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Spectrochimica Acta Part A 57 (2001) 613–614

SPECTROCHIMICA ACTA PART A

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Preface

Molecular spectroscopy plays an important role in astrophysics and in astrochemistry, as illustrated in this first issue of *Spectrochimica Acta, Part A* devoted to the topic. This is because photons carry most of the information that we are able to remotely access regarding the nature and the composition of stellar and interstellar objects that lie far away from Earth. The goal of this special issue is, thus, to bring to the readers of this journal an illustrative — although certainly not exhaustive — set of research papers dealing with current astrophysical issues. This topic is by definition strongly multi-disciplinary and it involves astronomers, laboratory chemists and physicists and theoretical chemists and physicists to mention a few.

Astrophysics covers a wide range of issues ranging from the study of our Solar System to the study of the interstellar medium. We have attempted to select a few papers illustrating the main components of this effort. The issue is, thus, divided along four lines of work. The first section (articles 1–3) covers astronomical observations taken over a wide range of wavelengths, from the visible (Snow) through the infrared (Sellgren) to the millimeter range (Dickens et al.). All articles highlight the current astronomical issues as well as the strong need for relevant, quantitative, electronic, vibrational, and rotational spectral information from laboratory experiments to assign the spectral bands seen in space.

This section is followed by articles 4–6 that describe the search for specific interstellar molecules and ions in both the solid and the gas phases through the combination of astronomical observations, laboratory and theoretical studies. The paper by Tennyson and Miller deals with small gas-phase molecular species, while d'Hendecourt and Dartois discuss solid interstellar ices. The paper by Charnley et al. examines the interface between the two phases. The authors also discuss the complex physico-chemical processes that occur in the various environments.

The next section, articles 7–18, deals with laboratory studies of interstellar analogs. This section represents the 'lion's share' of this special issue because of the key role of laboratory studies in modern astrophysics and astrochemistry. Core laboratory studies are not only aimed at securing spectral band assignments in extraterrestrial observations, but also at deciphering the nature of the physical and chemical processes in action in space environments. Laboratory studies on materials and processes in the Solar System and beyond provide a fundamental contribution to the understanding of observed phenomena. These are essential for testing and improving the existing astrophysical models. The objectives of laboratory astrophysical studies are to simulate as closely as possible the conditions known or expected to exist in a given space environment and to provide quantitative data that are relevant for the interpretation of astronomical observations. Some laboratory applications are given in this section. The study of collisions within small gas-phase molecular systems (Oesterling et al.) is followed by the study of the spectroscopy of larger molecules such as polycyclic aromatic hydrocarbon ions (Piest et

1386-1425/01/$ - see front matter © 2001 Published by Elsevier Science B.V.
PII: S1386-1425(00)00431-5

al.; Bréchignac et al.) and their derivatives (Beegle et al.) and carbon chains (Thaddeus and McCarthy; Szczepanski et al.). The simulation of cosmic dust grains in the laboratory is described for hydrocarbon and silicate grains (Mennella et al.), carbon nanoparticles (Reynaud et al.) and carbides (Henning and Mutschke). The variation of the spectral signature of cosmic ices with photon and/or ion bombardment is discussed in the papers of Strazzulla et al. and Moore et al.

The last section, articles 19–24, covers computational chemistry studies. These include more qualitative type studies, such as those by Hudgins et al., Weismann et al. and Lee and Adamowicz, that are designed to test if the existence of a class of compounds is consistent with observations. The goal of more accurate calculations, such as those reported by Dimur et al., is to supply results that aid in the identification of molecules by laboratory studies and by observation. The paper by Martin uses OH^- to illustrate the highest levels of accuracy currently possible for small molecules. The work of Schwenke and Partridge describes attempts to generate spectral line lists for conditions that are difficult to reproduce on Earth, but are relevant to astrophysics. The paper by Papoular tests a numerical simulation on model dust particles. Clearly, current computational studies are able to address many aspects of molecular spectroscopy in astrophysics, and we hope that this special issue brings astrophysical problems to the attention of computational chemists, so that the computational effort increases with time.

We should point out here that an important subfield has been left out of this special issue, namely astrophysical modeling. We made this choice in order to focus on more 'hard core' spectroscopic issues, but clearly there is a need for a strong interaction between spectroscopists and modelers. We hope that after reading this special issue, researchers will either find an overlap with their current research activities and/or a strong interest to contribute to the field. We also hope that we have illustrated the multi-disciplinary aspect of the field, which requires active collaborations between observers, laboratory experimentalists, and computational chemists and physicists to decipher the complex problems of astrophysics. We sincerely hope that this issue will play an informative, as well as an inspirational, role for the readers of the journal.

Finally, this special issue has only been made possible thanks to the overwhelmingly positive response to the project by the astrophysics community. All the authors agreed to present their recent research results together with a comprehensive introduction highlighting the current issues and challenges at hand in their particular field of study. This special issue has 18 contributions from observers and/or laboratory experimentalists (which were coordinated by F. Salama) and six contributions from theoretical chemists (which were coordinated by C.W. Bauschlicher). The geographical distribution — more than ten countries are represented in this special issue — is another indicator of the good health of the field of laboratory astrophysics and astrochemistry. It is also an indication of the many challenging issues that the scientific community faces in the understanding of cosmic phenomena and of the ability of this field to attract many motivated researchers. We would like to thank the authors for the high quality of the manuscripts and topics they submitted. The vast majority of authors (with a very few exceptions) have worked within the time constraints and these authors are thanked for their efforts. Many thanks are also due to the referees who have greatly contributed to the quality of this special issue.

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