Graph Theoretical Optimization for Self-Assembling DNA Nanostructures

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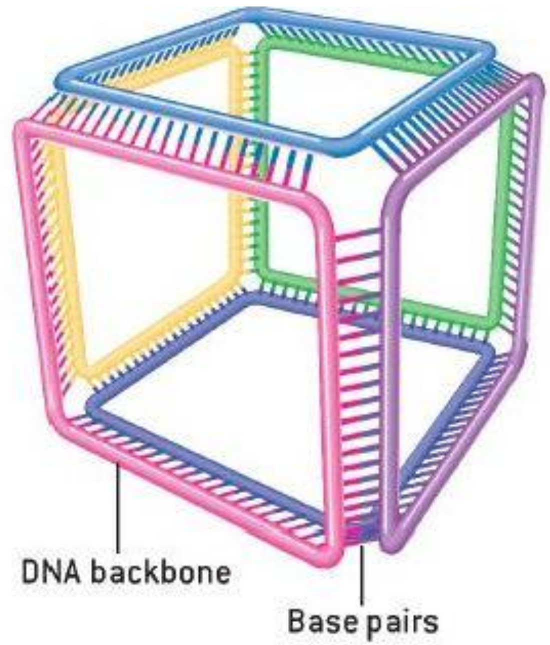
DNA Nanostructures and Their Uses

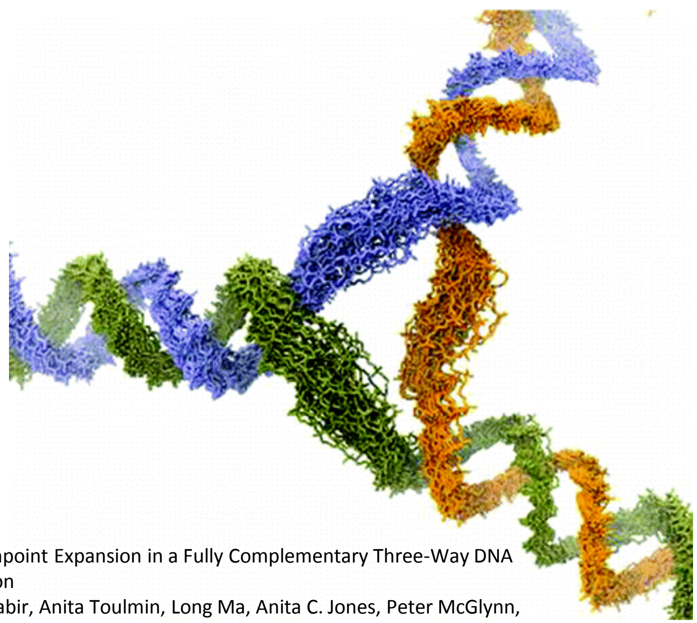
- Made of double stranded DNA
  - Utilize complimentary base pairing
- 2D and 3D geometric shape
- Applications
  - Pharmaceuticals
  - Biosensors
  - Biomolecular computing



https://sites.google.com/site/nanoselfassembly/linear-strand

Flexible Tiles: Building Blocks

- K-armed branched junction DNA molecules
  - Each branch has a sticky end
  - Join together with complimentary base pairing



Branchpoint Expansion in a Fully Complementary Three-Way DNA Junction
Tara Sabir, Anita Toulmin, Long Ma, Anita C. Jones, Peter McGlynn, Gunnar F. Schröder, and Steven W. Magennis
*Journal of the American Chemical Society*2012*134* (14), 6280-6285

