

Uncertainty and Regioselectivity in Chemistry

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This lecture begins with a consideration of uncertainty in chemistry. Physics and mathematics already have well established principles of uncertainty via the work of Schroedinger and Gödel, respectively. Chemistry likewise has inherent uncertainty, a fact illustrated by a potentially useful polymer-induced catalysis that, owing to complexity issues, cannot ever be understood at a fundamental level. The lecture then moves to a discussion of modeling enzyme-like regioselectivity. Enzymes are capable of differentiating among multiple positions of almost identical reactivity (such as reacting specifically at only one site in a long hydrocarbon chain). Chemists' ability to do this is only at a primitive stage, reflecting the fact that regioselectivity is actually a more difficult problem than stereoselectivity. An example in organic chemistry where only one of two nearly identical hydroxy groups is oxidized is presented.