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Research Interests

Spectroscopy and Dynamics of Molecules and Clusters; Chemical Kinetics and Reaction Dynamics; Shockwave interactions with molecules and materials; Hydrogen bonding; Intermolecular bonding/interactions; Astrochemistry and astrophysics.

Courses Taught

Graduate and undergraduate courses in: Physical Chemistry, Group Theory and Molecular Spectroscopy, Chemical kinetics and Dynamics, Classical and Statistical Thermodynamics

Education

Ph. D. in Physical Chemistry, August 1991. Advisor : Prof. D. W. Setser.
Kansas State University, Manhattan, KS.

Dissertation: Applications of infrared chemiluminescence in chemical reaction dynamics.

M. Tech. in Modern Methods of Chemical Analysis and Control, January 1986
Indian Institute of Technology, New Delhi, India.

Dissertation: Structural investigations of acrylic acid-methyl methacrylate copolymers.

M. Sc. in Chemistry July 1984, Indian Institute of Technology, Madras, India.

Dissertation: Synthesis of π -CS₂ complexes of Iron and phase transfer catalyzed reductions of nitroarenes.

B. Sc. in Chemistry June 1982, The American College, Madurai, India.

Work Experience

Chairman, Department of Inorganic and Physical Chemistry October 2018 -

Member JAM Advisory Committee of IISc from 2015

Vice-Chairman GATE/JAM, Indian Institute of Science 2013-2015

Coordinator for the Integrated Ph. D. Programme in Chemical Sciences 2010-

2014

- June 2009 – Present: Professor, Inorganic and Physical Chemistry Department, Indian Institute of Science, Bangalore, India
- Jun. 2003 – May 2009: Associate Professor, Inorganic and Physical Chemistry Department, Indian Institute of Science, Bangalore, India
- Jun. 1997 – May 2003: Assistant Professor, Inorganic and Physical Chemistry Department, Indian Institute of Science, Bangalore, India.
- Nov. 1994 - May 1997: Assistant Professor at Indian Institute of Technology, Kanpur, India.
- Apr. 1992 - Oct. 1994: Research Associate with Prof. H. S. Gutowsky at University of Illinois at Urbana-Champaign. Investigated weakly bound complexes using pulsed nozzle Fourier transform microwave spectroscopy.
- Aug. 1991 – Apr. 1992. Research Associate with Prof. D. W. Setser at Kansas State University; supervisory responsibilities between August 1991 - January 1992.
- Jun. 1988 – Jul. 1991. Research Assistant. Rebuilt the infrared chemiluminescence laboratory at K.S.U. in a new Chemistry building. Acquired experience in vacuum techniques, glass blowing, computing and other laboratory skills needed for research in experimental physical chemistry.
- Aug. 1986 - May 1988. Teaching Assistant. Involved in teaching undergraduate physical chemistry labs and grading undergraduate physical and organic chemistry courses at Kansas State University.
- Feb. 1986 – Jun. 1986. Project assistant with Prof. K. C. Patil, Inorganic and Physical Chemistry Department, Indian Institute of Science, Bangalore, India.

Awards and Activities

- Plenary Lecture at the 7th Asian Spectroscopy Conference, Singapore,**
Conducted online, National Technological University, Singapore
December 2020.
- Alumni Award for Excellence in Research for Science for the year 2020,**
awarded by the Indian Institute of Science.
- Editor,** Volume 100, issue 1 of the *Journal of the Indian Institute of Science*,
January 2020, on 100 years of hydrogen bonding.
- Member of the Editorial Board** for the *Journal of Molecular Spectroscopy*
2014-2017 and 2020-2023
- National Prize for Chemical Spectroscopy and Molecular Structure,** CNR
Rao Research Foundation, 2019
- International Advisory Board Member for the First International
Conference on Non-Covalent Interactions,** Given keynote lecture.
Lisbon, Portugal September 2019.
- Keynote Lecture at the European Congress on Molecular Spectroscopy
2018,** August 2018, Coimbra, Portugal.
- Editorial Board of the Journal of the Indian Institute of Science 2018 -
Plenary Lecture at the 22nd Horizons in Hydrogen Bond Research
Conference,** September 2017, Finland
- Editor of the Journal of Molecular Structure** May 2016 -
Fellow of the National Academy of Sciences, India, 2015

Guest Member of the Editorial Board 67th *Annual Reviews in Physical Chemistry* 2016

Fellow of the Royal Society of Chemistry 2014

Plenary Speaker at the Fourth Asian Spectroscopy Conference, Singapore
December 2013.

