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# Ockham's Razor and Chemistry*

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**Abstract:** We begin by presenting William of Ockham's various formulations of his principle of parsimony, Ockham's Razor. We then define a reaction mechanism and tell a personal story of how Ockham's Razor entered the study of one such mechanism. A small history of methodologies related to Ockham's Razor, least action and least motion, follows. This is all done in the context of the chemical (and scientific) community's almost unthinking acceptance of the principle as heuristically valuable. Which is *not* matched, to put it mildly, by current philosophical attitudes toward Ockham's Razor. What ensues is a dialogue, pro and con. We first present a context for questioning, within chemistry, the fundamental assumption that underlies Ockham's Razor, namely that the world is simple. Then we argue that in more than one pragmatic way the Razor proves useful, without at all assuming a simple world. Ockham's Razor is an instruction in an operating manual, not a world view. Continuing the argument, we look at the multiplicity and continuity of concerted reaction mechanisms, and at principal component and Bayesian analysis (two ways in which Ockham's Razor is embedded into modern statistics). The dangers to the chemical imagination from a rigid adherence to an Ockham's Razor perspective, and the benefits of the use of this venerable and practical principle are given, we hope, their due.

**Keywords:** *Ockham's Razor, reaction mechanism, principle of least action, principle of least motion, principal component analysis, Bayesian analysis.*

## Introduction

Scientists think they are born with logic; God forbid they should study this discipline with a history of more than two and a half millenia. Isn't it curious that some of our competitors and critics, pretty good scientists (except when they review our papers), seem to be strangely deficient in logic!

While scientists think they can do without philosophy, occasionally principles of logic or philosophy do enter scientific discourse explicitly. One of these philosophic notions is Ockham's Razor, generally taken to mean that one should not complicate explanations when simple ones will suffice. The context in which Ockham's Razor is used in science is either that of argumentation (trying to distinguish between the quality of hypotheses) or of rhetoric (deprecating the argument of someone else). Either way, we think that today appeal to the venerable Razor has a bit of a feeling of showing off, of erudition adduced for the rhetorical purposes. This attitude reveals a double ambiguity. The first is toward learning - today's science, no longer elitist, does not depend on men steeped in classical learning. And appeal to Ockham's Razor also points to a certain ambiguity in the relationship of science to philosophy.

We thought it would be interesting to learn something of the principle and its various meanings. We also present a personal discussion on the use of Ockham's Razor in chemistry, with specific reference to the analysis of reaction mechanisms.

# Ockham's Razor

To his peers and to the world of theology William of Ockham (ca. 1286 - 1347) was and is a leading 'scholastic' Philosopher.[1] This is the late period of the Middle Ages; the wisdom of the Greeks is reintroduced into Europe through Al Andalus, Islamic Spain. It is a time of great minds in the religions; the time of the Rabbis Moses ben Maimon (Maimonides) in Cordova and Egypt, Moses ben Nachman (Nachmanides) in Gerona, Shlomo Yitzhaki (Rashi) in Troyes. It is the time, or shortly after the time, of St. Thomas Aquinas, of Roger Bacon, of Duns Scotus. The philosophy of Aristotle, with its far-reaching rationality, finds a resonance in the agile minds of Catholic theologians. The glory of God merges in their work with the path of reason.

William of Ockham (or Occam) was not only a theologian, but a great logician. A case has been made for his awareness of many of the principles of mathematical logic that were not mathematicized until 600 years later.[2] One of the tools he used routinely in his reasoning is what is known in philosophy as the principle of parsimony, and popularly as Ockham's Razor.