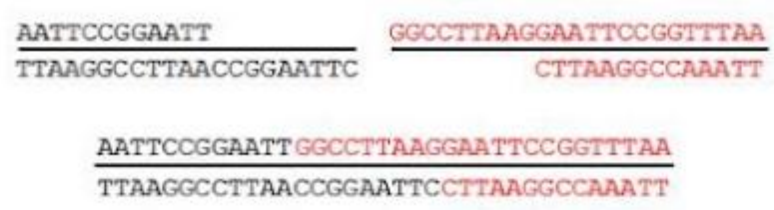
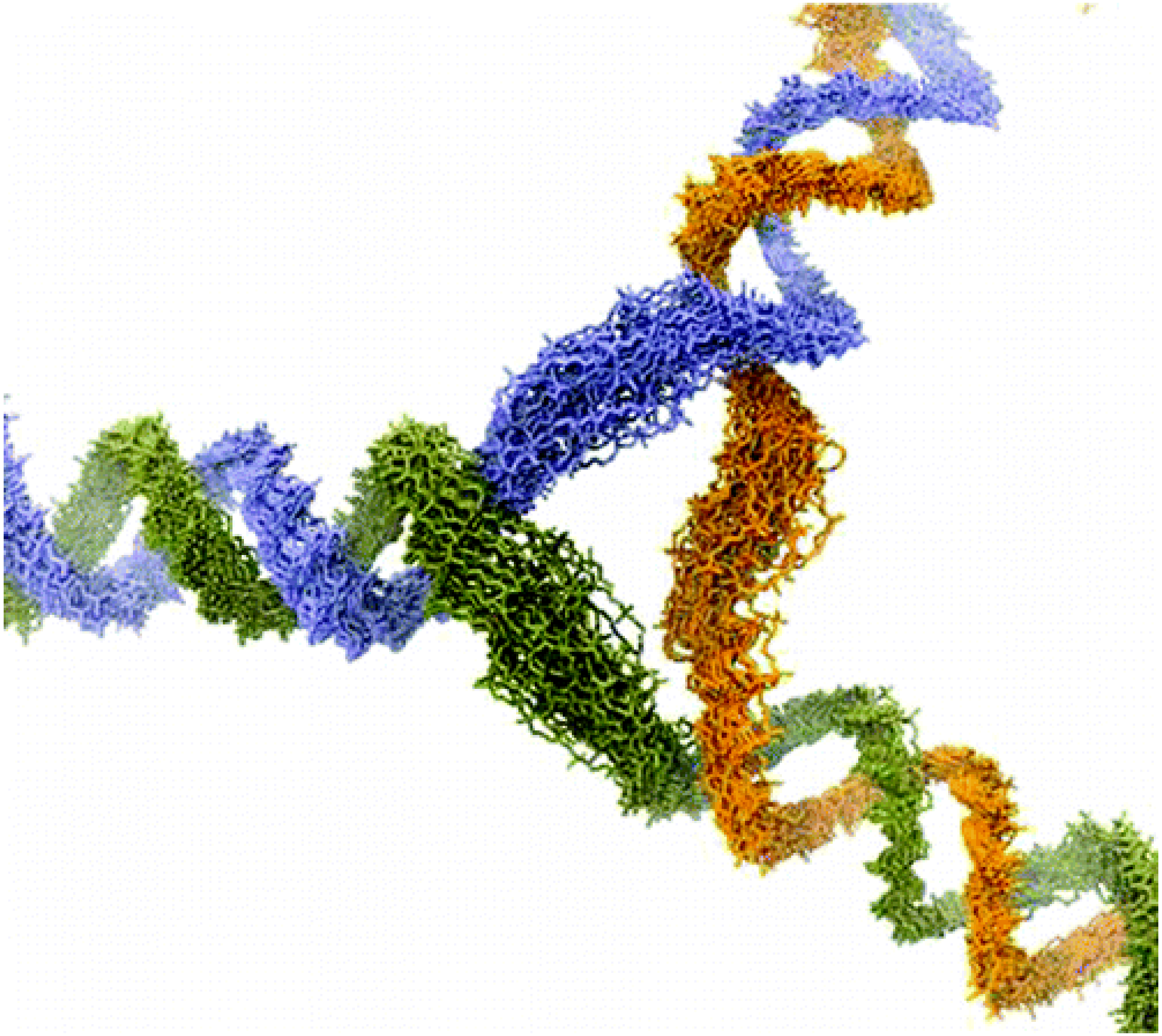
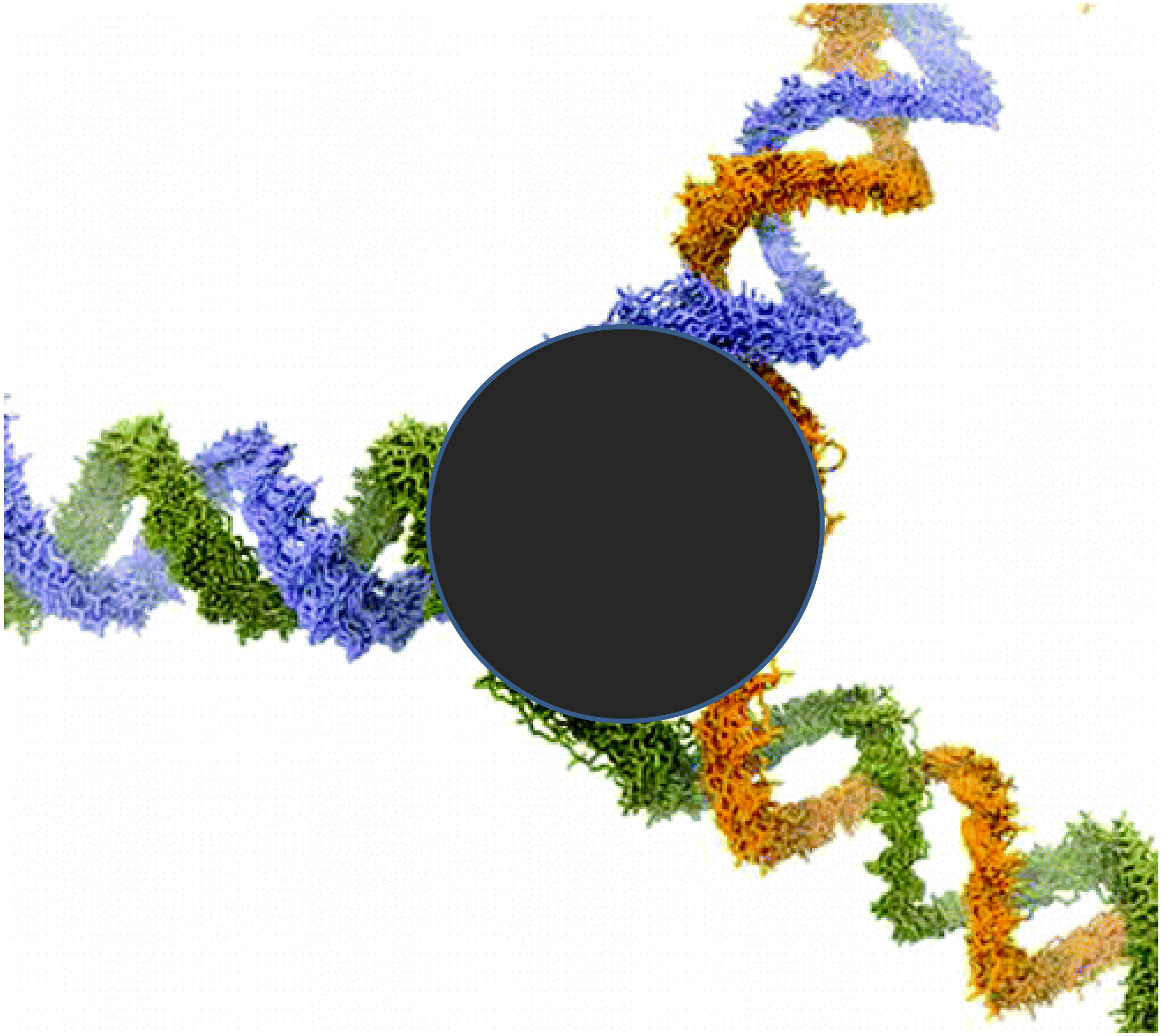
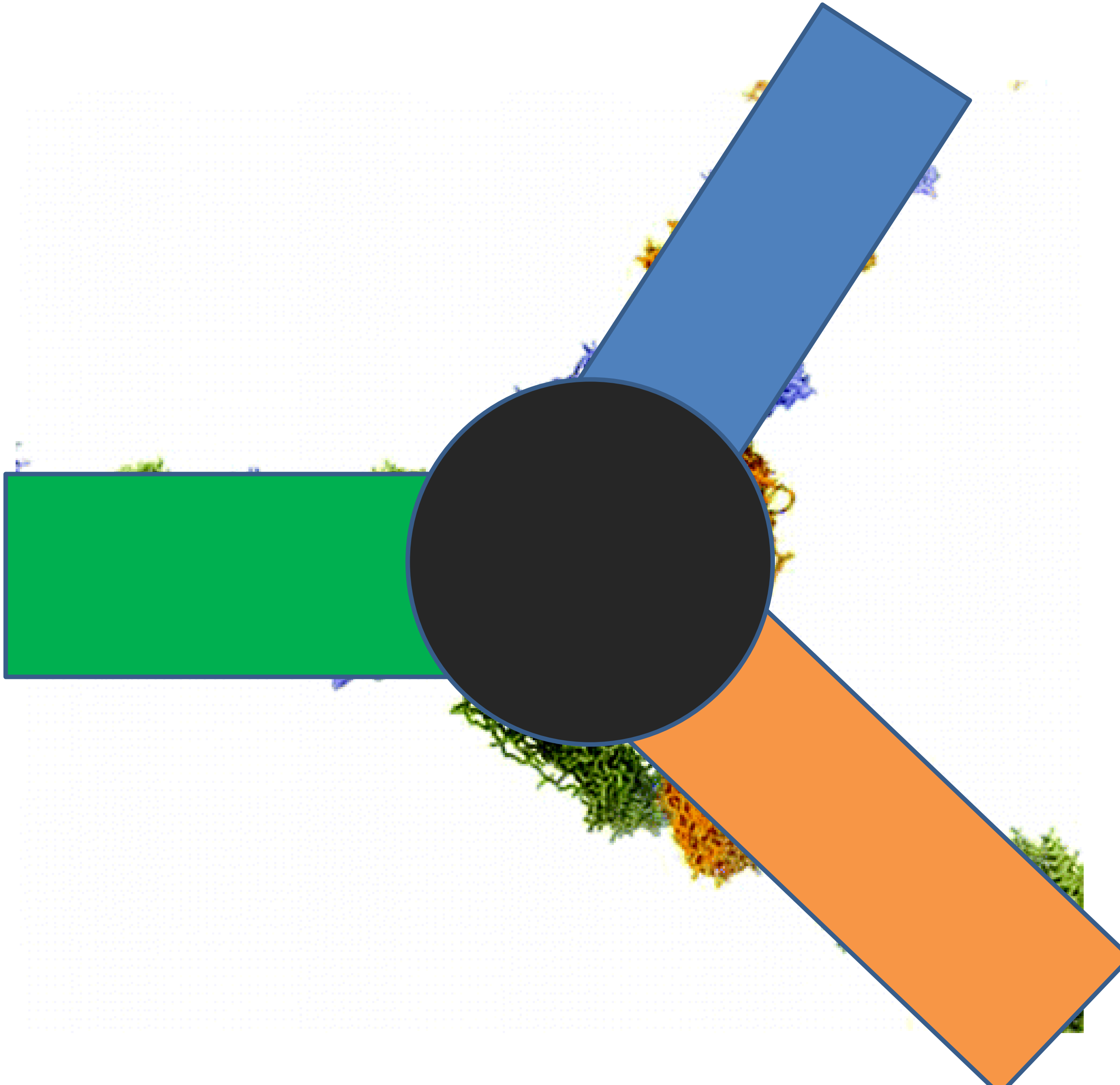


Figure 1: Joining two cohesive ends

https://sites.google.com/site/nanoselfassembly/branched-junction-molecule

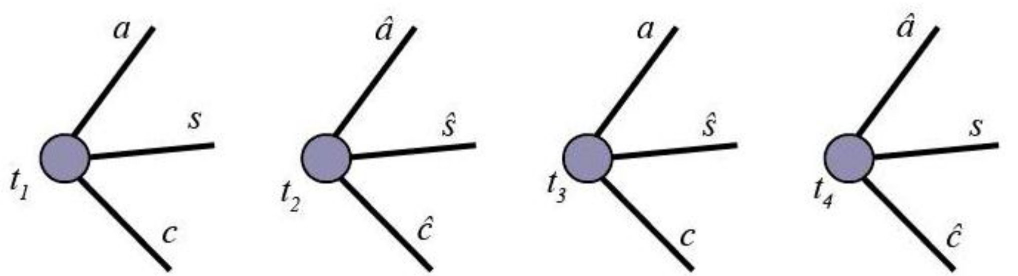






Graph Theoretical Definitions

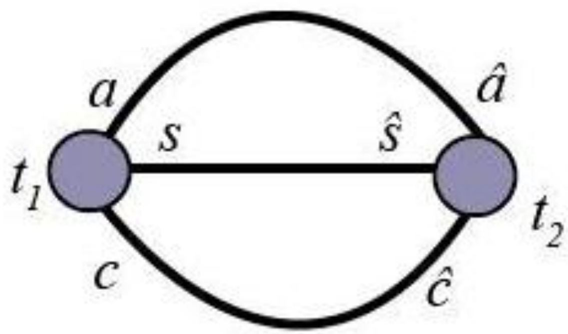
- **Tile:** k-branched junction molecule with cohesive ends fit to a vertex with half edges
- **Cohesive end types:** z is complimentary to ẑ
- **Bond-edge:** a cohesive end together with its complementary cohesive end
- **Pot:** a collection of tiles