PRL Colloquium at Physical Research Laboratory, Ahmedabad, 27 November 2013

ASET Colloquium at Tata Institute of Fundamental Research, Mumbai, 8 Nov 2013.

Royal Society Travel Grant to visit 12 Universities in the USA and attend Molecular Spectroscopy and Shock Wave symposium June-July 2013.

A. V. Ramarao Foundation Prize Lecture at the Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore. April 2013

Member of Science Education Panel of the Indian Academy of Sciences 2013-2018

Fellow of International Union of Pure and Applied Chemistry 2011

Plenary Lecture at the 28th International Symposium on Shock Waves,
Manchester 2011.

Member of the International Advisory Board for ‘Horizons in Hydrogen Bond Research’ Conference 2011 –

Member of the International Steering Committee for the Asian Spectroscopy Conference 2009-2013. Continuing in the Advisory Board Since 2013.

Fellow of the Indian Academy of Sciences, 2009

Member of the Programme Advisory Committee on Physical Chemistry, Department of Science and Technology 2008-2012.

Member of the International Advisory Editorial Board for Physical Chemistry Chemical Physics, Royal Society Publication, From 2005-2016.

Section Editor (Chemistry) for Current Science from 2018, Associate Editor 2013-2018 and in the editorial board since 2008

Associate Editor for Journal of Chemical Sciences from 2012-2015 in the editorial board since 2008

Recipient of Chemical Research Society of India Bronze Medal 2008

Chairman of IUPAC Task Group on Hydrogen bonding and other molecular interactions. Redefined hydrogen bonding in 2011.

Member of the International Advisory Board for the International Symposium on Shockwaves from 2005.

Vice-President/Founder Member of the Indian Society for Shockwave Research 2004.

Member of International Union of Pure and Applied Chemistry since 2004

Member of Chemical Research Society of India since inception, 1999

KSU Department of Chemistry Award for Excellence in Research, 1991.

KSU Phi Lambda Upsilon Graduate Student of the Year Award, 1989.

Member of Phi Lambda Upsilon, an Honourary Chemical Society in U.S.A. Since 1988

Member of the American Chemical Society since 1987

Invited Talks/Seminars/Lectures

Have organized several national/international conferences/symposia in the fields of spectroscopy, hydrogen bonding and shock wave applications. Have given numerous plenary, key note and invited lectures all over India and many countries in the world including U.S.A, U.K, France, Germany, Italy, Poland, Spain, Russia, Czech Republic, Finland, Portugal, China, Taiwan, Pakistan, Bangladesh, Singapore, Australia and South Korea. Given invited talks at most of the premier institutes in India and also in small colleges and high schools all over India. Given invited lectures at Universities, including at University of California, Berkeley; Stanford University; California Institute of Technology, Rowland Institute at Harvard University; University of Colorado, Boulder; Wesleyan University; University of Connecticut; Kansas State University; National Oceanographic and Atmospheric Agency, Colorado; University of Massachusetts, Amherst; Moscow State University, Moscow; Fritz Haber Institute, Berlin; Warsaw University, Poland; Milan Technical University, Italy; University of Rennes, France; Grenoble University, France; Hebrew University at Jerusalem, Israel; Universidad del País Vasco, Spain; Czech Academy of Sciences, Prague.

Research Highlights

- *Built the only pulsed nozzle Fourier transform microwave spectrometer in India and one of about 15 in the world.*
- *Our experimental results on weakly bound complexes of H₂O/H₂S eventually led to IUPAC redefining hydrogen bond through a task group formed and chaired by me.*
- *Microwave spectroscopic and theoretical results from our laboratory led us to define a 'carbon bond' analogous to hydrogen bond. This has helped the field of 'inter-molecular bonding' matured.*
- *Established shock tube facilities for chemical kinetics research in collaboration with Aerospace Engineering Department. This facility has been used to address problems of interest to ISRO and DRDO and eventually led to the formation of Center for Excellence in Hypersonic Research.*
- *Our research accomplishments on hydrogen bonding and carbon bonding have been featured in Science magazines and newspapers all over the world. Our laboratory is at the forefront of research in this area.*

