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Editorial

Scientific biography of Professor Boris Galabov

Boris Galabov was born on 24 February 1942 in Tzaribrod, Bulgaria. He received his M.S. degree in chemistry from the St. Kliment Ohridski University of Sofia in 1967 and the Ph.D. degree in 1975. He joined the Department of Chemistry, University of Sofia, as an Assistant Professor, becoming Professor of Organic Chemistry in 1989. He was Visiting Lecturer at the University of Salford several times during the 1970s. For the academic year 1986–1987 he was a Visiting Professor at the University of South Carolina. During the period 2000–2011, he held a similar position at the University of Georgia. In 1991 he became Vice-Rector for Academic Affairs of Sofia University. From 1993 to 1995 he was Deputy Minister of Education and Science for the Bulgarian Government, responsible for his country's higher education and research sectors. Boris Galabov married his wife Danka in 1969. Professor Danka Galabova is the Head of the Department of Microbial Biochemistry, Bulgarian Academy of Sciences, Sofia. They have two daughters living in the USA: Theodora (born 1970) and Violeta (born 1972), pursuing careers in diplomacy and medicine, respectively.

The scientific biography of Boris Galabov can be separated into two parts. The first period (1968–1996) is associated with developments in vibrational spectroscopy; while the emphases of his research activities during the second part (1997–present) of his career fall in the domains of physical organic chemistry and computational chemistry. Many of his early studies were devoted to analyzing the unusual spectroscopic properties of strained ring compounds. By combining experiments with normal coordinate analysis computations, Galabov showed that the higher characteristic IR frequencies in most typical strained ring systems are governed by two effects: (a) the purely geometric effect of reduced ring angles, which favor the vibrational coupling between the exocyclic bonds (e.g. C=O, C=N) and the neighboring cyclic bonds; (b) the strengthening of exocyclic bonds associated with increasing force constants (*Chem. Phys. Lett*. 1970, 1980, *J. Mol. Struct*. 1972).

A major theme in Professor Galabov's studies has been the development and application of new theoretical methods for the interpretation of vibrational intensities for infrared and Raman spectra. These studies were initiated during his numerous visits to University of Salford. Quantum mechanical computations revealed the very complex character of the intramolecular charge rearrangement accompanying molecular vibrations. These studies have shown that, unlike other spectroscopic techniques (UV–VIS, NMR), vibrational spectroscopy provides unique insights into the properties of individual chemical bonds. Galabov proposed (*J. Chem. Phys*. 1981) a procedure for the interpretation of IR intensities based on molecular quantities, *bond polar parameters*, associated with the stretching and angular vibrational distortions of individual chemical bonds. A number of successful applications showed their usefulness in characterizing the polar properties of different molecules. His later research on IR and Raman intensities concentrated on developments associated with the atomic polar (and polarizability) tensor approach. He defined the rotation-free atomic polar tensors and later used these quantities in a theoretical model for interpretation of IR and Raman intensities in terms of *effective bond charges* (or *bond polarizabilities*), invariants with respect to coordinate axis transformations of bond charge (bond polarizability) tensors (*Spectrochim. Acta A* 1993). His studies in this field culminated in publishing the definitive monograph *Vibrational Intensities* (Elsevier Science, 1996) together with Todor Dudev, a former Ph.D. student and research associate of Galabov at the University of Sofia. Galabov's last work in this field was published in 2002 in collaboration with Yukio Yamaguchi and treated the application of high-level *ab initio* electronic structure theory in predicting IR intensities and a number other molecular properties (*J. Phys. Chem. A*). This work revealed that truly reliable IR intensities can only be obtained from rather sophisticated wave functions. The accuracy of such high level theoretical predictions falls within the uncertainties of the reported gas-phase IR intensities for a series of small and medium size molecules.

During the second half of 1990s the emphasis of studies in the group of Professor Galabov changed significantly. This was mostly inspired by the desire to pursue research in broader areas of chemistry. In 1998 and 1999 Galabov and his student Petia Bobadova-Parvanova reported that theoretically evaluated electrostatic potentials at particular nuclei (EPN) predict with remarkable accuracy the reactivity of molecules for processes involving hydrogen bonding (*J. Phys. Chem. A*). This quantity was first defined by E.B. Wilson in 1962. However, its first application as a reactivity index was in the work of Galabov and collaborators. Later the EPN index was successfully applied in quantifying the features of a number of organic reactions: solvolytic reactions of esters and amides, S_N2 reactions, and proton transfer reactions (*J. Phys. Chem. A* 2004, 2008). Based on theoretically determined EPN values, an efficient computational method for the evaluation of substituent constants was developed (*J. Org. Chem*. 2006). The origin of the unusual reactivity of benzylic compounds in S_N2 reactions, known as the *benzylic effect*, was also explained (*J. Am. Chem. Soc*. 2008). Using state-of-the-art quantum mechanical computations Galabov and his coauthors showed that even very low energy conformational transitions can be satisfactorily predicted theoretically (*J. Phys. Chem. A* 2002, 2008). The origin of the higher rotational barriers in thioamides than in amides was definitively elucidated (*J. Phys. Chem. A* 2003).

