Cayley’s Theorem

Cayley’s Formula

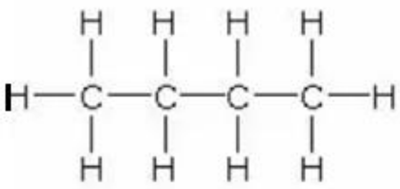
- In 1857, Arthur Cayley discovered trees while he was trying to count the number of structural isomers of the saturated hydrocarbons (or paraffin series) C_kH_{2k+2} .
- He used a connected graph to represent the C_kH_{2k+2} molecule. Corresponding to their chemical valencies, a carbon atom was represented by a vertex of degree four and a hydrogen atom by a vertex of degree one (pendant vertices). The total number of vertices in such a graph is

$$n = 3k + 2,$$

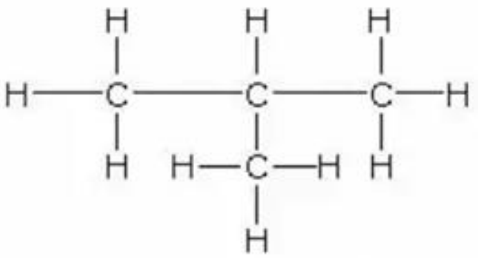
and the total number of edges is

$$\begin{aligned} e &= \frac{1}{2}(\text{sum of degrees}) = \frac{1}{2}(4k + 2k + 2) \\ &= 3k + 1. \end{aligned}$$

Since the graph is connected and the number of edges is one less than the number of vertices, it is a tree. Thus the problem of counting structural isomers of a given hydrocarbon becomes the problem of counting trees.



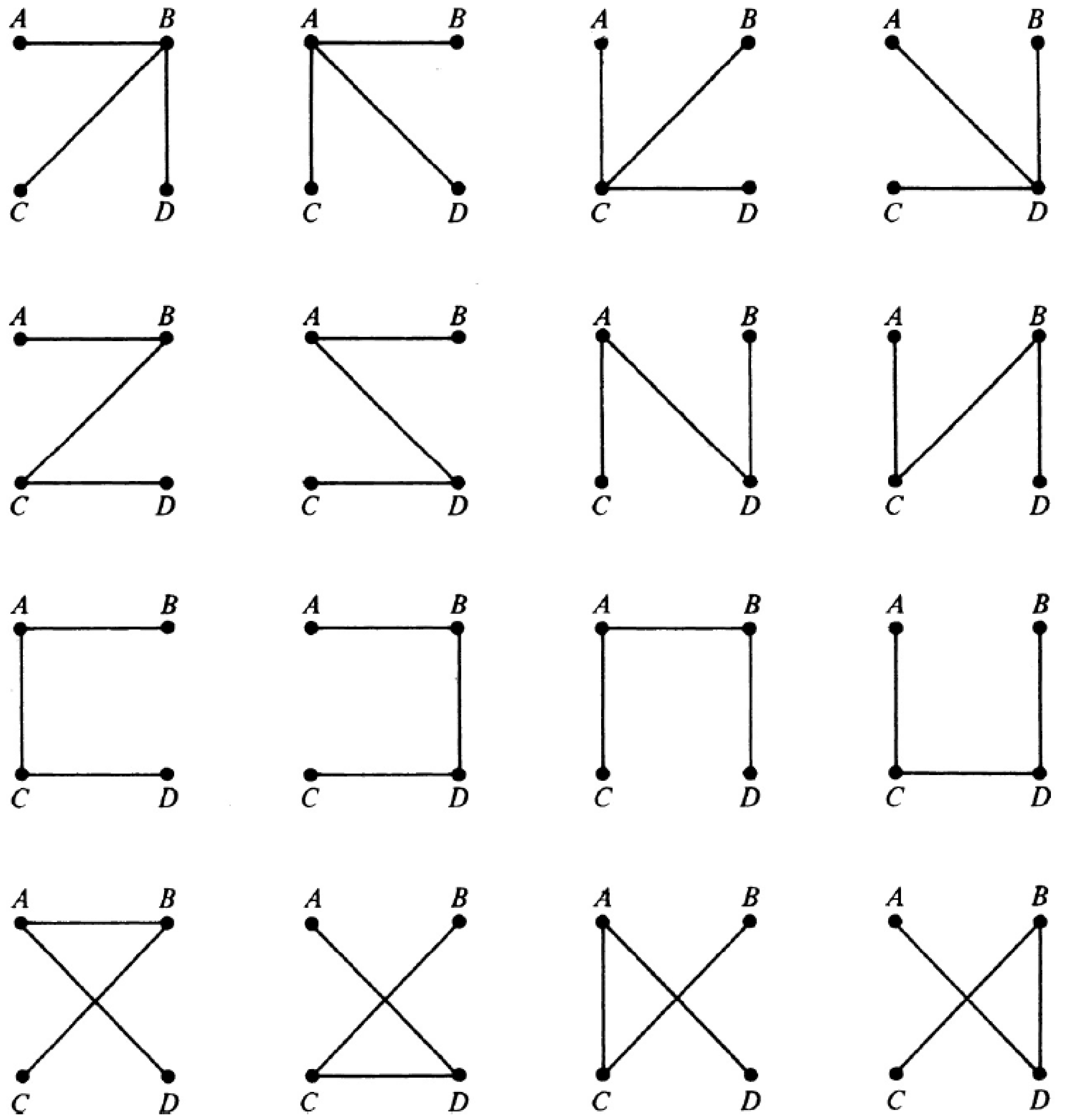
Butane (C_4H_{10})



