Curriculum Vitæ – Ponnadurai RAMASAMI
(*PhD, CSci CChem, FICCE, FRSC*)

Name Ponnadurai RAMASAMI

Date of Birth : 13 March 1969
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Educational Background

December 1996	PhD in Physical Chemistry; University of Delhi, India Title of thesis: "*Volume and Compressibility Studies of Some Aminocarboxylic acids and a Peptide in Water and Aqueous Solutions of Sodium Sulphate at 288.15, 298.15 and 308.15 K*"
July 1993	M.Sc. Chemistry; University of Delhi, India
July 1991	B.Sc. (Hons) Chemistry; University of Delhi, India
November 1987	Higher School Certificate; Royal College Port-Louis, Mauritius

Professional Career

Apr. 2012	Professor, Personal Chair in Computational Chemistry
Aug. 2006 to Apr. 2012	Associate Professor in Chemistry; University of Mauritius
Aug. 2003 to Aug. 2006	Senior Lecturer in Chemistry; University of Mauritius
Aug. 2000 to Sep. 2003	Lecturer in Chemistry; University of Mauritius
Jan. 1997- Jul. 2000	Teacher; Merton College, Mauritius

Teaching

(a) Merton College, Mauritius: Ordinary and Advanced levels Chemistry
(b) University of Mauritius:
    (i) Department of Chemistry
    (ii) Department of Chemical Engineering

Supervision

- 50 Undergraduate projects
- 10 Postgraduate projects

MPhil/PhD Supervision

Raj Kumar Sreeruttun, Completed
Ashwini Bundhun, Completed
Lydia Rhyman, On going
Naziah Jaufeerally, On going
Neelum Seeburrun, On going
Pravesh Gohee, On going

Research

My doctoral research work was done at, The Physical Chemistry Laboratory, University of Delhi, India, under the supervision of Late Dr. R. K. Wadi.

Theoretical methods based on *ab initio* computations are used to study molecules and clusters in vacuum and solution phases.

The optimised structures and conformations of the molecules and clusters are predicted.

Spectroscopic parameters such as infrared, Raman and NMR spectra are predicted.

The energetic of molecules and clusters are also studied leading to estimation of ionization energies and electron affinity among physical parameters.

The reactions involving these molecules and clusters are also probed with the objectives of shedding more light into mechanisms, activation barriers, thermodynamic properties and rate constants.

Studies are extended to novel, yet not synthesized, molecules and clusters.

Funded projects

1) University of Mauritius (September 2001): Rs 150,000 (US$ 5,000) (Completed)
2) Assessment of theoretical methods for the study of reactions involving global warming gas species degradation and byproduct formation (November 2007-2009): (US$ 6,000)
3) University of Mauritius (September 2011): Rs 150,000 (US$ 5,000) (Theoretical investigations of the gas phase reactions of DMSe with halogens)

Book

One of the editors of the book of proceedings, Bioresources Towards Drug Development, available on CD.

Chemistry Education in the ICT Age; M. Gupta-Bhowon, University of Mauritius, Reduit, Mauritius; S. Jhaumeer-Laulloo, University of Mauritius, Reduit, Mauritius; H. Li Kam Wah, University of Mauritius, Reduit, Mauritius; P. Ramasami, University of Mauritius, Reduit, Mauritius (Eds.) Published by Springer, 2009.

Chemistry for Sustainable Development; M. Gupta-Bhowon, University of Mauritius, Reduit, Mauritius; S. Jhaumeer-Laulloo, University of Mauritius, Reduit, Mauritius; H. Li Kam Wah, University of Mauritius, Reduit, Mauritius; P. Ramasami, University of Mauritius, Reduit, Mauritius (Eds.) Published by Springer, 2012.

