THE JOURNAL OF PHYSICAL CHEMISTRY A

 VOLUME 113, NUMBER 26, JULY 2, 2009

Preface to the Robert Benny Gerber Festschrift

"The purpose of computing is insight, not numbers"
R.W. Hamming

We are both humbled and honored by the opportunity to recognize Benny Gerber's contributions to Physical Chemistry, thus far, and to recognize his sixty-fifth birthday. Benny received his Ph.D. at Oxford in 1968, working with C. A. Coulson on scattering theory. This was a time when the introduction of computers into chemical studies was just starting, and anyone who worked with computers at that time has stories to tell about the lengths they went to in order to keep their computers running or finding ways to use spare cycles on university computers. Looking at this situation, Benny made the logical choice to focus his efforts on analytical theory and not involve himself with these computing machines. His Ph.D. and postdoctoral research was focused on the formal work, which he favored.

However, the new opportunities offered by computers were exciting. Although Benny did not favor programming himself, his first students at the Weizmann Institute and at the Hebrew University realized elegant computational schemes devised by Benny to address problems in scattering theory and in condensed phase energy transfer. Gradually, computational aspects of Benny's research become more and more important. Computers have enabled Benny to ask challenging questions about complex systems. In contrast to the level of technology used by his students and postdocs in their research, Benny remained more comfortable with ideas than working on the computer himself. All of us remember from our time in Jerusalem in the mid 1990s the VT100 terminal that Benny had in his office for checking his email. Only a couple years ago, Benny abandoned his beautifully prepared overhead projector transparancies and began to deliver his talks using PowerPoint. Many of us will miss his neat hand-written transparences.

Against this backdrop, Benny has pushed theoretical and computational chemistry into areas and systems that advance the limits of what is considered possible. Benny has also kept a keen eye on the important and interesting experimental problems, both fundamental and applied (e.g., epitaxial growth, atmospheric chemistry), that are being explored. Through this he has developed a large number of collaborations with

10.1021/jp902677a CCC: $40.75
Published on Web 06/25/2009

experimental groups. The range of his interests and his interest in experimental as well as theoretical work is reflected in the large number of experimental contributions to this volume. The breadth of his interests is really very extraordinary and ranges from understanding the chemistry of unusual rare gas containing compounds to gas phase spectroscopy and surface scattering.

A distinguishing feature of Benny's style is focus on insight and predictions rather than generating numbers reproducing experimental measurements. Indeed, the ability of computational methods to provide data complementary to the experimental measurements (or even replace the latter) is very valuable. However, the real power of theory is unraveled when it predicts novel phenomena and stimulates and guides the experimentalists, and this is one of the most important lessons that we learned from Benny. Two examples demonstrate this point: ultrafast matrix-induced spin-flip and novel rare-gas compounds, both challenging the conventional views.

Spin-forbidden processes have been perceived as slow relative to other types of electronic transitions. Thus, almost statistical population of different spin-states of HCl achieved on the sub-picosecond time scale was quite a surprising outcome of nonadiabatic simulations of HCl (and even lighter diatomics) photodissociation in Ar clusters. For example, triplet states were often judiciously excluded in the calculations. This prediction stimulated new experiments in the Schwentner group, who indeed observed ultrafast scrambling of spin states in the matrix.

One of the first chemistry lessons we learn in school is about a broad range of reactivity of chemical elements, and that some of them—noble gases—simply do not make chemical bonds. Indeed, since all the electrons are paired, shells are filled, and electron sharing with other elements necessary for a chemical bond formation is energetically unfavorable. A couple of counter examples, stable compounds of Xe and Kr with halogens, were regarded as esoteric exceptions. Imaginative computational studies of the Gerber group proved this wrong and predicted a number of stable molecules in which lighter rare gases form strong chemical bonds with a variety of other elements. These bold predictions stimulated experimental studies, which confirmed theoretical predictions and characterized new compounds.

When we think of Benny's work, we often focus on the specific systems and classes of problems that he has investigated, along the lines of the problems described above. He is also associated with a number of areas of method development. One such area that has run through his research for nearly thirty years is in the application of self-consistent field approaches to vibrational problems (VSCF). It also represented the start of a long-term collaboration and friendship between Benny and Mark Ratner. While in the 1980s and early 1990s this work focused on relatively small systems, typically in the gas phase, in the mid-1990s they extended this work to larger systems including solvated proteins! They also worked out ways to extend beyond simple Hartree product wave functions to include corrections using, for example, perturbation theory. The most exciting aspect of this work has been in determining how to minimize the number of electronic energies that need to be calculated to implement these VSCF calculations. In incorporating their VSCF codes into GAMESS, they have made this work available to the broader community.

We each spent two or more years in Benny's group, two of us as graduate students and one as a postdoctoral researcher. One of us has also been a colleague of Benny's at Hebrew University since returning to Israel in 1992. What has made working in the field of reaction dynamics so rewarding for many has been the generosity and support of the community. In our experience, Benny stands out among this community both in terms of his deep enthusiasm for science—something anyone who has seen him give a talk can attest to—and his concern for and support of the people who have worked with him. To date, 59 scientists have had the privilege to have had Benny as a graduate or postdoctoral mentor.

An exciting aspect of working in Benny's group was the large number of very different projects that were going on simultaneously. As faculty members ourselves, we cannot imagine how he was able to do it! Such a range of interests has also led to a large number of experimental and theoretical collaborators, many of whom have contributed to this volume.

We wish Benny a very happy sixty-fifth birthday and continued success as he finds new and interesting problems to study.

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