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Preface

Molecular spectroscopy and molecular structure – Selected communications presented at the 1st International Turkish Congress on Molecular Spectroscopy (TURCMOS 2013)



The First International Turkish Congress on Molecular Spectroscopy (TURCMOS 2013) took place at the Harbiye Cultural Center & Museum, Istanbul, Turkey, September 15–20, 2013. The main aim of the congress was to encourage the exchange of scientific ideas and collaborations all around the world, introduce new techniques and instruments, and discuss recent developments in the field of molecular spectroscopy. Among the different subjects covered, particular emphasis was given to the relevance of spectroscopy to elucidate details of the molecular structure and the chemical and physical behavior of systems ranging from simple molecules to complex biochemical molecules. Besides experimental spectroscopic approaches, related computational and theoretical methods were also considered. In this volume, selected contributions presented at the congress were put together.

Unsalan and Kuzucuoglu present an interesting report on the effects of hazardous pollutants on the walls of Valence Aqueduct (Istanbul), using a combined Raman Spectroscopy/SEM–EDX/Geographical Information System approach. They show that identification of air pollution rates and pollutants by means of spectroscopic methods might play an important role in the preservation of historical monuments. Glavcheva et al. describe a comprehensive spectroscopic study of samples obtained from a fourth century BC Thracian tomb wall paintings located at Alexandrovo (Bulgaria), providing a glance on the used ingenious construction and painting techniques. The Thracian tomb at Alexandrovo is one of the oldest examples in the world that has paintings executed with wax binder and, rather interestingly, the results revealed also the presence of various nano-size particles among the used materials, which are suggested to be a factor contributing to the optical effects and preservation of the wall paintings.

Todoran et al. propose a fast technique based on optical luminescence measurements as a method to evaluate the kinetics of adsorption processes, which might be applied to the optimization of the industrial froth flotation process. The method is illustrated by considering ethyl xanthate adsorption layers on the surface of sphalerite minerals.

The contributions by Arı and Özpozan, Aksabal, and Aksabal et al. focus on the investigation of silk materials. In the first study, the authors examine the structure of glycyglycylarginine (in both nonionic and zwitterionic forms) as a part of structural submotifs of spider silk spidroin, using theoretical and spectroscopic techniques, and evaluate the role of intra and intermolecular interactions in the stabilization of these systems. In the two last reports, ATR–FTIR spectroscopy is applied to the study of UV and

temperature effects on the recovery process in stretched *Bombyx mori* silk fibers. It is shown that changes in the absorbance ratios and shifts in the positions of some specific infrared bands suggest the formation of hydrogen bonds between polypeptide chains, especially in amorphous regions, and changes in the intra-sheet hydrogen bonds in β -sheet crystalline regions, as important structural changes leading to the recovery process.

Petkova et al. discusses the absorption spectra of cobalt-doped tungsten-based glasses, which are relevant materials in non-linear optics, to evaluate the effects of the doping on the electro-optical properties of the material. Effects of doping on crystalline materials properties are addressed by Ceylan and Tapramaz and by Yıldırım et al., in interesting contributions where EPR spectroscopy and X-ray diffraction are used as main experimental techniques. EPR spectroscopy is also used, together with photoluminescence spectroscopy, by Repp and Erdem, to investigate the possibility of controlling the exciton energy of zinc oxide quantum dots by changing of the confinement conditions.

The application of spectroscopic techniques, combined with quantum mechanics based theoretical methods, for elucidation of structural details of metal complexes is illustrated by the works of Vural et al., on a new chelidamate complex of nickel(II) with 4-methylpyridine, and Kartal, on two novel cyano-bridged heteropolynuclear complexes of nickel(II) and cobalt(II). In turn, interesting examples of application of spectroscopic techniques to the investigation of the structure and properties of organic molecules or of their complexes are presented by Polat, centering on the hydrogen bonding interactions of dimethyl sulfoxide, ethylene and pyrrole with water, and Abbas et al., dealing with 4-hexyloxy-3-methoxybenzaldehyde, an important alkoxy derivative of vanillin. In addition, Tanak and Toy present reports on the theoretical investigation of the molecular structures and vibrational spectra of derivatives of azobenzene and naphthalenone, where both density functional theory and *ab initio* methods are used.

Biologically-oriented spectroscopic investigations are illustrated by the contributions of Ildiz et al., which consider the use of FTIR spectroscopy and multivariate analysis as an auxiliary tool for diagnosis of mental diseases (bipolar and schizophrenia), Maciązek-Jurczyk et al. and Szkudlarek-Haśnik et al., which evaluate the alteration of methotrexate binding to human serum albumin induced by oxidative stress as well as the effects of non-enzymatic glycation on the structure of this protein, and Swiatkowska et al. that present a FRET investigation of the G-quadruplex folding ability of fluorescent oligonucleotide probes at lipid monolayer interfaces.

We hope this Special Issue can record faithfully the scientific richness of the meeting that led to its appearance and might also stimulate further research on the covered domains.

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Editor

James R. Durig

University of Missouri-Kansas City, USA

E-mail address: DurigJ@umkc.edu

Guest Editors

Rui Fausto

University of Coimbra, Portugal

E-mail addresses: rfausto@ci.uc.pt

Ozan Ünsalan

Istanbul University, Turkey

E-mail addresses: unsalan@istanbul.edu.tr

Associate Guest Editors

Sevgi Bayarı

Hacetepe University, Ankara, Turkey

Nihal Kuş

Anadolu University, Eskişehir, Turkey

Gülce Ö. Ildız

Kültür University, Istanbul, Turkey

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