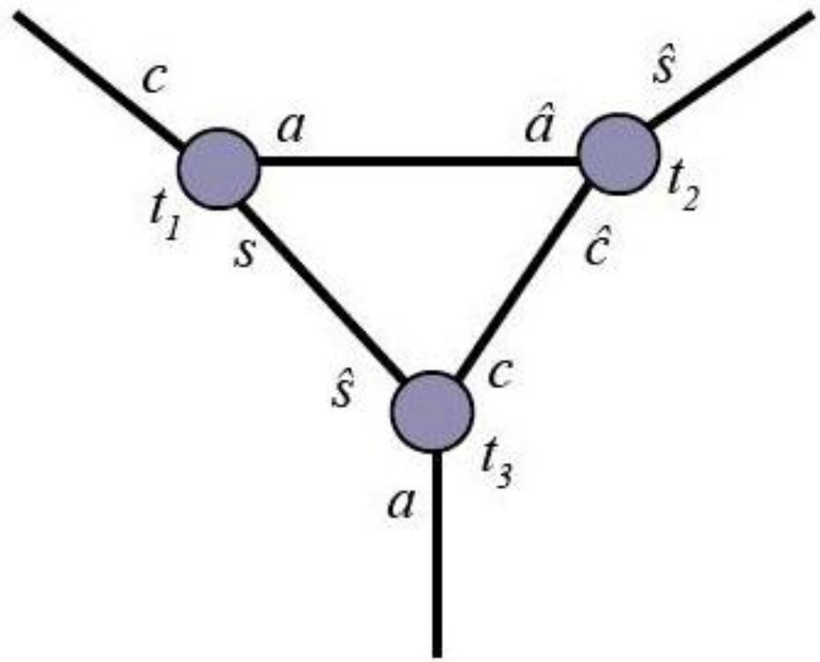
https://sites.google.com/site/nanoselfassembly/branched-junction-molecule

Graph Theoretical Definitions cont.

- **Complete complexes**:



complete complex



incomplete complex

https://sites.google.com/site/nanoselfassembly/branched-junction-molecule

The Problem

Given a target graph, what is the smallest pot which can realize the target in a complete complex

Conditions

- **Scenario 1**: complexes with fewer vertices than the target graph may be formed
- **Scenario 2**: only complexes with the same number of vertices as the target graph may be formed
- **Scenario 3**: no complexes with less than or equal to the number of vertices in the target graph may be formed

Scenario 1

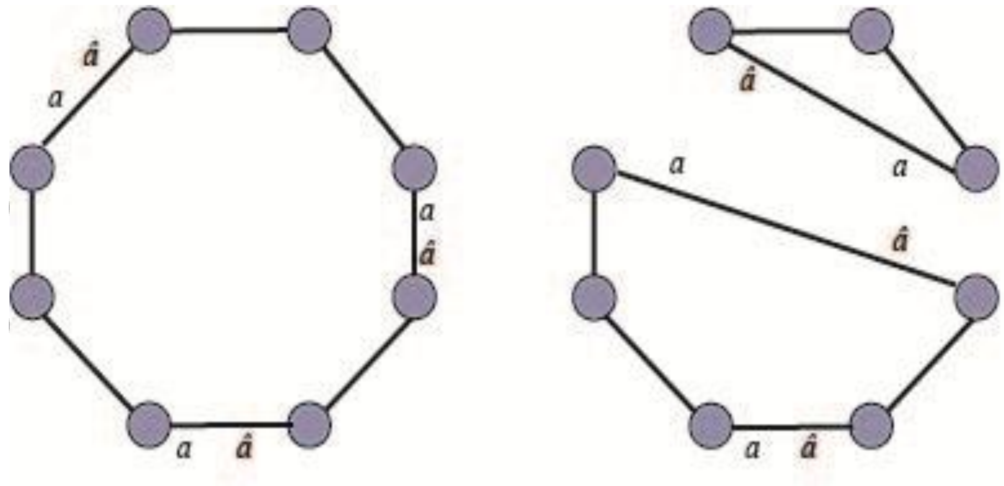


Fig. 5 Smaller graphs formed when there are three edges with the same bond-edge type.

Scenario 3

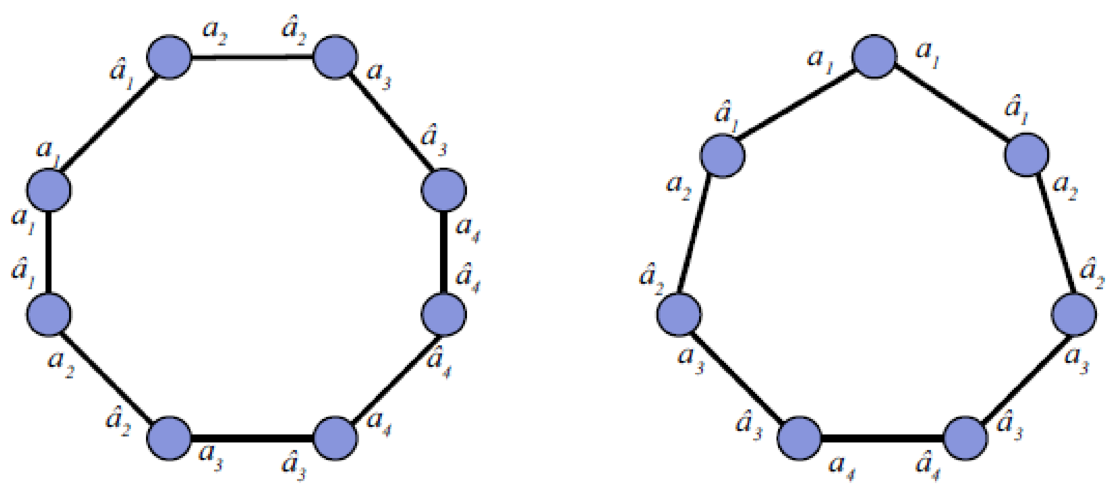
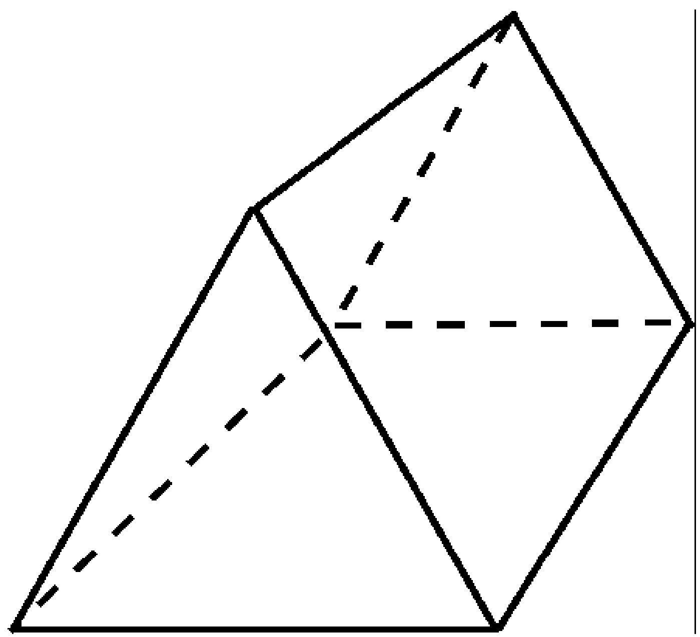


Fig. 6 Cycle constructions.

