

Reasoning and Representation: the Sketching of Organic Chemical Reaction Mechanisms

Position paper for CHI 2006 Workshop entitled "Sketching" Nurturing Creativity: Commonalities in Art, Design, Engineering, and Research

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For nearly a century organic chemists have developed a method of sketching chemical reaction mechanisms in order to reason-out the structural transformations that convert one set of molecules into another. Known informally as *pushing electrons (or curly arrows)*, it is a form of chemical illustration in which a sequence of structures is drawn to represent the movement of electrons and nuclei from starting materials to final products. By pushing electrons, organic chemists use illustrations as a way of phrasing an idea or to argue *what-if* scenarios for chemical events.

Figure 1 shows an example of a reaction mechanism for a simple molecular rearrangement. Beginning with knowledge of the starting material's structure (upper left) and end products (lower left), the chemist attempts to explain their distribution by postulating possible structural intermediates and rearrangement pathways. The imagery is standard chemical iconography of atoms (vertices) and bonds (edges) in which each two-dimensional drawing concisely communicates three-dimensional structural information that is firmly grounded in chemical theory. Each illustration acts as a 2D interface between its creator and the reader in which the three-dimensional model in the creator's mind is mapped onto the 2D image, which in turn is transformed into the reader's mental model employing his knowledge of stereochemistry.

Organic chemists use these diagrams as mathematicians or philosophers use abstract symbols to derive formulas or form proofs. Indeed, these sketches are structural geometric proofs, consistent with Plato's supposition that geometry is a

philosophical language. By definition, geometry is the formal study of spatial order through the measure and relationship of form. For Plato this meant that these chemical diagrams must operate within a hierarchy of abstraction. To him, the lowest level of abstraction would be a molecule's physical existence. On a higher level are the guiding models behind the construction of all molecules such as the structural chemical rules or theories - pure formal ideas or specifications without physical manifestation. On the highest level are the universal processes or dynamical patterns that can be considered independently of any structure or material form. The general chemical reaction patterns of oxidation-reduction, functional group transfer, hydrolysis, and isomerization, realized through specification and modification of a molecule's structural form, are examples of this highest level of abstraction. Hence, these diagrams support layers of representation, allowing chemists to freely move from physical entity to theory to process.

A strength of pushing electrons is that it requires only pencil and paper, and it may be performed by an individual or in groups. And because chemical iconography transcends medium, these diagrams may be combined with physical or computer rendered models to characterize molecular structure and dynamics at different time scales. In the end, all these depictions are underpinned by quantum mechanics as expressed through molecular orbital theory. This theory may be invoked at degrees of rigor ranging from complex quantitative computations to qualitative diagrams. As such, quantum theory supports levels of metaphorical representations of electrons from particles to clouds-of-probability. Ideally, the dragging of an electron dot across a

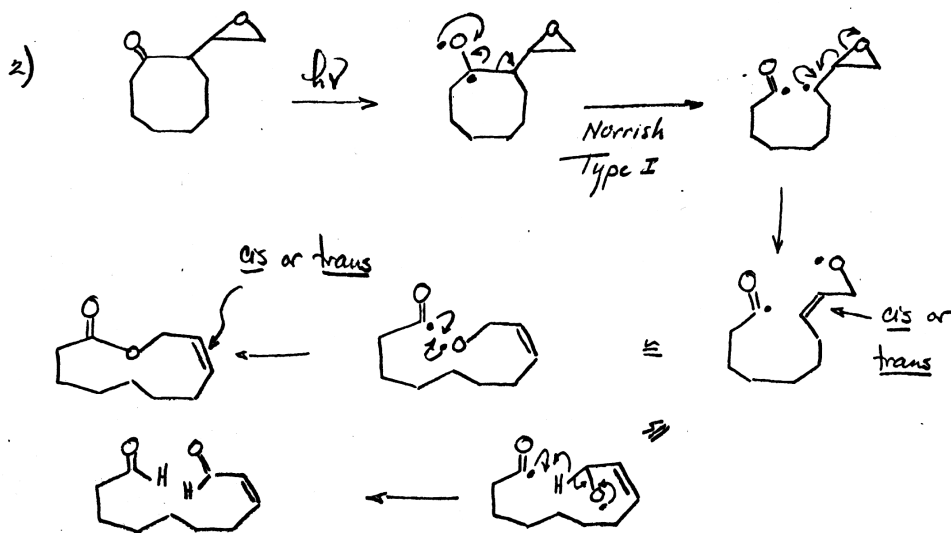


Figure 1 Simple example of pushing electrons.

computer display would trigger a calculation that instantly updates a sketch so that it presents the best theoretical account. However, these calculations are too time consuming for real-time manipulation and must be performed asynchronously. As a result, the scientist must rely on chemical intuition.

Like chemical intuition, the practice of pushing electrons is mastered over time. The most adept individuals are the researchers who possess a breadth and depth of synthetic chemical knowledge, and who have demonstrated creativity and ingenuity in synthesizing complex chemical structures. Figure 1 was created by such an individual whose deft hand is clearly revealed in the sureness and elegance of the sketch.

Finally, this illustration's artistic sense of symbolism is a reminder that synthetic chemistry has its origin in the black art of alchemy with its mystical signs, and imagery of smoke and fire. Organic chemists are still called *potboilers*, a term that conjures up these ancient practices, even though today's syntheses are highly sophisticated processes. Yet, these symbols make a cultural connection by binding the ancient art with contemporary science.