Conference Participation

Participated in 35 International conference giving oral presentations

Administration

1. Associate Editor Research Journal of Chemistry and Environment
2. Advisory Board Member of Asian Journal of Chemistry
3. Reviewer for Physical Chemistry Chemical Physics
4. Reviewer for Chemical Reviews
5. Reviewer for The Journal of Chemical Engineering Data
6. Reviewer for The Journal of Chemical Education
7. Reviewer for The Research Journal of Chemistry and Environment
8. Reviewer for The Asian Journal of Chemistry
9. Reviewer for Research in Space Science
10. Reviewer for Chemical Engineering Communications
11. Reviewer for Journal of Food Composition and Analysis
12. Committee member of Project ChemLab, Journal of Chemical Education
13. Member of the American Chemical Society
14. Member of the Royal Society of Chemistry (CSci CChem FRSC)
15. Fellow member of International Congress of Chemistry and Environment (FICCE)
16. Affiliate Member of International Union of Pure and Applied Chemistry
17. Organising member for "World Science Day" held on at the University of Mauritius
18. Scientific Secretary of IUPAC Satellite Symposium held at the University of Mauritius
19. Panelist for chemistry educational programme conducted by Mauritius College of the Air
20. Committee member at National level for "Promotion of Science and Technology at Primary level, conducted by Mauritius Research Council.
21. Committee member for student grievance cell at the University of Mauritius.
22. High power committee member for Scholarship, Ministry of Education, Culture and Human Resource, Mauritius
23. Coordinator for International Congress of Chemistry and Environment, Dec 2005 Indore, India.
24. Organiser of the first workshop "Computational Chemistry and Its Applications", part of ICCS 2006, 28^{th}-31^{st} May 2006, Reading, UK.
25. Organiser of the second workshop "Computational Chemistry and Its Applications", part of ICCS 2007, 27^{th}-30^{th} May 2007, Beijing, China.
26. Organiser of the third workshop "Computational Chemistry and Its Applications", part of ICCS 2008, 23^{rd}-25^{th} June 2008, Kraków, Poland.
27. Chairman of the 20^{th} ICCE (International Conference on Chemical Education), 3^{rd}-8^{th} August 2008, Mauritius.
28. Organiser of the fourth workshop "Computational Chemistry and Its Applications", part of ICCS 2009, 25^{th}-27^{th} May 2009, Baton Rouge, USA.
29. Organiser of the fifth workshop "Computational Chemistry and Its Applications", part of ICCS 2010, 31^{st} May – 2^{nd} June 2010, Amsterdam, The Netherlands.
30. Chairman of ICPAC (International Conference on Pure and Applied Chemistry), 26^{th}-30^{th} July 2010, Mauritius.
31. Organiser of the sixth workshop "Computational Chemistry and Its Applications", part of ICCS 2011, 1^{st} June – 3^{rd} June 2011, Singapore.
32. Chairman of ICPAC (International Conference on Pure and Applied Chemistry), 2^{nd}-6^{th} July 2012, Mauritius.

External Examiner

I am the external examiner for the Department of Chemistry of the University of Namibia.

I have also examined 15 PhD theses.

List of published papers

P1 R. K. Wadi and P. Ramasami: "Partial Molal Volumes and Adiabatic Compressibilities of Transfer of Glycine and DL-Alanine from Water to Aqueous Sodium Sulphate at 288.15, 298.15 and 308.15 K." (Journal of Chemical Society Faraday Transaction, 1997, 93, 243-247)

P2 P. Ramasami: "Students as Solids, Liquids and Gases" (Journal of Chemical Education, 2000, 77, 485)

P3 P. Ramasami: "Solubilities of Amino Acids in Water and Aqueous Sodium Sulphate and Related Apparent Transfer Properties" (Journal of Chemical Engineering Data, 2002, 47, 1164-1166)

P4 P. Ramasami and P. Ramburrun: "Applications of Conductimetric Titrations" (Research Journal of Chemistry and Environment, 2003, 7, 48-53)

P5 P. Ramasami: "A Concise Description of an old Problem: Application of Matrices to obtain the Balancing Coefficients of Chemical Equations." (Journal of Mathematical Chemistry, 2003, 34, 123-129)

P6 P. Ramasami and P. Ramburrun: "Non-aqueous Conductimetric Titrations of Phenolic Compounds with Tetrabutylammonium Hydroxide and Amines against Perchloric acid in Acetonitrile Solvent" (Asian Journal of Chemistry, 2003, 15, 1539-1544)

P7 S. Jhaumeer-Laulloo, P. Rondeau, F. Cadet and P. Ramasami: "Quantitative Determination of Sugar in some Common Fruits by Different Methods." (Chemistry, An Indian Journal, 2003, 1, 131-136)

P8 P. Ramasami, D. N. Moothoosamy and R. Goojha: "Kinetics of the Reaction between Peroxodisulphate (VI) and Iodide ions." (Asian Journal of Chemistry, 2004, 16, 85-88)

P9 P. Ramasami, S. Jhaumeer-Laulloo, P. Rondeau, F. Cadet, H Seepujak and A Seeruttun: "Quantification of Sugar in Beverages and Fruit Juices by Different Methods" (South African Journal of Chemistry, 2004, 57, 24-27)

P10 N. Salim and P. Ramasami: "Applications of Potentiometric Titrations" (Chemistry, An Indian Journal, 2004, 1, 607-609)

P11 S. Jhaumeer-Laulloo and P. Ramasami: "Monitoring Browning and Sugar Content Of Litchi After Post Harvest Treatment" (Chemistry, An Indian Journal, 2004, 1, 610-611)

P12 R. K. Sreeruttun, P. Ramasami, G Yan, C. S. Wannere, P. v. R. Schleyer and H. F. Schaefer: "The Alkylethynyl Radicals, $\bullet C{\equiv}C\text{-}C_nH_{2n+1}$ (n=1-4), and their Anions'" (International Journal of Mass Spectrometry, 2005, 241, 295-304)

