the mirrors, this time across the red mirror.

# Navigation



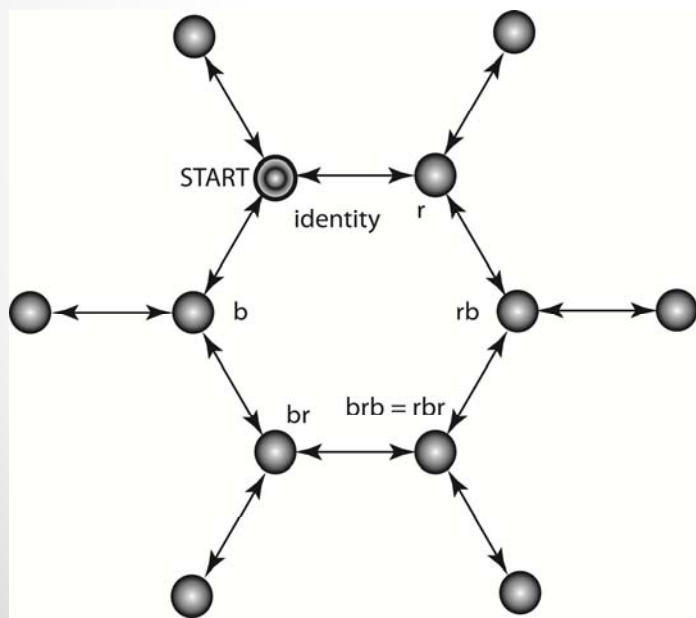
Moving counterclockwise, we reflect across the blue mirror ...

# Navigation



... to get to the node we label “brb” as we traversed a blue mirror, a red, and then a blue to get there.

# Navigation



... to get to the node we label “brb” as we traversed a blue mirror, a red, and then a blue to get there.

If we had gone clockwise, we would have reached that same node, labeling it “rbr”.



# Where do Crystallographers go from Here?

...

This approach appears productive in crystal structure prediction, and may have applications in structure analysis...

# Where do Crystallographers go from Here?

This apparatus is already being used for crystal prediction, but in a non-mainstream way.

# Where do Crystallographers go from Here?

This apparatus is already being used for crystal prediction, but in a non-mainstream way.

- Contemporary crystal prediction tends to be specific to the materials being used. This makes it an exercise in computational chemistry (actually, physics).

# Where do Crystallographers go from Here?

This apparatus is already being used for crystal prediction, but in a non-mainstream way.

- Contemporary crystal prediction tends to be specific to the materials being used. This makes it an exercise in computational chemistry (actually, physics).
- This apparatus is inherently geometric, and will show what can or cannot be done, regardless of the physics.

# Where do Crystallographers go from Here?

I know of two programs that rely on this approach.

# Where do Crystallographers go from Here?

I know of two programs that rely on this approach.

1. The **Symmetry-Constrained Intersite Bonding Search** (SCIBS) developed by Michael Treacy, Igor Rivin et al, uses von Dyck's reflection technique. SCIBS has generated several million "zeolitic" graphs, posted at the Hypothetical Zeolites database.

# Where do Crystallographers go from Here?

I know of two programs that rely on this approach.

1. The **Symmetry-Constrained Intersite Bonding Search (SCIBS)** developed by Michael Treacy, Igor Rivin et al, uses von Dyck's reflection technique. SCIBS has generated several million "zeolitic" graphs, posted at the Hypothetical Zeolites database.
2. The **Crystal Turtlebug**, developed by Edwin Clark and Greg McColm, is still under development. It has generated several hundred novel crystal nets, none of which has been synthesized (yet).

# Where do Crystallographers go from Here?

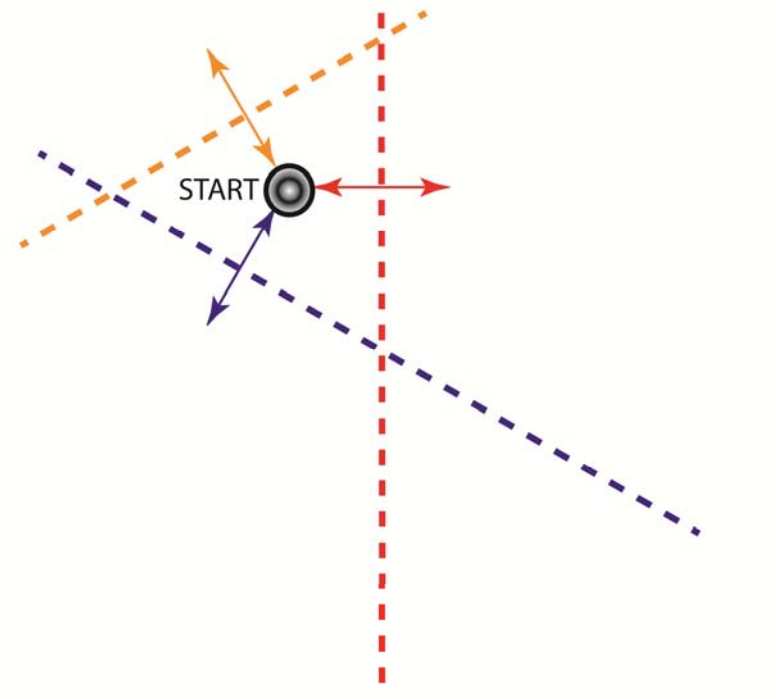
Both generate crystals somewhat as follows ...



