LIVING APART TOGETHER: ON GRAPH THEORY AND POLYMER CHEMISTRY

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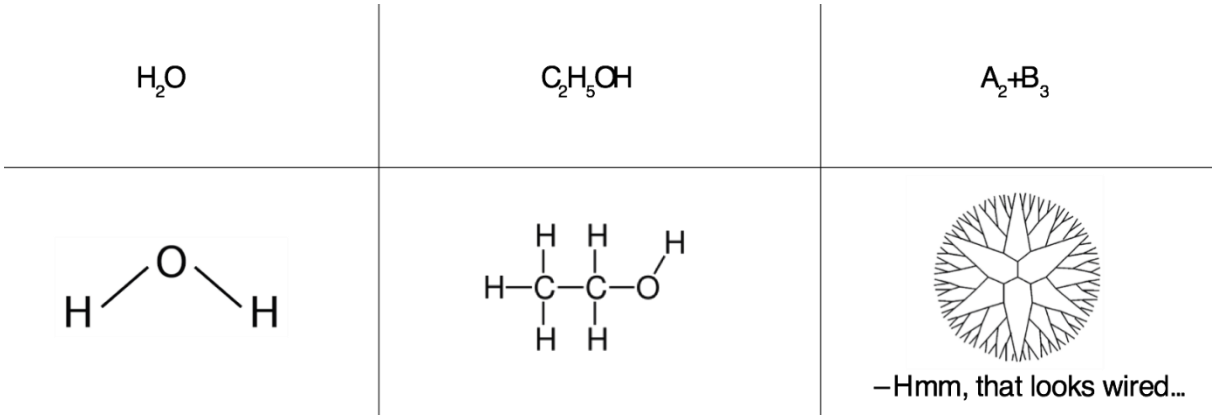

Graph theory and chemistry has always been bound by intricate relationships. This theory centers its attention on the connectivity between atoms but not their spatial configurations. Graph theory is attractive not just due to pure convenience of representing a molecule as a diagram made of nodes and sticks. On many occasions such reduction revealed a deep connection between the structure and the properties, that is to say, a connection between the chemistry and the physics. Notably, differences in boiling temperatures of isomers, formation heats of conjugated hydrocarbons, and vibrational potential energy of proteins has been successfully explained by graph theory.

Of course, to apply the theory one must exactly know the molecular graph to start with. Such a prerequisite seems to be non-restrictive, however, it is quite fatal for the graph theory when one considers branched polymers or gels. The situation with polymers is radically different, as we cannot talk about molecules with a specific molecular graph. Distinct polymers undergo different degree of polymerization and one possibly ends up with as many different irregular molecular structures as molecules in the system.

In this talk, I will discuss various results appearing in Refs.[1-5] and review the recent developments in a quite young filed of *random graphs*, a branch of graph theory that operates with probability distributions over graphs. Random graphs allow us to efficiently handle the variability and randomness of polymer structures and, more importantly, to connect experimental observables with the polymerization conditions.

References

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