

ASTROPHYSICS AND SPACE SCIENCE PROCEEDINGS

R.K. Chaudhuri
M.V. Mekkaden
A.V. Raveendran
A.S. Narayanan
Editors

Recent Advances in Spectroscopy

Theoretical, Astrophysical and
Experimental Perspectives

 Springer

Astrophysics and Space Science Proceedings

For further volumes:
<http://www.springer.com/series/7395>

Recent Advances in Spectroscopy

Theoretical, Astrophysical and Experimental
Perspectives

Editors

R.K. Chaudhuri

M.V. Mekkaden

A.V. Raveendran

A. Satya Narayanan

Indian Institute of Astrophysics, Bangalore, India

Editors

R.K. Chaudhuri

Indian Institute of Astrophysics
II Block, Koramangala
Sarjapur Road
Bangalore-560034
India
rkchaudh@iiap.res.in

M.V. Mekkaden

Indian Institute of Astrophysics
II Block, Koramangala
Sarjapur Road
Bangalore-560034
India
mvm@iiap.res.in

A.V. Raveendran

Indian Institute of Astrophysics
II Block, Koramangala
Sarjapur Road
Bangalore-560034
India
avr@iiap.res.in

A. Satya Narayanan

Indian Institute of Astrophysics
II Block, Koramangala
Sarjapur Road
Bangalore-560034
India
satya@iiap.res.in

ISSN 1570-6591

e-ISSN 1570-6605

ISBN 978-3-642-10321-6

e-ISBN 978-3-642-10322-3

DOI 10.1007/978-3-642-10322-3

Springer Heidelberg Dordrecht London New York

Library of Congress Control Number: 2010924625

© Springer-Verlag Berlin Heidelberg 2010

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilm or in any other way, and storage in data banks. Duplication of this publication or parts thereof is permitted only under the provisions of the German Copyright Law of September 9, 1965, in its current version, and permission for use must always be obtained from Springer. Violations are liable to prosecution under the German Copyright Law.

The use of general descriptive names, registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

Cover design: eStudio Calamar S.L.

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Preface

Spectroscopy is the basic tool employed in astronomy to derive physical parameters, like temperature, density, chemical composition, velocity and magnetic fields, that give insights into the physical processes that are operative in the celestial objects. Much of our understanding of stellar atmospheres and even low-density collisionally excited plasma, such as supernova remnants, is based on the understanding of plasma processes in the solar atmosphere. Although some of these processes can be studied by high spatial resolution images of the sun, our knowledge of the temperature, densities and dynamics of different regions of the solar atmosphere is based on the high-resolution spectroscopy in the X-ray, UV and optical spectral regions.

The atomic and molecular spectroscopy plays a key role in understanding astrochemistry. For example, the carbon bearing molecules, such as polycyclic aromatic hydrocarbons (PAHs), are now thought to be widespread in the interstellar medium in their neutral and ionized forms. Identifying the carriers responsible for several observed interstellar bands will allow us to derive important information on cosmic elemental abundance as well as on the physical conditions reigning in specific interstellar environments. The identifications of these carriers are the key for a correct understanding of the energetic mechanisms that govern the origin and evolution of the interstellar medium.

Comprehensive and accurate transition probability data are needed to determine the abundances of neutral atom and all of its ions in different astrophysical environments. Determination of radiative lifetimes can provide the absolute scale for converting the branching fractions into atomic transition probabilities and vice versa. Since the derivation of the physical parameters of the prevailing astrophysical conditions is an inverse problem, accurate theories of line formation under widely varying conditions that one encounters in celestial objects have to be developed.

It is imperative that a multi-disciplinary approach, by combining astrophysical observation with laboratory simulations and theoretical modeling, is essential to address the complex issues involved in interpreting the data for a better understanding of the physical conditions prevalent in celestial

objects. Also for a proper interpretation of the high-resolution data that we obtain from space missions, it has become necessary to improve the accuracy of the theory of line formation to a great extent. It is with this idea that the *International Conference on Recent Advances in Spectroscopy : Theoretical, Experimental, and Astrophysical Perspectives* was organized at Kodaikanal, India. Peers in the areas of theoretical and experimental atomic physics, and observational astrophysics were brought together during the conference.