# Where do Crystallographers go from Here?

Both generate crystals somewhat as follows ...

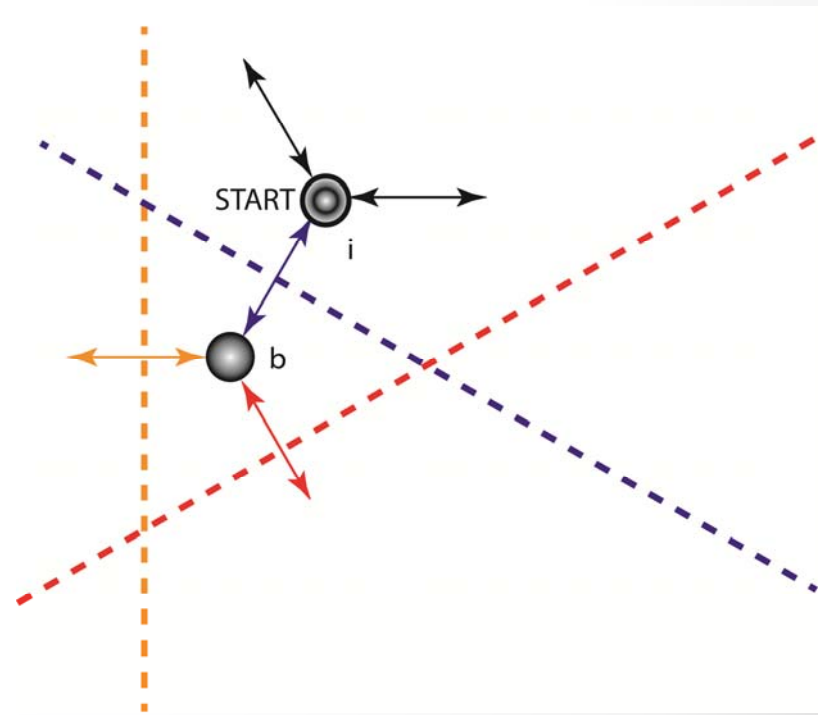
Start at the beginning:



# Where do Crystallographers go from Here?

Both generate crystals somewhat as follows ...

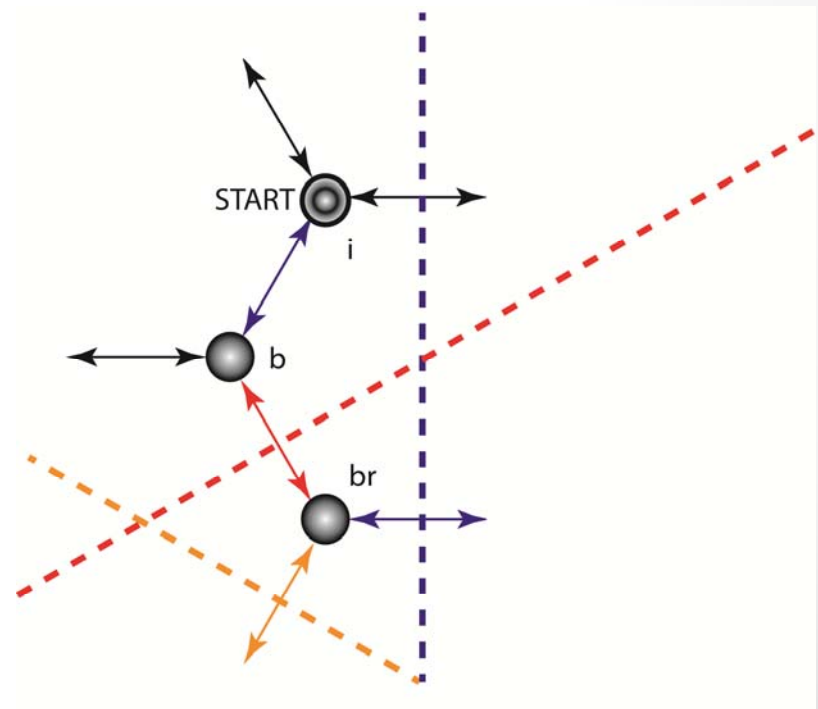
Add a vertex:



# Where do Crystallographers go from Here?

Both generate crystals somewhat as follows ...