Publications in Journals

1. A. S. Brar, E. Arunan and G. S. Kapur, (1989) "Sequence determination in acrylic acid-methyl methacrylate copolymers by ¹³C and ¹H NMR spectroscopy", *Polym. J. (Tokyo)* 21, 689.
2. E. Arunan, S. J. Wategaonkar and D. W. Setser, (1991) "HF/HCl vibrational and rotational distributions from three- and four-centered unimolecular elimination reactions", *J. Phys. Chem.* 95, 1539.
3. E. Arunan and D. W. Setser, (1991) "HCN infrared chemiluminescence from the H + ICN reaction", *J. Phys. Chem.* 95, 4190.
4. E. Arunan, D. W. Setser and J. F. Ogilvie (1992) "Vibration-rotational Einstein coefficients for HF/DF and HCl/DCl", *J. Chem. Phys.* 97, 1734.

5. E. Arunan, D. Raybone and D. W. Setser (1992) "Vibrational relaxation rate constants for HF($v=1-4$) by CO, CO₂ and HCN with product identification by infrared emission", , *J. Chem. Phys.* 97, 6348.
6. E. Arunan and H. S. Gutowsky (1993) "The rotational spectrum, structure and dynamics of a benzene dimer", *J. Chem. Phys.* 98, 4294.
7. E. Arunan, G. Manke II and D. W. Setser, (1993) "Infrared chemiluminescence studies of H + BrCN and H abstraction by CN reactions: importance of the HNC channel", *Chem. Phys. Lett.* 207, 81.
8. H. S. Gutowsky, T. Emilsson and E. Arunan. (1993) "Low J rotational spectra, internal rotation, and structures of several benzene-water dimers", *J. Chem. Phys.* 99, 4883.
9. E. Arunan, T. Emilsson and H. S. Gutowsky, (1993) "Rotational spectrum and structure of Ne-C₆H₆-H₂O, an aromatic sandwich", *J. Chem. Phys.* 99, 6208.
10. E. Arunan, C. Liu, D. W. Setser, J. V. Gilbert and R. D. Coombe, (1994) "Infrared chemiluminescence studies of H + NFCl₂ and H + NFCl reactions", *J. Phys. Chem.* 98, 494.
11. E. Arunan, R. Rengarajan and D. W. Setser, (1994) "Infrared chemiluminescence studies of the reactions of H atoms with CCl₃, CF₂Cl and CH₂CH₂Cl radicals at 300 and 475 K: addition-elimination vs abstraction reaction mechanisms", *Can. J. Chem.* (J. C. Polanyi Special Issue) 72, 568.
12. E. Arunan, T. Emilsson and H. S. Gutowsky, (1994) "Rotational spectra and structure of Rg-C₆H₆-H₂O (Rg = Ne, Ar or Kr) trimers and Ne-C₆H₆ dimer", *J. Chem. Phys.* 101, 861.
13. E. Arunan, T. Emilsson and H. S. Gutowsky, (1994) "Rotational spectra, structure and dynamics of Ar_n(H₂O)_m clusters: Ar₂-H₂O, Ar-(H₂O)₂, Ar₃-H₂O and Ar-(H₂O)₃" *J. Am. Chem. Soc.* 116, 8418.
14. J. -U. Grabow, A. S. Pine, G. T. Fraser, F. J. Lovas, R. D. Suenram, T. Emilsson, E. Arunan, and H. S. Gutowsky, (1995) "Rotational spectra and van der Waals potentials of Ne-Ar", *J. Chem. Phys.* 102, 1181.
15. E. Arunan, T. Emilsson, and H. S. Gutowsky, (1995) "Excited v_3 vibrational state of the Ar-HCN and Kr-HCN dimers", *J. Chem. Phys.* 103, 493.
16. H. S. Gutowsky, E. Arunan, T. Emilsson, S. L. Tschopp, and C. E. Dykstra, (1995) "Rotational spectra and structures of the C₆H₆-HCN dimer and Ar₃-HCN tetramer", *J. Chem. Phys.* 103, 3917.
17. E. Arunan, C. E. Dykstra, T. Emilsson, and H. S. Gutowsky, (1996) "Rotational spectra, structures, and dynamics of small Ar_m-(H₂O)_n clusters : the Ar₂-H₂O trimer", *J. Chem. Phys.* 105, 8495.
18. H. S. Gutowsky, T. Emilsson, and E. Arunan (1997) "Rotational spectra, structure, and internal dynamics of Ar-H₂S isotopomers", , *J. Chem. Phys.* 106, 5309.
19. E. Arunan (1997) "The C-C bond is stronger than the C-Cl bond in CH₃COCl" *J. Phys. Chem. A.* 101, 4838.
20. A. Srivatsava, E. Arunan, G. Manke II, D. W. Setser, and R. Sumathi, (1998) "Unimolecular reaction dynamics of CH₃COCl and FCH₂COCl :