The conference began with a welcome note and opening remarks by M. V. Mekkaden. The conference had 12 sessions spread over three and half days. The first two sessions were devoted to the general aspects of Atomic and Molecular Spectroscopy. They were followed by three sessions on theoretical aspects of spectroscopy. One session was devoted to line formation in stellar atmospheres. There were two sessions on observations and analysis on Solar spectroscopy and three sessions on similar topics in Stellar spectroscopy. The conference was summarized by T. P. Prabhu, while the vote of thanks was delivered by R. K. Chaudhuri.

We would like to acknowledge the sponsors, Indian Institute of Astrophysics (IIA), Department of Science and Technology (DST), Council of Scientific and Industrial Research (CSIR), and Board of Research in Nuclear Sciences (BRNS), without whom the conference would not have materialized. We thank Prof. Siraj S Hasan, Director, IIA, for his whole-hearted support, encouragement, and advice, right from the planning of this conference. Dr K. Sundararaman and his colleagues of the Kodaikanal Observatory are thanked for their unstinted support during the conference. Dr C. Kathiravan helped us in designing the cover pages for both the abstract book and the proceedings. The untiring support of the LOC and SOC members is gratefully acknowledged.

Bangalore,
August 2009

R K Chaudhuri
M V Mekkaden
A V Raveendran
A Satya Narayanan

Contents

X-Ray Spectroscopy of Highly Charged Ions in Laboratory and Astrophysical Plasmas <i>E. H. Silver, N. S. Brickhouse, T. Lin, G. X. Chen, K. Kirby, J. D. Gillaspy, J. N. Tan, and J. M. Laming</i>	1
X-ray Spectroscopy of Astrophysical and Laboratory Z-pinch Plasmas <i>A. Dasgupta, R. W. Clark, J. Davis, and J. G. Giuliani</i>	11
Computational Interstellar Chemistry <i>So Hirata, Peng-Dong Fan, Martin Head-Gordon, Muneaki Kamiya, Murat Keçeli, Timothy J. Lee, Toru Shiozaki, Jan Szczepanski, Martin Vala, Edward F. Valeev, and Kiyoshi Yagi</i>	21
State specific calculation of dissociation potential energy curve using multireference perturbation theory <i>Uttam Sinha Mahapatra and Sudip Chattopadhyay</i>	31
C–H···O Hydrogen Bonded Complexes Between Chloroform and Cyclic Ketones: Correlation of Spectral Shifts and Complex Stability with Ring Size <i>Anamika Mukhopadhyay and Tapas Chakraborty</i>	43
Infrared spectroscopic demonstration of cooperative and anti-cooperative effects in C-H--O hydrogen bonds <i>Amit K. Samanta and Tapas Chakraborty</i>	53
The Single Surface Beyond Born-Oppenheimer Equation for the Excited States of Sodium Trimer <i>Amit Kumar Paul, Biplab Sarkar, and Satrajit Adhikari</i>	63