Just as for the Golden Rule, there are many ways of stating Ockham's Razor. Here are four that William of Ockham used in his works:[3]

> (A) It is futile to do with more what can be done with fewer. [*Frustra fit per plura quod potest fieri per pauciora.*]
>
> (B) When a proposition comes out true for things, if two things suffice for its truth, it is superfluous to assume a third. [*Quando propositio verificatur pro rebus, si duae res sufficiunt ad eius veritatem, superfluum est ponere tertiam.*]
>
> (C) Plurality should not be assumed without necessity. [*Pluralitas non est ponenda sine necessitate.*]
>
> (D) No plurality should be assumed unless it can be proved (a) by reason, or (b) by experience, or (c) by some infallible authority. [*Nulla pluralitas est ponenda nisi per rationem vel experientiam vel auctoritatem illius, qui non potest falli nec errare, potest convinci.*]

Philosophers and historians are generally puzzled as to why the principle of parsimony should be called Ockham's Razor. The principle is not original to William of Ockham. Versions of it are to be found in Aristotle, and nearly verbatim variants occur in the work of most scholastic philosophers.[4] Though Ockham used it repeatedly and judiciously, "he clearly does not regard it as his principal weapon in the fight against ontological proliferation"[5].

We suspect that the association is due to the strength of the razor metaphor rather than anything else. Scholastic and theological arguments were complex; to cut through them, to reach the remaining core of truth quickly, was desperately desirable. Whoever rechristened the principle of parsimony as Ockham's Razor (the earliest reference appears to be to Etienne Bonnot de Condillac in 1746)[6] was creating an easily imagined image. Metaphor reaches right into the soul.

The last, most extensive formulation of Ockham's Razor, (D) above, is intriguing. Note the 'religious exclusion' in it. It refers to the Bible, the Saints and certain pronouncements of the Church. This testimony to the faith of William did not stop him from questioning the reasoning of Pope John XXII, when the Pope's writings came in conflict with earlier church authority. In the context of science, especially interesting is part (b) of version D of the Razor, that experience (*experientia*) can serve to justify plurality. There is no reason not to think of 'experience' here as 'experiment', even though the idea of a scientific experiment lies centuries in the future. William of Ockham's method (and that of Aristotle) empowers the human senses as arbiters. His method accepts what we now call science.[7]

## Reaction mechanisms

Six and a half centuries is a lot of time; it is also very little time. In the Middle Ages one had protochemistries - fermentation, metallurgy, ceramics, alchemy, dyeing. People have always transformed matter in ingenious ways. The Renaissance came, then the Industrial and Scientific Revolutions. Now there is chemistry, a true science, an industrial empire, a profession. Beautiful molecules are made, fifteen million of them unknown to Nature. People ask questions "How does this reaction run?" "What is the mechanism (a very Newtonian clock-work type of question) of that reaction?" And remarkably, six hundred and fifty years after he died, they invoke William of Ockham's restatement of the principle of parsimony, that old Ockham's Razor, to help them reason out what happens.

Let us first define what is to be meant by the term 'reaction mechanism'. The notion of the mechanism of a chemical reaction consists of a description of all 'elementary' steps in the transformation of reactants into products. On the molecular level the mechanism includes, in principle, knowledge of the geometry and relative energy of all structures involved, including isolable or potentially isolable intermediates and transition states, the latter representing the turning points along the minimal energy paths connecting all interconverting species. Following another line of thinking, the reaction mechanism traces the evolution of a chemical system along the reaction trajectory, *i.e.*, the line linking reactant and product molecules in the space of all nuclear coordinates. The concept of a potential energy surface (PES), with all its attendant limitations, is essential to this definition.

## Minimal action, least motion

Given the definition of a reaction mechanism, the drawing of an analogy with the mechanical description of moving particles is obvious. A predictable consequence was the early application of the principles and methods developed so successfully in classical mechanics to the treatment of mechanisms of chemical reactions. Before the idea of a molecule ever took hold, there had been developed the *principle of minimal action*, first introduced by Pierre Louis Morveau de Maupertuis and universally applied by Leonhard Euler in ballistics, central force motion, etc. According to this principle, spontaneous movements are always associated with minimal changes in the quantity of 'action', the latter a well-defined physical variable. Reporting in 1744 to the Académie des Sciences of Paris on the principle of minimal action, de Maupertuis stressed, in particular, that light chooses neither the shortest line, nor does it follow the fastest path. Instead, light takes the path which gives real *economy* (*cf.* the law of parsimony), *i.e.*, where the quanitity of action is minimal.[8] Minimal action is itself a beautiful, economic way to get at the heart of physical motion. And it found a place in the new quantum mechanics, most elegantly in the work of de Broglie, Schwinger, and Feynman.[9]