- An infrared chemiluminescence and *ab initio* study", *J. Phys. Chem.A.* **102**, 6412.
21. E. Arunan*, T. Emilsson, H. S. Gutowsky, and C. E. Dykstra (2001) "Rotational spectra and structures of the Ar₃-H₂O and Ar₃-H₂S symmetric tops", *J. Chem. Phys.* **114**, 1242.
 22. P. K. Mandal and E. Arunan (2001) "Hydrogen bond radii for the hydrogen halides and van der Waals radius of hydrogen", *J. Chem. Phys.* **114**, 3880.
 23. K. R. Shamaundar and E. Arunan (2001) "Hydrochlorofluoroamines: Ab initio and DFT studies on their unimolecular reaction pathways" *J. Phys. Chem.A.* **105**, 8533
 24. E. Arunan*, T. Emilsson, and H. S. Gutowsky, (2002) "Rotational Spectra, structures, and dynamics of small Ar_m-(H₂O)_n clusters II : the Ar-(H₂O)₂ trimer" *J. Chem. Phys.* **116**, 4886.
 25. S. P. Vijayalakshmi, E. Arunan*, R. Valesa and D. W. Setser. (2002) "Infrared chemiluminescence studies of the H + ICH₂X and N + CH₂X (X = Cl/F/I/H) reactions" *Phys. Chem. Chem. Phys.* **4**, 51.
 26. E. Arunan*, A. P. Tiwari, P. K. Mandal, and P. C. Mathias, (2002) "Pulsed nozzle Fourier transform microwave spectrometer: Ideal to define hydrogen bond radius", *Curr. Sci.* **82**, 533
 27. B. Rajakumar, K. P. J. Reddy and E. Arunan*, (2002) "Unimolecular HCl elimination from 1,2-dichloroethane: A single pulse shock tube and ab initio study" *J. Phys. Chem. A.* **106**, 8366
 28. E. Arunan*, T. Emilsson, H. S. Gutowsky, G. T. Fraser, G. de Oliviera and C. E. Dykstra (2002) "Rotational dynamics of the weakly bonded C₆H₆-H₂S dimer and comparisons to C₆H₆-H₂O" *J. Chem. Phys.* **117**, 9766.
 29. B. Rajakumar, D. Anandraj, K. P. J. Reddy, and E. Arunan (2002). "Chemical kinetics studies at high temperatures using shock tubes" *J. Ind. Inst. Sci.* **82**, 37.
 30. B. Rajakumar and E. Arunan (2003) "Ab initio, DFT and transition state theory calculations on HF, HCl and ClF elimination from CH₂XCH₂Y:X/Y=F/Cl", *Phys. Chem. Chem. Phys.* **5**, 3897.
 31. B. Rajakumar, K. P. J. Reddy and E. Arunan, (2003) "Thermal decomposition of 2-fluoroethanol: Single pulse shock tube and ab initio studies." *J. Phys. Chem. A.* **107**, 9782.
 32. Naba K. Karan and E. Arunan, (2004) "Chlorine bond distances in ClF and Cl₂ complexes" *J. Mol. Structure* **688**, 203).
 33. E. Arunan, Sagarika Dev, P. K. Mandal, (2004) "Pulsed nozzle Fourier transform microwave spectrometer: Advances and applications" *Appl. Spectrosc. Rev.* **39**, 131.
 34. M. Goswami, P. K. Mandal, D. Ramdass and E. Arunan, (2004) "Rotational spectra and structure of the floppy C₂H₄-H₂S complex: Bridging hydrogen bonding and van der Waals interactions" *Chem. Phys. Lett.* **393**, 22.
 35. B. Lakshmi, A. G. Samuelson, K. V. Jovan Jose, S. R. Gadre, and E. Arunan, (2005) "Is there a hydrogen bond radius? Evidence from

