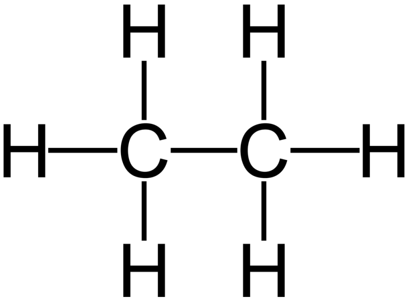
From Graphs to Graphite!

Modelling Molecules with Graphs

Abhilash Saha (21MS)
as21ms054@iiserkol.ac.in

July 4, 2022

Why does C_2H_6 look like this?



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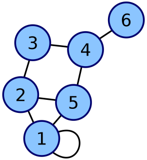

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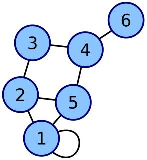

Definition of a Graph

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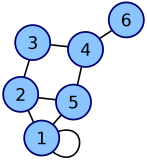

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A **graph** G consists of a finite set V of **vertices** and a collection E of pairs of vertices called **edges**.

The vertices are represented by points on the plane, and the edges by lines (not necessarily straight) joining the vertices.

Some Terms Related to Graphs :)

- If an edge e joins vertices x and y then x and y are adjacent and e is incident with both x and y.
- Any edge joining a vertex x to itself is called a loop.
- Note that E is a collection, not necessarily a set. This is to allow repeated edges. If two or more edges join the same two vertices, they are called multiple edges.
- A graph is said to be simple if it has no loops or multiple edges.
- The number of edges incident with a vertex v in a graph without loops is called the degree or valency of v and is denoted by $d(v)$.

The Handshaking Lemma

When a graph contains a loop, the loop is considered to contribute twice to the degree of its incident vertex.

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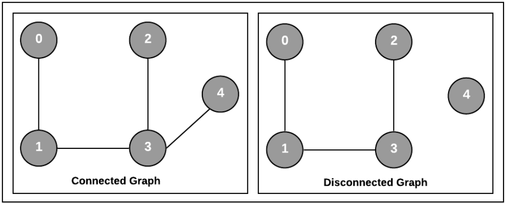
At a party, the total number of hands shaken is twice the number of handshakes. It has an immediate corollary: *In any graph, the sum of the vertex degrees is even.*

Connected Graphs

Path: A sequence of edges which joins a sequence of vertices which are all distinct (and since the vertices are distinct, so are the edges).



Connectedness

A graph is connected if, for each pair x, y of vertices, there is a path from x to y . A graph which is not connected is made up of a number of disconnected pieces, called components.

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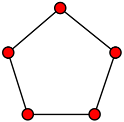

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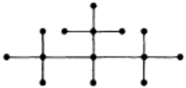

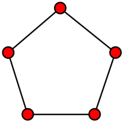

"Pendant vertices": Vertex of degree 1.

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Consider the path that starts at l, and follows to any other vertex v. If v is a leaf, we are done. Otherwise it must be adjacent to at least another vertex u. Repeat the reasoning for u.

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Thereby, our path can only end in a leaf or in an already visited vertex creating a cycle (which is not possible by assumption since the graph we consider is a tree).

What is a "tree-like" molecule?

Let T be a simple graph with p vertices. Then the following statements are equivalent:

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2. T has $p-1$ edges and no cycles.
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$$1 \implies 2 \implies 3 \implies 1$$

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- Remove w and its incident edge from T to obtain a tree T' with k vertices.
- By the induction hypothesis, T' has $k - 1$ edges; so T has $(k - 1) + 1 = k$ edges as required.

Proof: If a simple graph T with p vertices has $p-1$ edges and no cycles then it is connected.

- Suppose T has $p-1$ edges and no cycles, and suppose it consists of t components, $T_1, \ldots, T_t$, each of which has no cycles and hence must be a tree.

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- Then $\sum_i p_i = p$, and the number of edges in T is $\sum_i (p_i - 1) = p - t$.
- So $p - t = p - 1 \implies t = 1$, so that T is connected.

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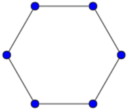

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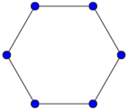

- The resulting graph must be a tree, with p vertices and $q < p-1$ edges, contradicting the previous result.

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- The degree of a vertex is the "valency" of that atom– the number of atoms that it is connected with.
- In case an atom makes multiple bonds, its valency is reduced by one, per bond.

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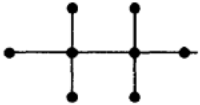

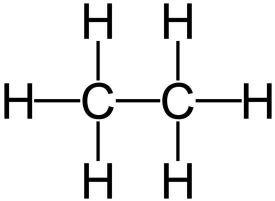

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a	b	q
1	2	8
3	0	9

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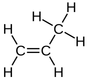
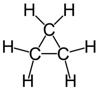


1-propene



cyclopropane

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There is no edge connecting v_{n-1} and v_n, which means there is no path from v_{n-1} to v_n. This contradicts the fact that G is connected.

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- As the molecule is a connected graph, number of edges $q \geq 3n+2-1 = 3n+1$.
- Thus $q = 3n+1 = p-1$, which means that all our inequalities must attain the maximum. Thus all carbon atoms have degree four and the molecule is a tree.

References

- *A First Course in Discrete Mathematics*, Ian Anderson.
- *Introduction to Graph Theory*, Douglas B. West.

Thank You!