Letters

Behavioral Sciences: Benign Neglect?

It is difficult to take issue with what Erich Bloch says in "Basic research and economic health: The coming challenge" (Articles, 2 May, p. 595), but it is no less feasible to remain tranquil about the absence of any reference to the behavioral and social sciences. While many of the same trends of precipitous enrollment declines exist as in what Bloch terms the "basic sciences" and "engineering base," he evinces little interest or urgency in policies that would assist both the "best and the brightest of our young people" or "the latent talent of women and minorities" in these areas of behavioral and social research.

What makes this silence especially disquieting, apart from Bloch's role as director of the National Science Foundation (NSF), is his recognition that "new demands often require a new approach to social organization." Just where are such innovations to be generated if not in the behavioral and social research areas of our universities?

This de-emphasis on the behavioral sciences has not evolved in a vacuum. The partial (and one must emphasize that word "partial") transformation of social science into generalized ideological expressions of displeasure and discontent have provided the legitimacy of this new NSF environment of benign neglect. Social and behavioral scientists are probably more culpable of smuggling into their findings extrinsic and even irrelevant conclusions and recommendations than are investigators in the physical and engineering sciences. By the same token, it is precisely this taken-for-grantedness of the political and economic realms that social research is charged, in part at least, with disabusing.

In the interim, Bloch would be better served by a frank recognition that his very own concern with science policy and science organization is itself a subdiscipline of the sociology of science.

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Methylene: Experiment and Theory

H. F. Schaefer (Articles, 7 Mar., p. 1100) describes the methylene saga, emphasizing the contributions of theory. The viewpoint of a participating experimentalist may provide an additional perspective.

A striking feature of the story is how little influence theory had on the experimental determination of the structure of the ground state. For example, the first experimental demonstration of the now accepted geometry (*1*) was carried out at Bell Laboratories without input from the calculation of Bender and Schaefer (*2*). Apparently, the two efforts were independent and largely simultaneous (*3*).

A reason for the lack of impact may have been the diversity of opinion in the theoretical community. I attended the 1959 conference in which Boys presented his methylene calculations. Some in the audience had clear, negative responses. In the following decade calculations that agreed with those of Boys but apparently disagreed with experiment seemed to be leaving the authors uneasy. My rationalization was that theory was having difficulties with a triatomic triplet state.

Compounding the confusion was a statement by Foster and Boys in their 1960 paper (*4*, p. 306). They indicated that more elaborate studies were unlikely to change their conclusions: "In order not to miss unsuspected features in the wave functions, the eigenvector calculation was carried out with large numbers of determinantal expansion functions . . . . the results suggest that this was very unnecessary since many small terms were found and these appeared *very unlikely to affect any physical prediction*" (emphasis mine). Since the authors predicted an essentially correct geometry, I find this a most impressive statement.

Bender and Schaefer as well as Harrison (*5*) clearly and correctly questioned an earlier experimental conclusion, an important role for theory. In the future even more benefits might be obtained when, in the design and interpretation of specific projects, theory and experiment are combined. In both areas we often seek information near the limits of our current tools. Both have had failures among their many successes. Together they might provide us with an increased ability to deal with complex problems.

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REFERENCES AND NOTES

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2. C. F. Bender and H. F. Schaefer, *J. Am. Chem. Soc.* **92**, 4984 (1970).
3. An article by W. A. Goddard [*Science* **227**, 917 (1985)] may also lead to a misinterpretation on this point.
4. J. M. Foster and S. F. Boys, *Rev. Mod. Phys.* **32**, 305 (1960).
5. J. F. Harrison, *J. Chem. Phys.* **54**, 5413 (1971).

Response: Our prediction of the bent structure of triplet CH_2 (*1*) appeared in the 12 August 1970 issue of the *Journal of the American Chemical Society*. The paper by E. Wasserman, W. A. Yager, and V. J. Kuck was received on 9 September 1970 and published in the 15 November issue of *Chemical Physics Letters* (*2*). The paper by Wasserman *et al.* cites as reference 16 the earlier paper by Bender and Schaefer. The relationship between the two papers is clearly one in which theory precedes experiment.

If I erred in the assignment of credit in this matter, the error was made in favor of the 1970 Wasserman paper. It is now better understood that the use of zero-field splitting parameters D and E to deduce the geometry of a molecule is a dubious procedure (*3*). From this perspective the first definitive experimental determination of the structure of triplet methylene did not appear until 1983 (*4*).

The inability of electron spin resonance spectroscopy to provide a definitive experimental molecular structure for methylene led us in 1972 to attempt to improve upon our 1970 theoretical prediction of 135.1° for the CH_2 bond angle. The result (*5*) was a prediction of 134.0° for the HCH angle, with the exact result stated to be 134° ± 2° with error bars. This prediction was ultimately confirmed 11 years later by Bunker and Jensen (*4*), who reported 133.8° ± 0.1° from their laser magnetic resonance experiments.

I am in agreement with Wasserman's closing comments on the combined efforts of theory with experiment. In fact, my *Science* article gives eight examples of the constructive interplay between theory and experiment under the heading "Theory and experiment: Symbiosis."

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3. J. F. Harrison and R. C. Liedtke, *J. Chem. Phys.* **58**, 3106 (1973).
4. P. R. Bunker and P. Jensen, *ibid.* **79**, 1224 (1983).
5. D. R. McLaughlin, C. F. Bender, H. F. Schaefer, *Theor. Chim. Acta* **25**, 352 (1972).

Royal Greenwich Observatory

Readers of David Dickson's briefing "British telescope dogged by British weather" (News & Comment, 4 Apr., p. 19) may be forgiven for believing there is a good scientific reason for moving the Royal