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EDITORIAL

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Laser Analysis and Control of Complex Molecular Systems

Rainer Weinkauff,^{*,[a]} Mattanah S. de Vries,^{*,[b]} and Klaus Müller-Dethlefs^{*,[c]}

This special issue is dedicated to Karl Kleinermanns on the occasion of his 60th birthday. Karl Kleinermanns studied chemistry at the Rheinisch-Westfälische Technische Hochschule Aachen and graduated in 1974 in Theoretical Organic Chemistry by investigating Diels–Alder reactions. Subsequently, he focussed on experimental work, producing his PhD thesis on "IR laser-induced dissociation of N₂F₄ and isomerization of H₃NC"



in the group of Prof. H. Gg. Wagner at the Max-Planck Institut für Strömungsforschung in Göttingen.

During two years at the IBM research laboratories in San José, California (USA), Karl Kleinermanns investigated elementary chemical reactions in crossed molecular beam experiments. He moved to Göttingen and continued the study of similar reactions but now employing laser photolysis and laser product analysis. These studies were continued and refined by

him in Heidelberg at the Chair of Jürgen Wolfrum, achieving high selectivity in state and kinetic energy of the collisional partners. For this sophisticated work, Karl Kleinermanns was awarded the Heinz-Meier-Leibnitz prize in 1984, one of the highest-ranked prizes for scientists in Germany.

In 1990 Karl Kleinermanns started the investigation of molecular clusters in supersonic jet expansions. Such molecular clusters are seen as a bridge between isolated molecules and the solution phase, but it soon became clear that cold molecular homo- or hetero-clusters can also be new species with different structures and properties compared to the solution phase. The great advantage of these gas-phase studies, however, is that high-resolution spectroscopy can be combined with mass selection to provide new and very precise data of molecular complexes to serve as calibration data for theory. This synergy with computational quantum chemistry has become very important because in parallel with increasing experimental sophistication, as showcased in Karl Kleinermanns' work,

theory also rapidly developed with new algorithms and increasing computer power.

In 1989 Karl Kleinermanns was appointed to a Chair for Physical Chemistry at the Heinrich-Heine-Universität in Düsseldorf (Germany). Here, he initiated innovative work in the new field of multi-colour laser spectroscopy of complex molecular systems in the gas phase. A major emphasis is on molecules and complexes of small bio-related compounds. Although the gas-phase results themselves do not model biological processes, they can shed light on very fundamental properties and spectroscopy of basic biomolecular building blocks. Examples include the chromophores of amino acids, complete amino acids as well as small model peptides with two up to ten moieties, and tautomers of nucleic acid bases as well as their clusters with each other and with water. A highlight of these investigations is the study of the many tautomeric nucleic acid dimers.

To discriminate between different conformers and tautomers, Karl Kleinermanns developed sophisticated double-resonance methods. In order to provide confident assignments—and to gain a deeper insight into intermolecular bonds—his measurements have been increasingly accompanied by his own high-level theoretical calculations.

Karl Kleinermanns is well known in a broad scientific community for his work, combining laser desorption, mass spectrometry, double-resonance laser spectroscopy and theoretical

calculations. The theme and the papers of this special issue represent a cross-section of this field. In addition to this signature work he has demonstrated great scientific breadth, spanning from solution-phase experiments, scanning tunnelling microscopy, and analytical methods to research on semiconductor quantum dots for the construction of solar cells.

Karl Kleinermanns is a very good friend, an excellent mentor and an inspiring scientist. He has pushed and continues to push the frontiers of basic and applied science in many ways as researcher, as lecturer, as instructor for many PhD students, as journal editor, as organizer of conferences and as one of the main reviewers for the *Deutsche Forschungsgemeinschaft*. The contributions to this issue are dedicated by former and current collaborators and friends. The international and broad scope of this special issue is a reflection of his engagement and his open mindedness in science.

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