Right Prisms in Scenario 2

Goal: Find a pot with the minimum number of tiles for right prisms



http://www.narragansett.k12.ri.us/resources/necap%20support/gle_support/Math/resources_geometry/3d_shapes.htm

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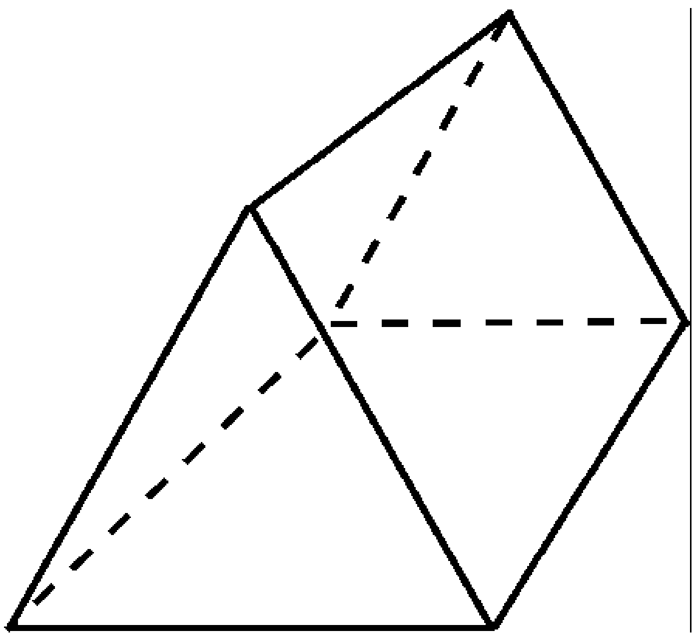

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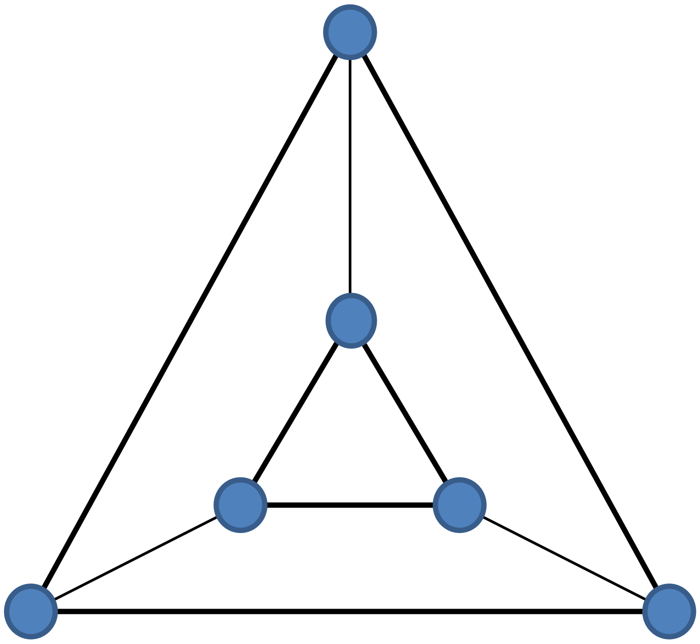

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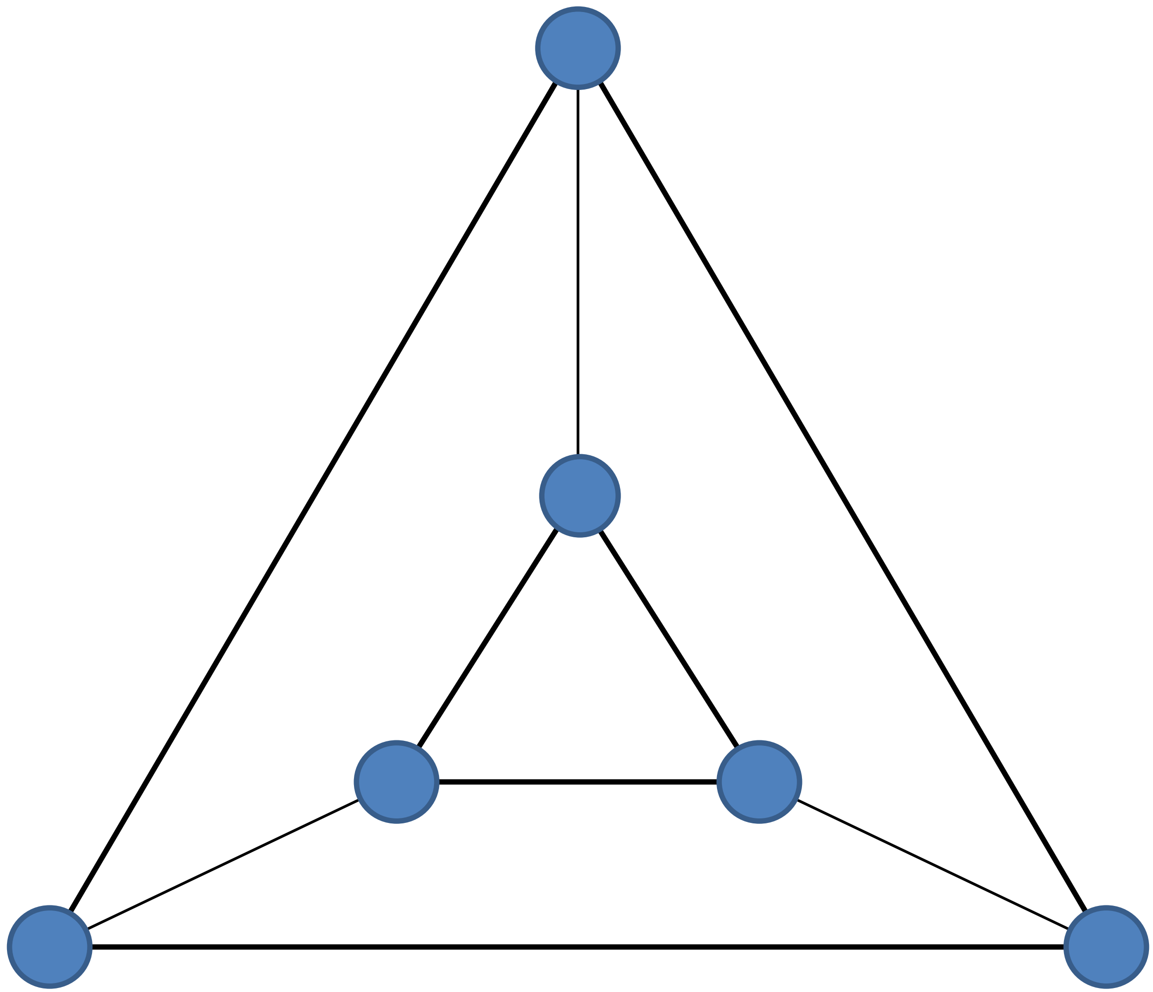
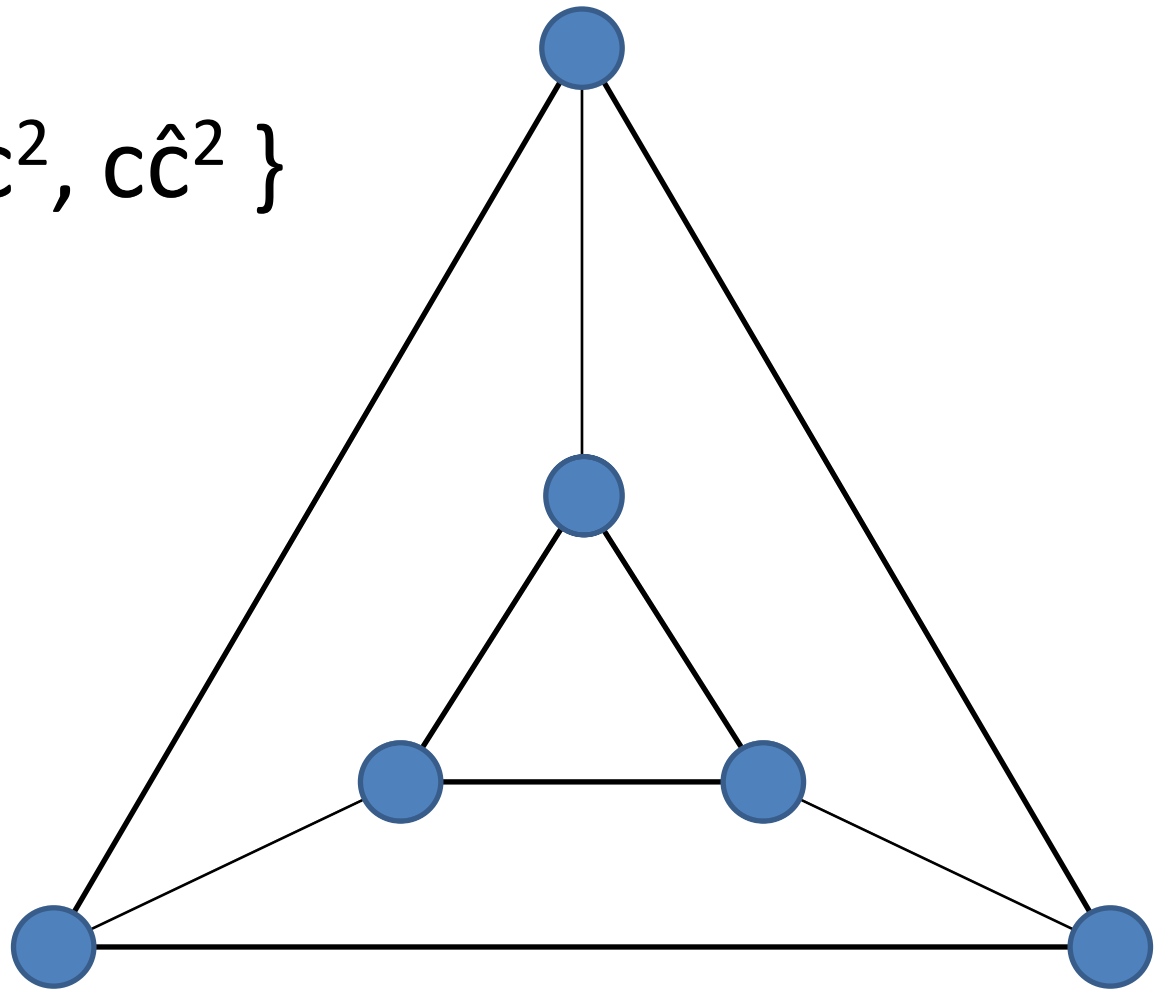