Kubo Oscillator and its Application to Stochastic Resonance: A Microscopic Realization <i>Jyotipratim Ray Chaudhuri and Sudip Chattopadhyay</i>	75
Spectra of Conjugated Polymer Aggregates <i>K. Banerjee and G. Gangopadhyay</i>	85
Studies of parity and time reversal violations in heavy polar molecules <i>Malaya K. Nayak</i>	91
Static hyper-polarizability of open shell molecules computed at the FSMRCCSD level using constrained variational approach <i>A. Bag, S. Bhattacharya, and S. Pal</i>	99
Chemical shielding of closed-shell molecules using Extended Coupled-cluster theory <i>Lalitha Ravichandran, Sayali Joshi, and Nayana Vaval</i>	111
Multi-Disciplinary Role of Atomic Astrophysics: From Stellar Interiors to Cancer Research Via Nanotechnology <i>Anil K. Pradhan, Sultana N. Nahar, Maximiliano Montenegro, Enam A. Chowdhury, Kaile Li, Chiranjib Sur, and Yan Yu</i>	123
Recent Developments in Polarized Line Formation in Magnetic Fields <i>K. N. Nagendra, M. Sampoorna, and L. S. Anusha</i>	139
Discrete Space Theory of Radiative Transfer: Application <i>M. Srinivasa Rao</i>	155
Solar Spectroscopy and (Pseudo-)Diagnostics of the Solar Chromosphere <i>Robert J. Rutten</i>	163
High-resolution spectroscopy of the R Coronae Borealis and Other Hydrogen Deficient Stars <i>N. Kameswara Rao and David L. Lambert</i>	177
Simultaneous X-ray and Optical Observations of the T Tauri star TW Hya <i>Sushma V. Mallik, N. S. Brickhouse, and A. K. Dupree</i>	193
Element Abundance Determination in Hot Evolved Stars <i>Klaus Werner</i>	199

Elemental abundances in CEMP stars: r - and s -process elements
Aruna Goswami, Subramania P. Athiray, and Drisya Karinkuzhi 211

Spectroscopic survey of emission line stars in open clusters
Subramaniam A and Mathew B 217

An improved Technique to Explore Disk Accretion Process in PMS Stars
Padmakar Parihar 223



List of Participants

Adhikari S, Department of Physical Chemistry, Indian Association for the Cultivation of Science
Jadavpur Kolkata 700032, India
pcsa@iacs.res.in

Arunan E, Department of Inorganic and Physical Chemistry
Indian Institute of Science
Bangalore 560012, India
arunan@ipc.iisc.ernet.in

Ashok N M, Physical Research Laboratory
Ahmedabad 380009, India
ashok@prl.ernet.in

Bagare S P, Indian Institute of Astrophysics
Bangalore 560034, India
bagare@iiap.res.in

Banerjee D, Indian Institute of Astrophysics
Bangalore 560034, India
dipu@iiap.res.in

Banerjee D, Department of Physics, Shibpur Dinobundhoo Institution (College), Shibpur
Howrah 711102, India
banerjee.debi@gmail.com

Banerjee K, S.N. Bose National Centre for Basic Sciences, Salt Lake
Kolkata, India
kinshukb@bose.res.in

Chatterjee S, Department of Chemistry, Bengal Engineering and Science University, Shibpur
Howrah 711103, India
sudipchattopadhyay@rediffmail.com

Chatterjee S, Indian Institute of Astrophysics
Bangalore 560034, India
chat@iiap.res.in

Chaudhuri R, Indian Institute of Astrophysics
Bangalore 560034, India
rumpa@iiap.res.in

Chaudhuri R K, Indian Institute of Astrophysics
Bangalore 560034, India
rkchaudh@iiap.res.in

Dasgupta A, Plasma Physics Division, Naval Research Laboratory, 4555 Overlook Avenue
SW Washington, DC 203755346
USA
dasgupta@ppdmail.nrl.navy.mil

Goswami A, Indian Institute
of Astrophysics
Bangalore 560034, India
aruna@iiap.res.in

Hirata S, Quantum Theory Project
Department of Chemistry and
Department of Physics University
of Florida, USA
hirata@qtp.ufl.edu

Mallik D C V, Indian
Institute of Astrophysics
Bangalore 560034, India
dcvmlk@iiap.res.in

Mallik S V, Indian
Institute of Astrophysics
Bangalore 560034, India
sgvmlk@iiap.res.in

Mekkaden M V, Indian
Institute of Astrophysics
Bangalore 560034, India
mvm@iiap.res.in

Mukhopadhyay A, Department
of Physical Chemistry, Indian
Association for the Cultivation
of Science, Jadavpur
Kolkata 700032, India
pcam@iacs.res.in

Mukhopadhyay M, Department
of Physical Chemistry, Indian
Association for the Cultivation
of Science, Jadavpur
Kolkata 700032, India
pcmm@iacs.res.in