- microwave spectroscopy, neutron scattering and X-ray diffraction results” *New. J. Chem* **29**, 371.
36. B. Ram Prasad, Mangala Sunder Krishnan and E. Arunan, (2005) “Rotational Spectrum of mono-substituted asymmetric C₆H₆-H₂O dimers” *J. Mol. Spectrosc.* **232**, 308.
 37. P. K. Mandal, D. Ramdass and E. Arunan (2005) “Rotational spectra and structure of Ar₂-H₂S complex: PNFTMW spectroscopic and ab initio studies”. *Phys. Chem. Chem. Phys.* **7**, 2740.
 38. P. K. Mandal, Mausumi Goswami and E. Arunan (2005) “Rotational Spectra and Structure of Ar-(H₂S)₂ trimer: Microwave spectroscopic and ab initio investigation”, *J. Ind. Inst. Sci.* **85**, 353.
 39. E. Arunan, P. K. Mandal, M. Goswami, and B. Raghavendra, (2005) “Rotational Spectra of weakly bound H₂O/H₂S complexes: Hydrogen bonding vs van der Waals interactions” *Proc. Ind. Nat. Sci. Acad.* **71 A**, 377.
 40. P. K. Mandal, B. Raghavendra and E. Arunan, (2006) “Ab initio and AIM theoretical analysis of Hydrogen-Bond radius of HD(D=F,Cl,Br,CN,OH,SH and CCH) donors and some acceptors” *Phys. Chem. Chem. Phys.* **8**, 5276-5286.
 41. B. Raghavendra and E. Arunan. (2007) “Unpaired and sigma bond electrons as H, Cl and Li bond acceptors: An anomalous one-electron blue-shifting chlorine bond”, *J. Phys. Chem. A* **111**, 9699.
 42. Prasanta Das, E. Arunan and P. K. Das, (2008) “Infrared Spectra of dimethylnaphthalenes in the gas phase”, *Vibrational Spectroscopy*, **47**, 1-9,.
 43. M. Nagaboopathy, C. Vijayanand, G. Hegde, K. P. J. Reddy, and E. Arunan (2008) "Single pulse shock tube for ignition delay studies" *Curr. Sci.*, **95**, 78-82,
 44. V. Kulkarni, G. M. Hegde, G. Jagadeesh, E. Arunan and K. P. J. Reddy. (2008) “Aerodynamic drag reduction by heat addition into the shock layer for a large angle blunt cone in hypersonic flow” *Phys. Fluid*, **20**, 081703.
 45. B. Raghavendra and E. Arunan (2008) “Hydrogen bonding with a hydrogen bond: The methane-water complex and the pentacoordinate carbon”, *Chem. Phys. Lett.* **467**, 37.
 46. L. Biennier, R. Georges, V. Chandrasekaran, B. Rowe, T. Bataille, V. Jayaram, K. P. J. Reddy and E. Arunan, (2009) “Characterization of circumstellar carbonaceous dust analogs produced by pyrolysis of acetylene in a porous graphite reactor” *Carbon*, **47**, 3295.
 47. M. Goswami and E. Arunan (2009) “The Hydrogen Bond: A molecular beam microwave spectroscopist’s view with a universal appeal”, *Phys. Chem. Chem. Phys.* **11**, 8974.
 48. Deepak Chopra, T. N. Guru Row, E. Arunan and R. A. Klein (2010) “Crystalline ethane-1,2-diol Does Not Have Intramolecular Hydrogen Bonding: Experimental and Theoretical Charge Density Studies”, *J. Mol. Struct.* **964**, 126.