2-methyl propane (C_4H_{10})

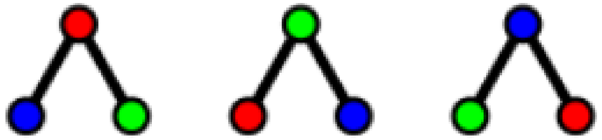
what is the number of different trees that one can construct with n distinct (or labeled) vertices?

n=4



n=1

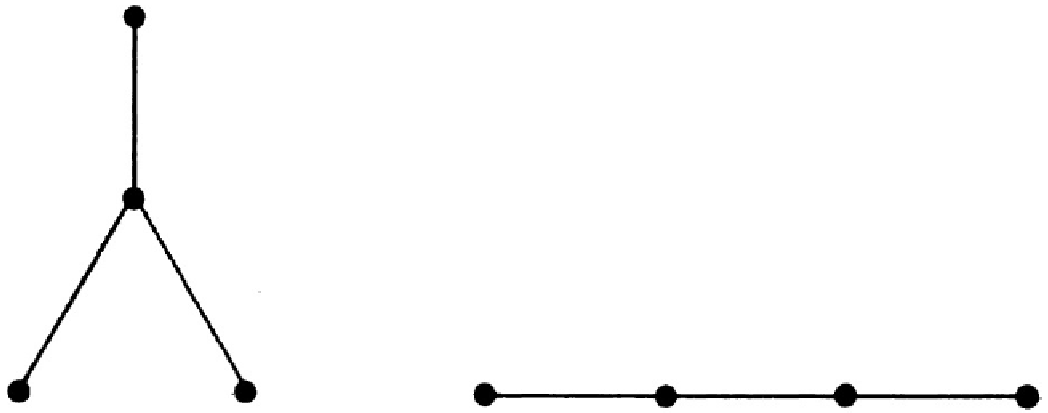
n=2



n=3

Cayley’s Theorem

- The number of labeled trees with n vertices ($n \geq 2$) is n^{n-2}.



All trees of Unlabeled vertices, n=4

Proof of Cayley's

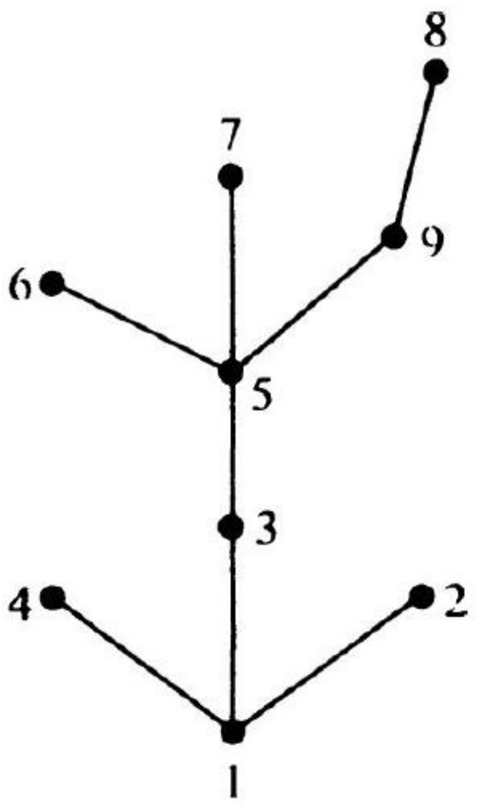
- Let the n vertices of a tree T be labeled 1, 2, 3, . . . , n.
- Remove the pendant vertex (and the edge incident on it) having the smallest label, which is, say, a1. Suppose that b1 was the vertex adjacent to a1. Among the remaining n − 1 vertices let a2 be the pendant vertex with the smallest label, and b2 be the vertex adjacent to a2. Remove the edge (a2, b2).
- This operation is repeated on the remaining n − 2 vertices, and then on n − 3 vertices, and so on.
- The process is terminated after n − 2 steps, when only two vertices are left. The tree T defines the sequence

$$B = (b_1, b_2, \ldots, b_{n-2})$$

- Conversely, given a sequence of n − 2 labels, an n-vertex tree can be constructed uniquely, as follows:
- Determine the first number in the vertex sequence that does not appear in the sequence.

$$(b_1, b_2, \ldots, b_{n-2})$$

- This number clearly is a1. And thus the edge (a1, b1) is defined. Remove b1 from B sequence and a1 from vertex sequence. In the remaining vertex sequence find the first number that does not appear in the remainder of B. This would be a2, and thus the edge (a2, b2) is defined.
- The construction is continued till the sequence B has no element left.
- Finally, the last two vertices remaining in the vertex sequence are joined.



- Nine-vertex labeled tree, which yields sequence

  (1, 1, 3, 5, 5, 5, 9).