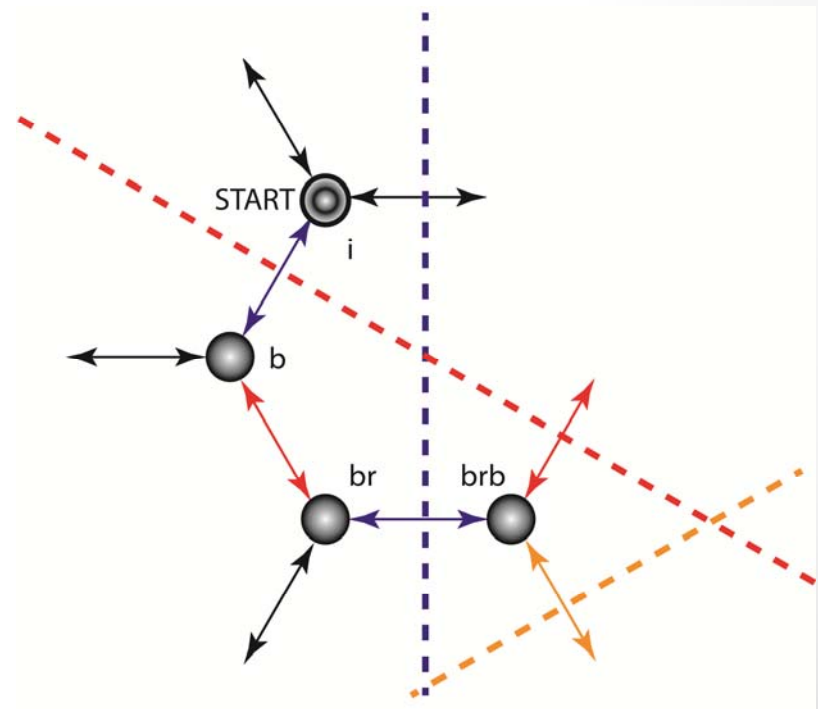
And another:



# Where do Crystallographers go from Here?

Both generate crystals somewhat as follows ...

And keep on going:



# Where do Crystallographers go from Here?

But is this all science fiction?

# Where do Crystallographers go from Here?

In 1980, according to legend, an Escher print inspired Ned Seeman to try to synthesize a structure of DNA.

# Where do Crystallographers go from Here?

Making *a cube* took a decade ...

# Where do Crystallographers go from Here?

DNA is highly controllable, and that's what inspired computer scientist Len Adleman to talk about ...

**“DNA computation”**



# Where do Crystallographers go from Here?

The dream was to make a desktop DNA computer that outperformed ordinary computers. Very quickly, this became a campaign to compute NP-complete queries ...

(Stephen Cook, Mr. NP-completeness.)

# Where do Crystallographers go from Here?

But a DNA computation of an NP-complete query meant constructing graphs out of DNA: the graphs generated would be the solution to the problem...

(Ron Fagin: NP and graphs...)

# Where do Crystallographers go from Here?

During the 1990s, a lot of graph-theoretic architecture was developed by a number of mathematicians, many of which visited Ned Seeman's lab and kibbitzed.

(USF's Natasa Jonoska, who kibbitzed)

# Where do Crystallographers go from Here?

During the 2000s, there appeared new design techniques for DNA origami and other DNA structures.

# Where do Crystallographers go from Here?

There's no sign of DNA computers, but there is a LOT of DNA construction...

# Where do Crystallographers go from Here?

DNA is extremely “tunable”, as Metal Organic Framework people would put it.

# Where do Crystallographers go from Here?

DNA is extremely “tunable”, as Metal Organic Framework people would put it.

Metal ions and organic ligands are not as tunable, but we have had enough success with them to suggest that *the next step is designing metal organic materials* – and then *synthesizing* them.

# Where do Crystallographers go from Here?

DNA is extremely “tunable”, as Metal Organic Framework people would put it.

Metal ions and organic ligands are not as tunable, but we have had enough success with them to suggest that **the next step is designing metal organic materials** – and then *synthesizing* them.

And that will include developing new design principles.



# Thank you

Places to go ...

- M. Behzad, G. Chartrand & L. Lesniak-Foster, ***Graphs & Digraphs***. Graduate but still accessible introduction to many of the issues.
- I. Herstein, ***Topics in Algebra***. The grand old undergraduate text in the subject.
- K. Hoffman & R. Kunze, ***Linear Algebra***. The monster book with all the toys.
- J. Meier's ***Graphs, Groups and Trees***. Probably the most accessible of the geometric group theory books.
- P. Yale, ***Geometry and Symmetry***. The most accessible book I've found that connects the group theory and the geometry.

(All these are at the math major senior / 1st year grad level.)