49. Prasanta Das, S. Manogaran, E. Arunan and P. K. Das (2010) "Infrared Spectra of Dimethylquinolines in the Gas Phase: Experiment and Theory", *J. Phys. Chem. A* **114**, 8351.
50. D. Mani, P. Aiswaryalakshmi and E. Arunan (2010) "Measuring rotational constant of a molecule without dipole moment and confirming low frequency vibrations using microwave spectroscopy" *Asian J. Spectrosc. Special issue*, 31. *Invited article for an issue honoring Dr. K. P Nair, a microwave spectroscopist from Kerala.*
51. M. Goswami and E. Arunan, (2011) "Microwave Spectrum and Structure of C₆H₅CCH--H₂S complex", *J. Mol. Spectrosc.* **268**, 147.
52. E. Arunan*, G. R. Desiraju, R. A. Klein, J. Sadlej, S. Scheiner, I. Alkorta, D. C. Clary, R. H. Crabtree, J. J. Dannenberg, P. Hobza, H. G. Kjaergaard, A. C. Legon, B. Mennucci and D. J. Nesbitt (2011) "Defining the hydrogen bond: An Account" *Pure Appl. Chem.* **83**, 1619.
53. E. Arunan*, G. R. Desiraju, R. A. Klein, J. Sadlej, S. Scheiner, I. Alkorta, D. C. Clary, R. H. Crabtree, J. J. Dannenberg, P. Hobza, H. G. Kjaergaard, A. C. Legon, B. Mennucci and D. J. Nesbitt (2011) "Definition of the hydrogen bond" *Pure Appl. Chem.* **83**, 1637.
54. M. Goswami and E. Arunan (2011) "Microwave Spectroscopic and Theoretical Studies on phenylacetylene· H₂O Complex: CH---O and OH---p Hydrogen Bonds as Equal Partners", *Phys. Chem. Chem. Phys.* **13**,14153.
55. V. Chandrasekaran, L. Biennier, E. Arunan, D. Talbi and R. Georges, (2011) "Direct Infrared Absorption Spectroscopy of Benzene Dimer", *J. Phys. Chem. A* **115**, 11263.
56. P. Das. E. Arunan, and P. K. Das, (2012) "Infrared Spectra of Dimethylphenanthrenes in the Gas phase", *J. Phys. Chem. A* **116**, 5769.
57. D. Mani, V. T. Bhat, K. J. Vinoy and E. Arunan (2012) "Towards the broadband microwave spectrometer", *Ind. J. Phys.* **86**, 225 (*Invited article for an issue honoring Prof. Mihir Chowdhuri*)
58. D. Koley, E. Arunan and S. Ramakrishnan, (2012) "Computational investigations on covalent dimerization/oligomerization of polyacenes: Is it relevant to soot formation?" *J. Comput.l Chem.* **33**, 1762.
59. A. Gardez, G. Saidani, L. Biennier, R. Georges, E. Hugo, V. Chandrasekaran, V. Roussel, B. Rowe, K. P. J. Reddy, and E. Arunan, (2012) "High-temperature kinetics of the reactions between CN and hydrocarbons using a novel high enthalpy flow tube" *Int. J. Chem. Kinetics* **44**, 753.
60. D. Mani and E. Arunan, (2013) "Microwave Spectroscopic and Atoms in Molecules Theoretical Investigations on the Ar···Propargyl Alcohol Complex: Ar···H - O, Ar···π, and Ar···C Interactions" *ChemPhysChem* **14**, 754.
61. R. Parajuli and E. Arunan, (2013) "Comprehensive Investigations on DNa···A (D=H/F) Complexes Show Why 'Sodium Bonding' is not Commonly Observed" *Chem. Phys. Lett.* **568-569**, 63.