Right Prisms in Scenario 2

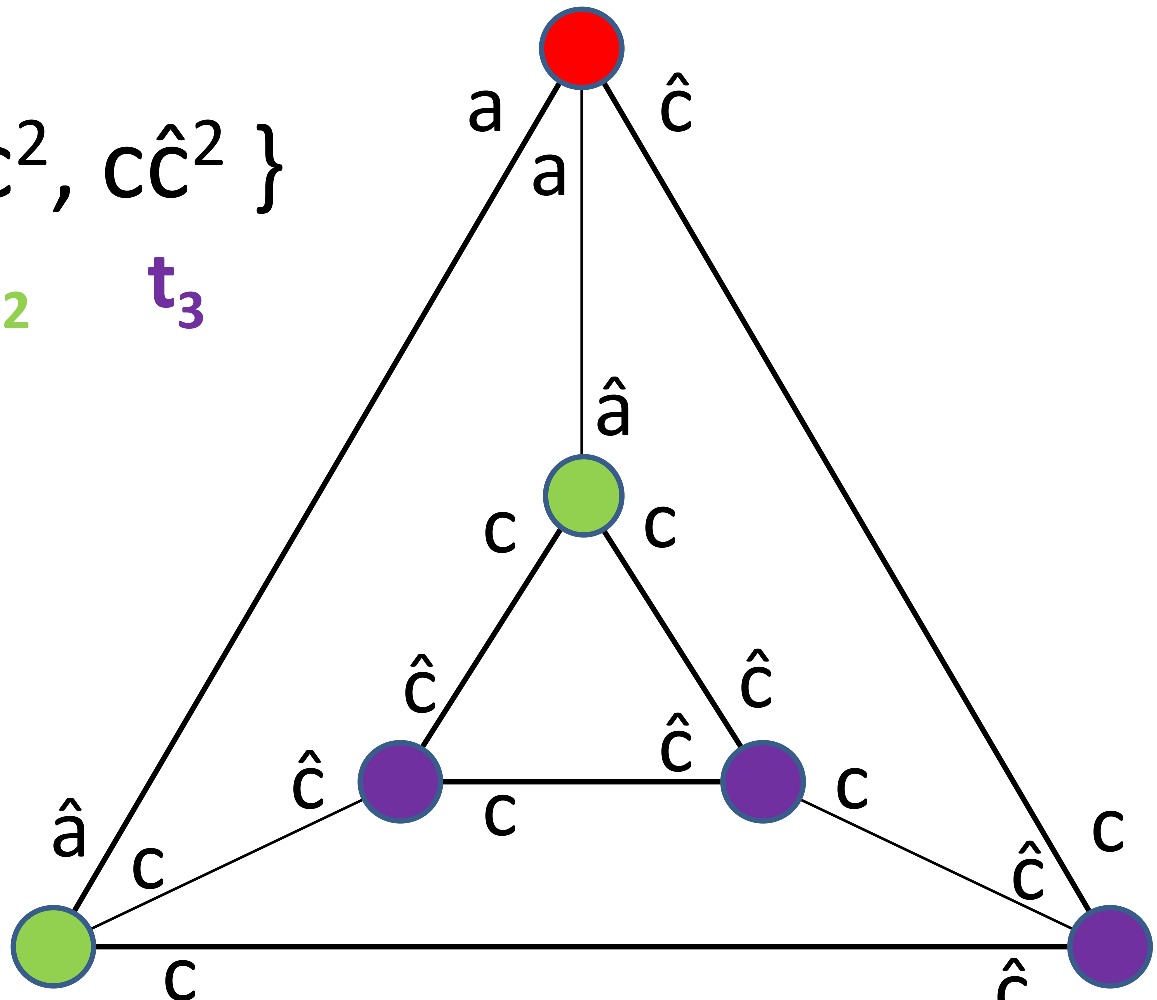
P = { a^2c, $\hat{a}c^2$, $c\hat{c}^2$ }



Right Prisms in Scenario 2

$P = \{ a^2\hat{c}, \hat{a}c^2, c\hat{c}^2 \}$

t_1 t_2 t_3



Right Prisms in Scenario 2

Prove: *P* makes nothing smaller

$P = \{ a^2\hat{c}, \hat{a}c^2, c\hat{c}^2 \}$

$$2r_1 - 1r_2 = 0$$
$$-1r_1 + 2r_2 - 1r_3 = 0$$
$$r_1 + r_2 + r_3 = 1$$

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$$\begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$

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$$\begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 0 & 0 & \frac{1}{6} \\ 0 & 1 & 0 & \frac{1}{3} \\ 0 & 0 & 1 & \frac{1}{2} \end{bmatrix}$$

$S(P) = \{ 1/6 , 1/3 , 1/2 \}$

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Proposition: smallest complete complex created from a pot is the LCM in the denominators of the spectrum

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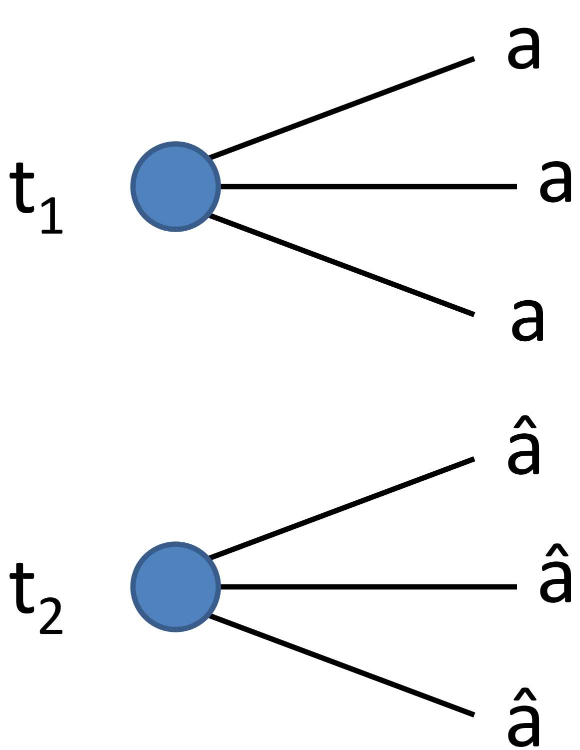
→ Need 6 vertices

