Character analysis of a science

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Chemists, like other specialists, ought to make it clearer what hypotheses they are framing and testing. They will thus avoid the suggestion that they are over-fond of empirical generalizations.

Do chemists deserve the reputation in some quarters that they are over-fond of elevating generalizations into natural laws[1]? I have taken a sample of 167 papers from four successive issues of the *Journal of the American Chemical Society* published in 1990, together with the 73 general articles published in four issues of *Nature* in 1990. I assigned papers to four categories: high-level explanatory theories, empirical generalizations, observations and technological reports — this last category consisted of papers in which known chemical principles have been applied to technology (Table 1). I also ranked my sample for generality of subject matter, using an arbitary scale and again including a category for technological products (Table 2). As I anticipated, the papers in both samples described highly specialized work: because their subject matter was restricted in range, so were their conclusions.

The objectives of the chemists writing in *JACS*, a refereed, general-interest journal, surprised me: almost half were trying to find out the mechanisms of chemical reations. If this journal is any guide, chemistry is well past the stage where the most effort goes into making new compounds and determining their chemical structure. These tasks now consume only 18% (synthetic) and 14% (structural) of the sample. Papers about the internal structure of molecules (electronic structure) represented 11%, and the rest (14%) were mainly devoted to measuring and explaining physical properties, including spectroscopy and general chemistry.

Unless the clearly unrepresentative nature of the sample invalidates my conclusions, I judge that chemistry is a mature science — almost as many contributors to *JACS* are seeking high-level explanations as those in *Nature*. Although articles in *Nature* tend to report major discoveries and *JACS* papers continuing projects, there is a remarkable similarity in the explanatory process which the two sets of contributors follow.

Despite Maddox's impression[1], my analysis revealed very little daring in the *JACS* generalizations. Most of them were the reverse — explanations in the process of being made. Because the explanations still lacked sufficient corroboration, the claims had to be muted. Thus, several papers dealt with biological processes involving compounds too fragile to isolate. So the researchers made model molecules and reported on the similarities and regularities in the behaviour of the natural and artificial compounds[2]. Ultimately the high-level explanation will come, but not yet.

It is true that chemists do not seem to move in the classical manner, from observation to generalization to explanation. The pattern seems to be that the explanation is known in advance and is adapted to the phenomenon in question. Most of the conclusions classified as 'generalizations' gained that category by default: they were qualitative; neither bare observations nor explanations.

Surprisingly, my sample contained no mathematically fitted generalizations. There were however, generalizations of the classical kind: genuinely predictive statements, like Kepler's laws, with important implications for the ultimate explanation but with no real explanatory content themselves. For example, the chemists who measured the Langmuir adsorption isotherms of mixtures of optical isomers on a column[3] found two kinds of sites, one with a preference for the D isomer, the other indifferent. The separation of the isomers is partially explained but the explanation is not chemical and does not reach my "explanatory theory" designation.

TABLE 1 PAPERS RANKED BY LEVEL OF UNDERSTANDING

	JACS	*Nature*
Explanatory theory	44	51
Generalization	47	34
Observations	7	12
Technological report	2	3

Values in per cent.

TABLE 2 PAPERS RANKED BY GENERALITY OF SUBJECT MATTER

	JACS	*Nature*
Perfectly general	3	6
Restricted class	4	3
Single category	90	89
Technological product	3	3

Values in per cent.

A chemical explanation is usually an explanation at the atomic, molecular or electronic level. An example is the explanation of the effectiveness of a technique to attach a substituent to a specific site in a steroid molecule by calculation of the 'stiffness' of the transition state in the reaction[4]. This is a 'molecular' explanation: classical 'molecular mechanics' is sufficient to obtain it. Chemists do indeed "want a picture of what has happened"[1]. 'Chemical' explanations are often pictorial, or if quantum phenomena intervene to make that impossible, at least describable by means of standard concepts.

Explanations at the electronic level have become much more common in the chemical literature now that 'user-friendly' electronic structure packages are so readily available. Specialist investigations of electronic structure represented 11% of my *JACS* sample, for example the use of geometry optimization (searching the conformational 'space' to find the minimum energy geometry for a molecule) to resolve a discrepancy between the theoretical and experimental structures reported for vinyl alcohol. The theoretical 'experiment' led to re-analysis of the experimental data, so removing the discrepancy[5].

It is clear that chemists are not "elevating empirical generalizations into natural laws": their explanations are visions about molecular motions and electron clouds that have come down from the heavens. The explanatory theories of the gods (quantum mechanics and statistical mechanics) are too hard for the real chemical world, so chemists have made approximate models of them, separately adapted for each application. Hartree–Fock/Born–Oppenheimer electron-cloud theory is one; molecular mechanics is another; the collision theory of what makes molecules reactive is another. Chemistry, very much a theory-driven discipline, uses these models all the time.

If the *JACS* sample is a proper guide, the chemists who do the experiments are the ones who make the explanations. I did not find any papers by theorists making explanations for other people's data. High-level explanations were almost always supported by observational evidence in the same paper. In many cases, the empirical generalization stage was left out altogether.

Chemists should be grateful to Maddox for reminding them that their science has a structure. After wading through the papers in a sample this size, it occurs to me that chemistry would profit if chemists paid more attention to the character of their science, saying explicitly what hypothesis they have tested, what the tests were and how well it survived. Making science understandable to non-specialists is an important responsibility, but making it assessable is also important. Away from the physical sciences, the processing of 'soft' data forces researchers to pay stringent attention to validity and reliability. It may be time for the rest of us also to acknowledge that our science is provisional, and to learn the proper way to frame, test and report hypotheses. □

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