62. N. K. Reddy, V. Jayaram, E. Arunan, Y. B. Kwon, W. J. Moon, and K. P. J. Reddy (2013) "Investigations on high enthalpy shock wave exposed graphitic carbon nanoparticles" *Diamond and Related Materials*, **35**, 53.
63. P. Aiswaryalakshmi, Devendra Mani, and E. Arunan (2013) "Fe as hydrogen/halogen bond acceptor in square pyramidal Fe(CO)₅" *Inorg. Chem.*, **52**, 9153.
64. D. Mani and E. Arunan, (2013) "The X-C---Y (X = O/F, Y = O, S, F, Cl, Br, N, P,) Carbon bond and hydrophobic interactions" *Phys. Chem. Chem. Phys.* **15**, 14377.
65. S. K. Reshmi, K. P. Vijayalakshmi, D. Thomas, E. Arunan and C. P. R. Nair (2013) "Glycidyl azide polymer crosslinked through triazoles by click chemistry: curing, mechanical and thermal properties." *Propellants, Explosives, Pyrotechniques* **38**, 525.
66. M. Goswami, J. L. Neill, M. Muckle, B. H. Pate, and E. Arunan (2013) "Microwave, infrared-microwave double resonance, and theoretical studies of C₂H₄···H₂S complex" *J. Chem. Phys.* **139**, 104303.
67. A. Shahi and E. Arunan, (2014) "Hydrogen bonding, halogen bonding and lithium bonding: An atoms in molecule and natural bond orbital perspective towards conservation of total bond order, inter- and intra-molecular bonding" *Phys. Chem. Chem. Phys.* **16**, 22935-22952. (Perspective article featured in back-cover and highlighted).
68. N. Sharath, K. P. J. Reddy and E. Arunan (2014) "Thermal Decomposition of Propargyl Alcohol: Single Pulse Shock Tube Experimental and ab initio Theoretical Study" *J. Phys. Chem. A* **118**, 5927-5938.
69. S. Reshmi, C. P. Reghunadhan Nair, E. Arunan (2014) "Azide and Alkyne Terminated Polybutadiene Binders: Synthesis, Crosslinking and Propellant Studies" *J. Ind. Eng. Chem.* **53**, 16612-16620.
70. D. Mani and E. Arunan (2014) "Rotational Spectra of Propargyl Alcohol Dimer: A Dimer Bound with Three Different Types of Hydrogen Bonds" *J. Chem. Phys.* **141**, 164311.
71. D. Mani and E. Arunan (2014) "The X-C···π (X=F, Cl, Br, CN) Carbon Bond" *J. Phys. Chem. A* **118**, 10081-10089.
72. D. Mani and E. Arunan (2015) "Dynamics of a chemical bond: inter and intra-molecular hydrogen bonding" *Faraday Discussions* **177**, 51-64.
73. Govinda P. Khanal, R. Parajuli, E. Arunan, Shinichi Yamabe, Kenzo Hiraoka, Eiko Torikai (2015) "Study of structures, energies and vibrational frequencies of (O₂)ⁿ⁺ (n=2-5) clusters by GGA and meta-GGA density functional methods" *Comp. Theor. Chem.* **1056**, 24-36.
74. Lakshmipriya Anamalagundam, Sachin Rama Chaudhari, Abhishek Shahi, E. Arunan and Suryaprakash Nagaraja Rao (2015) "Three Centered Hydrogen Bond of the type C=O···H(N)···X-C in diphenyloxalimide derivatives involving halogens and a rotating CF₃ group: NMR, QTAIM, NCI and NBO Studies" *Phys. Chem. Chem. Phys.* **17**, 7528-7536.

75. N. Sharath, P. K. Bharai, K. P. J. Reddy and E. Arunan (2015) "Ignition delay of 3-carene: Single Pulse Shock Tube Study", *Curr. Sci.* **108**, 2083-2087.
76. R. Parajuli and E. Arunan (2015) "X-H...C hydrogen bonds in n-alkane-HX (X = F, OH) complexes are stronger than C-H...X hydrogen bonds" *J. Chem. Sci.* **127**, 1035-1045.
77. S. K. Pandey, Prasanta Das, P. K. Das, E. Arunan* and S. Manogaran* (2015) "Intramolecular Hydrogen Bond: Can it be Part of the Basis Set of Valence Internal Coordinates in Normal Mode Analysis?" *J. Chem. Sci.* **127**, 1127-1134.
78. Prasanta Das, P. K. Das and E. Arunan (2015) "Conformational Stability and Intramolecular Hydrogen Bonding in 1,2-Ethandiol and 1,4-Butanediol" *J. Phys. Chem. A* **119**, 3710-3720.
79. Abhishek Shahi and E. Arunan (2015) "Microwave Spectrum of Hexafluoro-isopropanol and Torsional Behavior of Molecules with a CF₃-C-CF₃ Group" *J. Phys. Chem. A* **119**, 5650-5657.
80. S. Reshmi, K. P. Vijayalakshmi, R. Sadhana, B. K. George, E. Arunan, C. P. Reghunadhan Nair (2015) "Inter molecular azide-diisocyanate coupling: new insights for energetic solid propellants" *RSC Advances* **5**, 50478-50482.
81. Abhishek Shahi and E. Arunan (2015) "Microwave Spectroscopic and Theoretical Investigations of the Strongly Hydrogen Bonded Hexafluoroisopropanol-Water Complex" *Phys. Chem. Chem. Phys.* **17**, 24774-24782.
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