Muneer S, Indian Institute
of Astrophysics
Bangalore 560034, India
muneers@gmail.com

Nagaraju S, Indian Institute
of Astrophysics
Bangalore 560034, India
nagaraj@iiap.res.in

Nagendra K N, Indian
Institute of Astrophysics
Bangalore 560034, India
knn@iiap.res.in

Nataraj H S, Indian Institute
of Astrophysics
Bangalore 560034, India
nataraj@iiap.res.in

Nayak M, Theoretical Chemistry
Section, Bhabha Atomic
Research Centre, Trombay
Mumbai-400085, India
mknyak@barc.gov.in

Pal S, Physical Chemistry Division,
National Chemical Laboratory
Pune 411008, India
spal@ncl.res.in

Pandey G, Indian Institute
of Astrophysics
Bangalore 560034, India
pandey@iiap.res.in

Parihar P, Indian Institute
of Astrophysics
Bangalore 560034, India
psp@iiap.res.in

Prabhu T P, Indian Institute
of Astrophysics
Bangalore 560034, India
tpp@iiap.res.in

Pradhan A K, Department
of Astronomy, The Ohio State
University, Columbus, Ohio 43210
USA
pradhan@astronomy.ohio-state.
edu

Priya S, Department of
Astronomy, Osmania University
Hyderabad, India
shantipriya@osmania.ac.in

Ramya S, Indian Institute
of Astrophysics
Bangalore 560034, India
ramya@iiap.res.in

Rangarajan K E, Indian Institute
of Astrophysics
Bangalore 560034, India
rangaraj@iiap.res.in

Rao J V S V, Indian Institute
of Astrophysics, Kodaikanal, India
jvsv52@gmail.com

Rao M S, Indian Institute
of Astrophysics
Bangalore 560034, India
msrao@iiap.res.in

Rao N K, Indian Institute
of Astrophysics
Bangalore 560034, India
nkrao@iiap.res.in

Raveendran A V, Indian
Institute of Astrophysics
Bangalore 560034, India
avr@iiap.res.in

Ray Chaudhuri J P, Department
of Physics, Katwa College, Katwa
Burdwan 713130, India
jprc_8@yahoo.com

Rutten R J, Sterrekundig Instituut
Utrecht University, Utrecht
The Netherlands Instituut
for Teoretisk Astrofysikk
Oslo University, Oslo, Norway
R.J.Rutten@uu.nl

Samanta A K, Department
of Physical Chemistry, Indian
Association for the Cultivation
of Science, Jadavpur
Kolkata 700032, India
pcaks@iacs.res.in

Sarkar B, Department
of Chemistry, North Eastern
Hill University, Shillong 793022 India
s.biplot@gmail.com

Satya Narayanan A, Indian
Institute of Astrophysics
Bangalore 560034, India
satya@iiap.res.in

Sengupta S, Indian Institute
of Astrophysics
Bangalore 560034, India
sujan@iiap.res.in

Silver E, Harvard-Smithsonian
Center for Astrophysics, 60 Garden
Street, Cambridge, MA 02138, USA
esilver@cfa.harvard.edu

Sinha Mahapatra U, Department
of Physics, Taki Government College
Taki, North 24 Parganas, India
uttam.sinhamahapatra@
rediffmail.com

Subramaniam A, Indian
Institute of Astrophysics
Bangalore 560034, India
purni@iiap.res.in

Sundararaman K Indian Institute
of Astrophysics, Kodaikanal, India
sundar@iiap.res.in

Sutherson D, Indian Institute
of Astrophysics, Kodaikanal, India
mailsuther@gmail.com

Vaval N, Physical Chemistry
Division, National Chemical
Laboratory, Pune 411008, India
np.vaval@ncl.res.in

Werner K, Institute for Astronomy
and Astrophysics, Kepler Center
for Astro and Particle Physics
University of Tubingen, Sand 1
72076 Tubingen, Germany
werner@astro.uni-tuebingen.de