Right Prisms in Scenario 2

Prove: < 3 tiles won't work

Case: 1 bond edge type, 2 tile types



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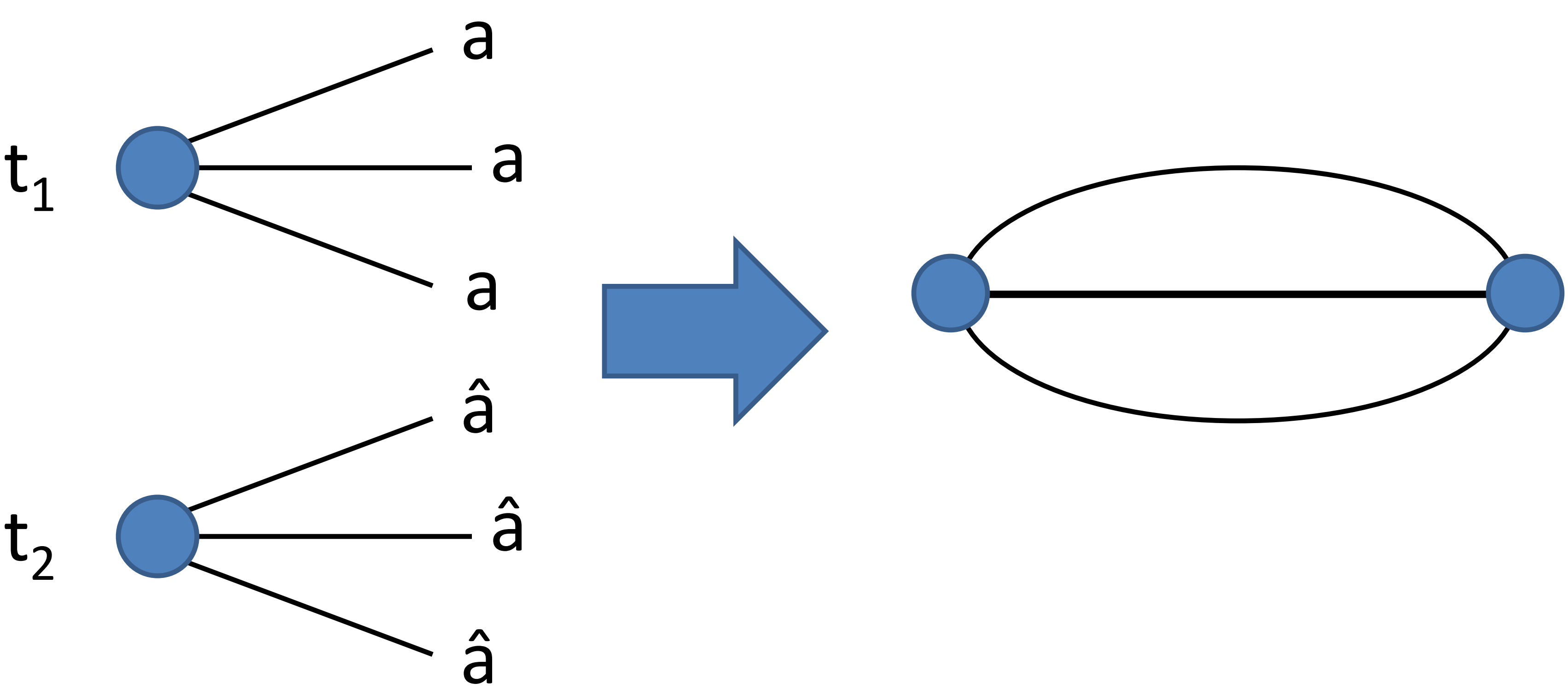

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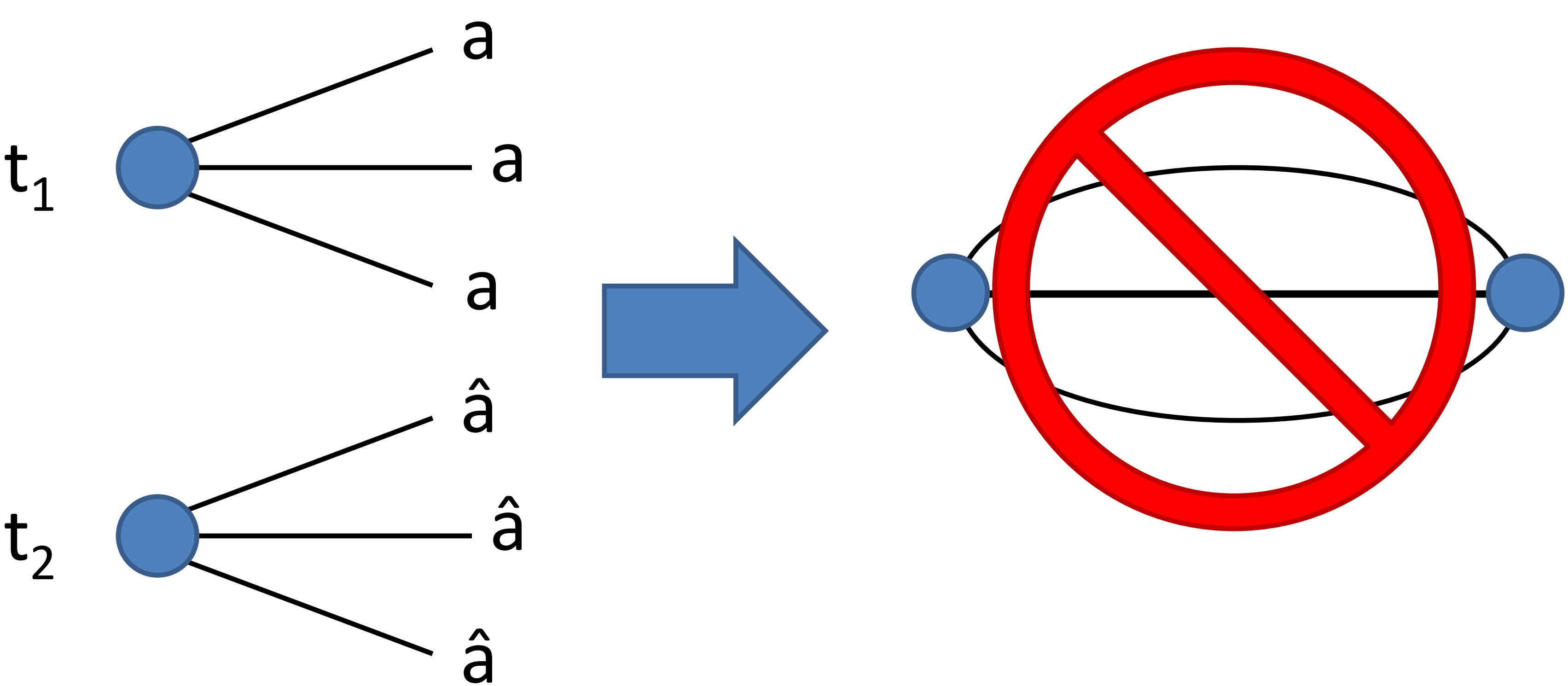
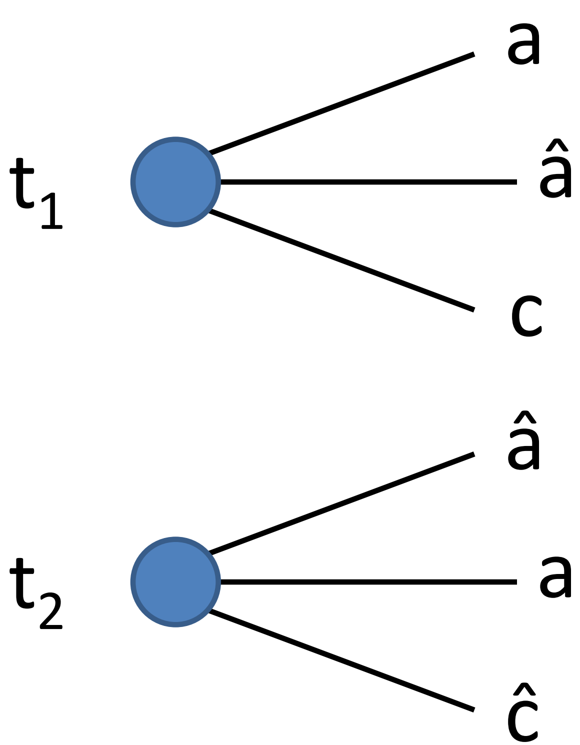