His research on the reactivity of organic molecules was then extended to electrophilic aromatic substitution reactions. A new theoretical concept, *electrophile affinity*, which quantifies the reactivity of aromatic compounds in their most typical reactions, was introduced (*J. Am. Chem. Soc.* 2009, *J. Org. Chem.* 2010). In a very

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recent development, Galabov's work has resulted in several groundbreaking papers on the mechanism of electrophilic aromatic substitution (*Angew. Chem. Int. Ed.* 2011, *J. Am. Chem. Soc.* 2011). Computational results and NMR experiments reveal that in the absence of catalysts or highly polar media, the halogenation of arenes with molecular Br_2 and Cl_2 proceeds in the context of a competition between direct substitution and addition of X_2 followed by HX elimination, leading to the same final substitution products. Moreover, in contrast to conventional interpretations, the direct substitution proceeds via concerted pathways, which do not involve arenium ion (σ complex) intermediates. For some activated aromatic compounds (e.g., anisole) the addition–elimination process has much lower reaction barriers than the direct substitution path and, hence, is the only plausible mechanistic pathway. Advanced NMR experiments provide compelling evidence that addition processes indeed take place during the chlorination of anisole.

The sulfonation of aromatic compounds with SO_3, an important laboratory and industrial process, also proceeds in an unusual way. The rate-determining step of the reaction involves attack by two SO_3 molecules. In non-complexing solvents ($CFCl_3$, CCl_4) the reaction follows a concerted pathway and does not involve a Wheland intermediate. In contrast, in complexing solvents (e.g., CH_3NO_2), the reaction proceeds along the classic S_EAr mechanism with the intermediate formation of a σ complex. Further work on other reactions of aromatic systems is underway in the Galabov laboratory.

The scientific carrier of Boris Galabov has benefited from a number of successful international collaborations. His research on vibrational intensities was initiated during his postdoctoral stays in the group of Prof. W.J. Orville-Thomas, a collaboration that lasted for many years (25 joint publications). During the 1986/1987 academic year, he was a Visiting Professor in the laboratory of Prof. James R. Durig at the University of South Carolina. The joint research activities also continued for a number of years (13 published joint papers). The visit as a Fulbright Scholar to the Center for Computational Chemistry, University of Georgia in 2000 played a significant role in the gradual shift of Galabov's research interests towards computational chemistry. The collaboration with Fritz Schaefer, Paul Schleyer, and Wesley Allen resulted in a number of joint papers, published in highly visible chemistry journals.

The principal motivation in the work of Professor Galabov is the joy of doing research in chemistry. In comparison with athletic events, Boris Galabov says that doing research is like participating in a continuous world competition, with the advantage of many winners. Having passed for a short period through several heavy administrative positions, he is now able to appreciate how much more challenging and fulfilling are his current research activities, with many possibilities to share scientific experiences with colleagues and students.

Professor Galabov has been the supervisor of ten successful Ph.D. students and a considerable number for Master's degree students. Some of his former associates have successful careers as researchers and teachers. Todor Dudev is a Senior Scientist in computational biochemistry at Academia Sinica, Taiwan; Sonia Ilieva is a full Professor of Chemistry at the University of Sofia; Boriana Hadjieva is Associate Professor of Chemistry at the University of Sofia; Petia Bobadova-Parvanova is Assistant Professor of Chemistry at Rockhurst University, Kansas City; Todor Gounev is Assistant Professor of Chemistry at the University of Missouri – Kansas City.

During his career, Boris Galabov has published 150 scientific papers, mostly in international journals, plus a few book chapters. He has delivered over 70 invited lectures and seminars at international conferences and foreign universities. He is a member of the Editorial Boards of three international journals. In 1986 Boris Galabov was awarded a Doctor of Science degree for his achievements in the field of vibrational intensities. He is the first recipient of the Grand Science Prize of the University of Sofia (2008), for his contributions to physical organic chemistry.

In addition to his research, Boris Galabov has been one of the most distinguished teachers at the Department of Chemistry, University of Sofia. There he has introduced a number of new courses: Applied Molecular Spectroscopy, Quantum Chemistry and Spectroscopy, Computational Chemistry, and Computational Methods in Spectroscopy. Following his name-only retirement as a Professor in 2009, he continues to teach and holds the position of Research Projects Supervisor at the University of Sofia.

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