Right Prisms in Scenario 2

Prove: < 3 tiles won't work

Case: 2 bond edge types, 2 tile types



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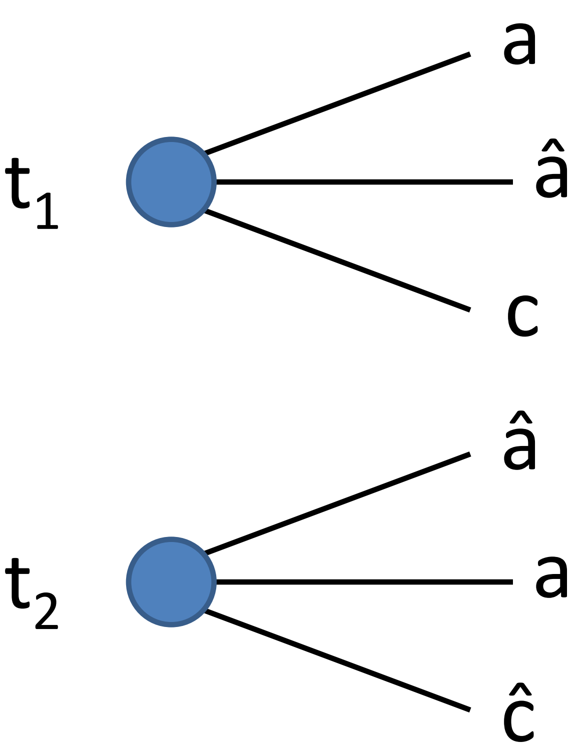
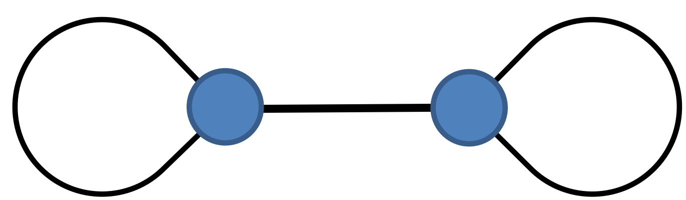


$$\begin{bmatrix} 0 & 0 & 0 \\ 1 & -1 & 0 \\ 1 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & \frac{1}{2} \\ 0 & 1 & \frac{1}{2} \\ 0 & 0 & 0 \end{bmatrix}$$

$S(P) = \{ ½ , ½ \}$



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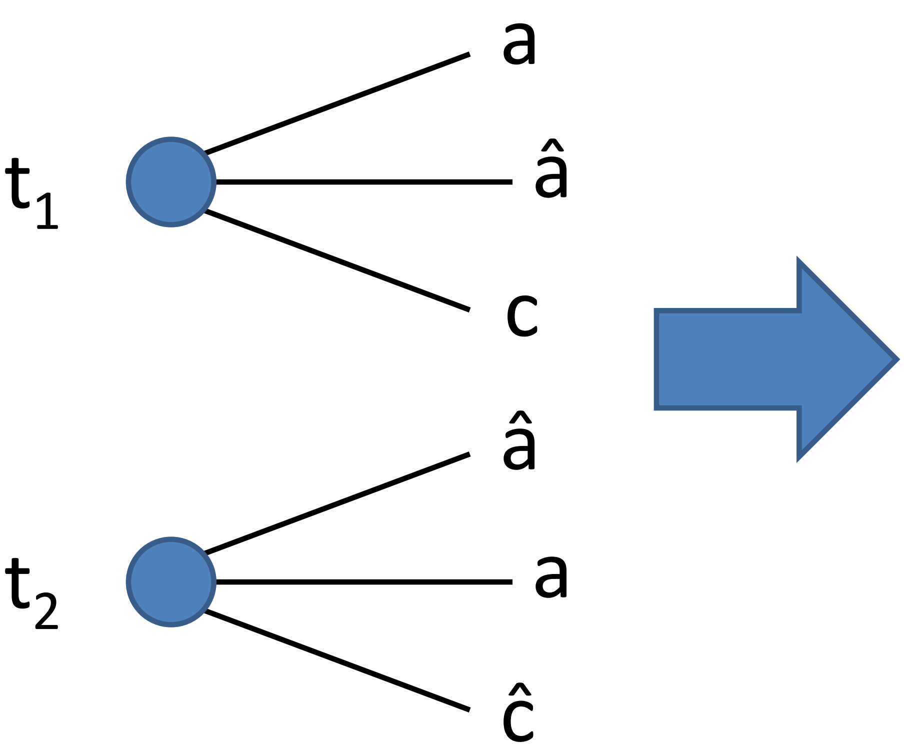

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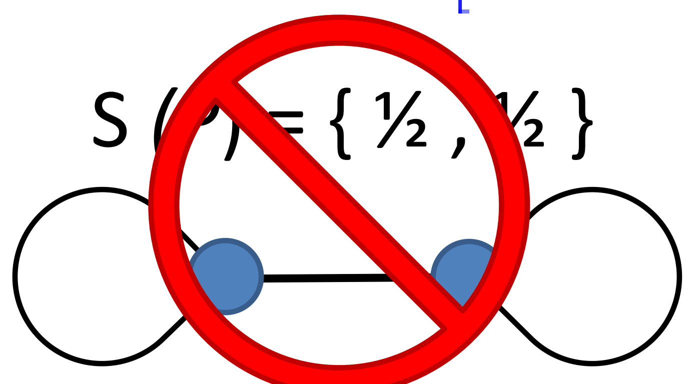

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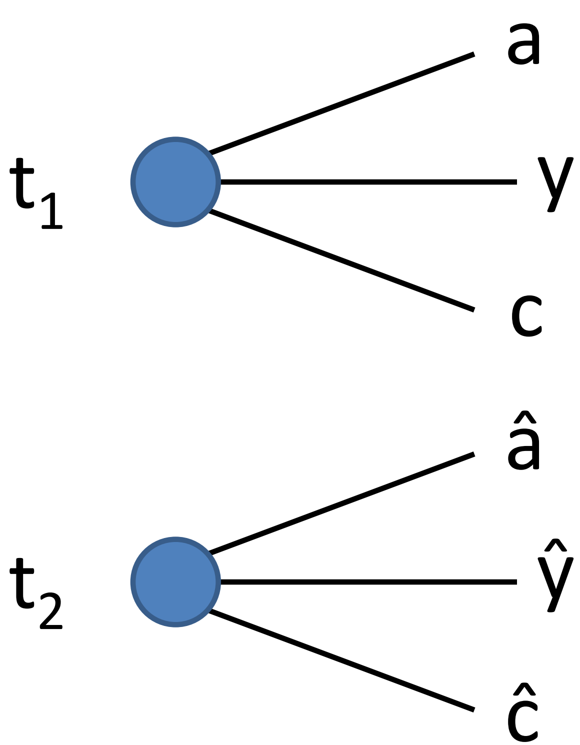

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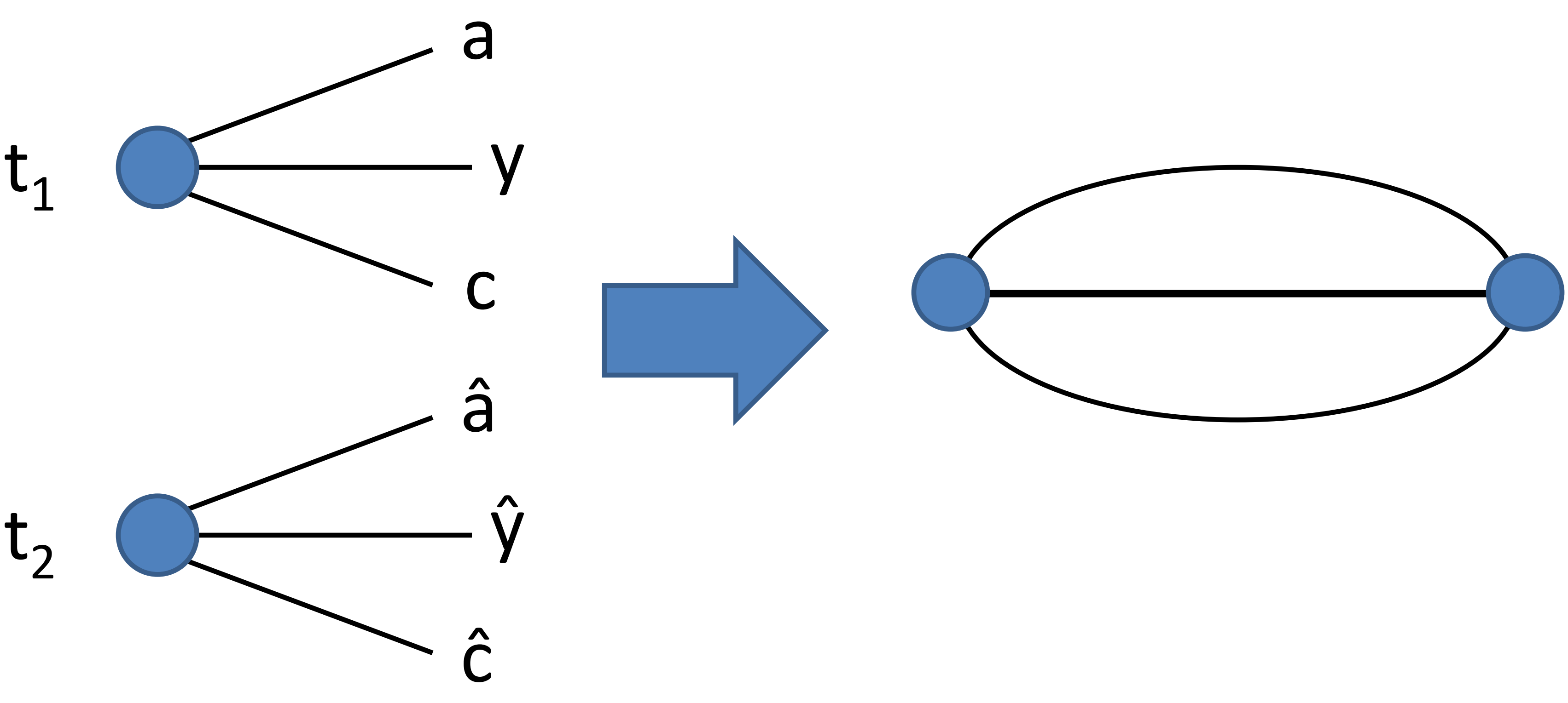

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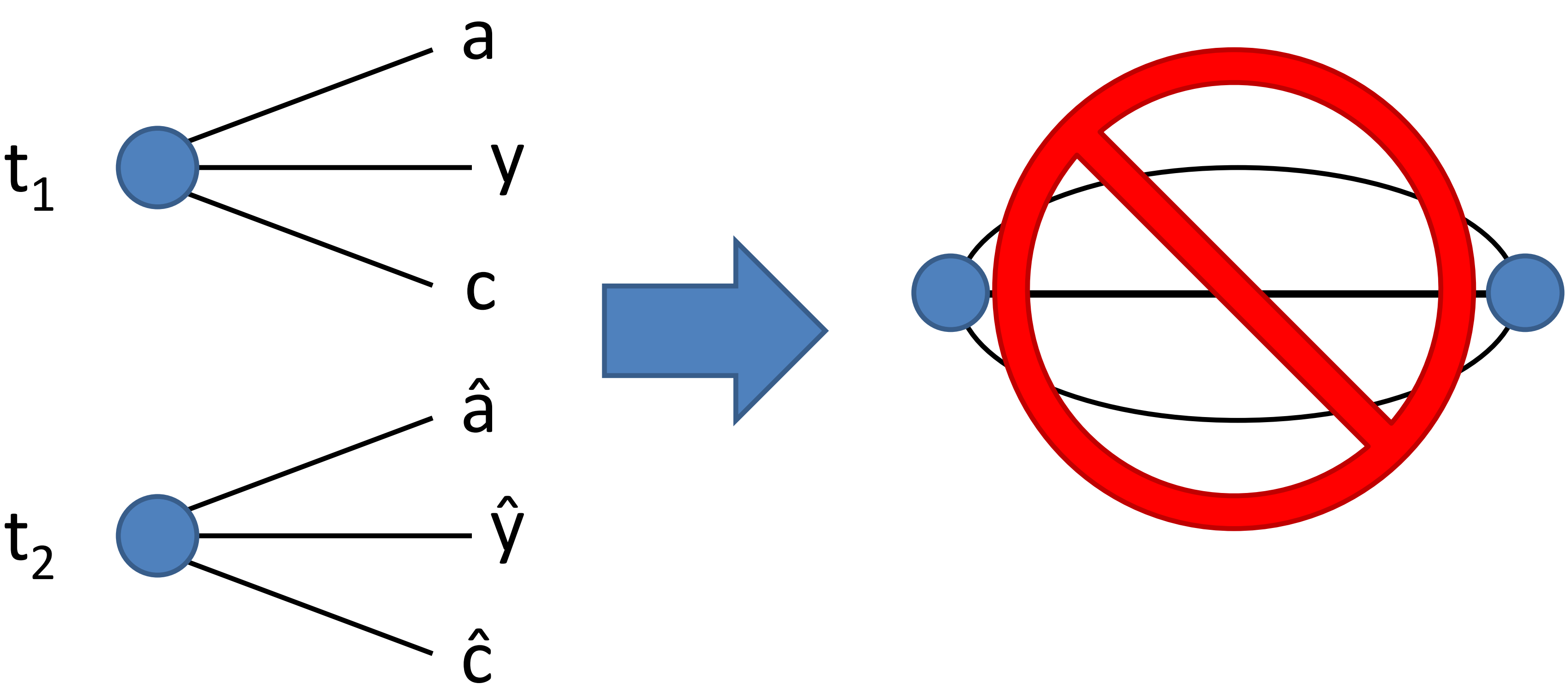
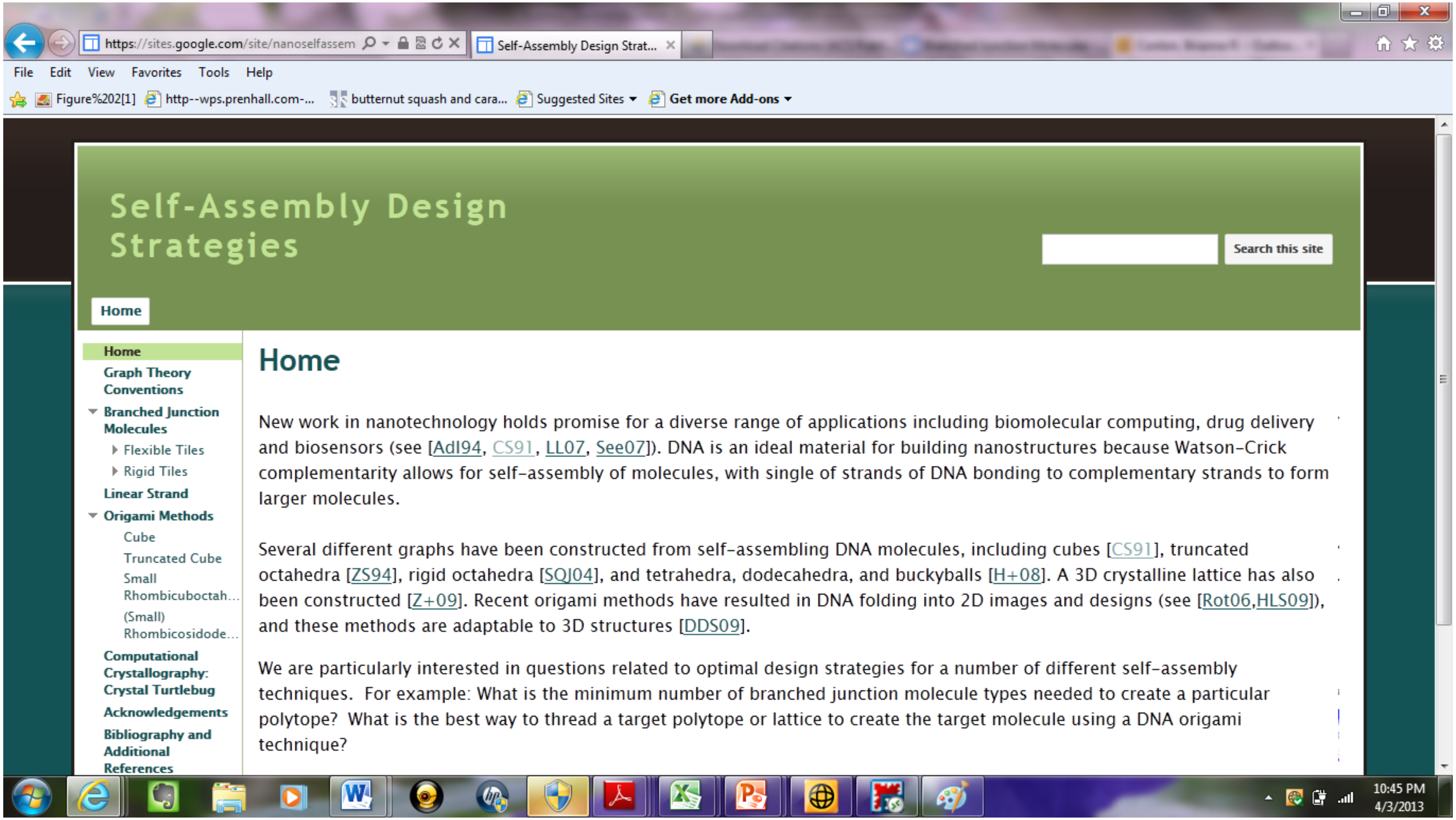


Right Prisms in Scenario 2

For triangular prisms: $P = 3$ tile types

Goal: extend to n-gon based prisms



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Questions?