P13 P. Ramasami, S. Jhaumeer-Laulloo, F. Cadet, P. Rondeau and Y. Soophul: "Quantification of Alcohol in Beverages by Density and Infrared Spectroscopy Methods" (International Journal of Food Sciences and Nutrition, 2005, 56, 177-183)

P14 P. Ramasami: "A Learning Experience: Conformational Studies of Ethane and 1,2-Disubstituted Ethanes Using Molecular Mechanics" (Australian Journal of Chemical Education, 2005, 65, 16-19)

P15 P. Ramasami: "Changing Culture with Virtual Meetings" (Accepted for IRFD World Forum (Side Events and Virtual Conference) on Small Island Developing States: Challenges, Prospects and International Cooperation for Sustainable Development, Mauritius, January 2005) (This is not a scientific publications)

P16 P. Ramasami: "Theoretical Studies of 1,2-Dichloroethane and 1,2-Dibromoethane in Gaseous Phase, Liquid Phase and Alcohol as Solvent" (Mansoura Journal of Chemistry, 2005, 32, 127-137)

P17 P. Ramasami and S. Jhaumeer-Laulloo: "Spectroscopic Quantitative Analysis of Food: Chemometrics is a Vital Tool" (Proceedings of the 7th Meeting of Agricultural Scientists, Mauritius, 2005, 35-42)

P18 S. Jhaumeer-Laulloo and P. Ramasami: "Infrared Spectroscopy: An Analytical Tool in Food Science" (Proceedings of the 7th Meeting of Agricultural Scientists, Mauritius, 2005, 43-50)

P19 B. A. Dilmohamud, J. Seeneevassen, S. D. D. V. Rughooputh and P. Ramasami: "Surface Tension and Related Thermodynamic Parameters of Alcohols using Traube Stalagmometer" (European Journal of Physics, 2005, 26, 1079-1084)

P20 P. Ramasami "Gauche and Trans Conformers of 1,2-Dihaloethanes: A Study by *Ab initio* and Density Functional Methods" (Lecture Series on Computer and Computational Sciences, 2005, 4, 732-734) (This is a conference proceedings)

P21 R. K. Sreeruttun, P. Ramasami, C. S. Wannere, A. Paul, P. v. R. Schleyer and H. F. Schaefer III "Effects of Fluorine on the Structures and Energetics of the Propynyl and Propargyl Radicals and Their Anions" (Journal of Organic Chemistry, 2005, 70, 8676-8686)

P22 P. Ramasami "Heat of Reaction of the Gas Phase Catalytic Decomposition Processes of Ozone: A comparison of Theoretical Methods" (Proceedings of the International Congress of Chemistry and Environment (ICCE-2005), India, 2005, 294-296) (This is a conference proceedings)

P23 P. Ramasami and R. Kakkar "Partial Molar Volumes and Adiabatic Compressibilities at Infinite Dilution of Aminocarboxylic acids and Glycylglycine in Water and Aqueous Solutions of Sodium Sulphate at 288.15, 298.15 and 308.15 K" (Journal of Chemical Thermodynamics, 2006, 38, 1385-1395)

P24 R. K. Sreeruttun and P. Ramasami "Conformational Behaviour of 1,2-Dichloroethane and 1,2-Dibromoethane: ^{1}H-NMR, IR, Refractive index and Theoretical Studies" (Physics and Chemistry of Liquids, 2006, 44, 315-328)

P25 P. Ramasami "Theoretical Gas Phase Study of the Gauche and Trans Conformers of 1-Fluoro-2-haloethanes CH_2F-CH_2X (X=Cl, Br, I) by *Ab initio* and Density Functional Methods: Absence of Gauche Effect" (Lecture Notes in Computer Science. 2006, 3993, 153-160) (This is a conference proceedings)

P26 P. Ramasami "A Theoretical Gas Phase Study of the Molecular Structures and Vibrational Spectra of Novel Penta-1,4-diyne-3-thioketone and Penta-1,4-diyne-3-selenoketone" (Journal of Molecular Structure THEOCHEM, 2006, 767, 19-22)

P27 P. Ramasami "Novel 1,5-Difluoropenta-1,4-diyn-3-one, its Sulfur and Selenium Analogues: MP2 and DFT Gas Phase Study of their Molecular Structures and Vibrational Spectra" (Journal of Molecular Structure THEOCHEM, 2006, 775, 87-92)

P28 K. Khodabux, M. S. S. L'Omelette, S. Jhaumeer-Laulloo, P. Ramasami and P. Rondeau "Chemical and Near-infrared Determination of Moisture, Fat and Protein in Tuna Fishes" (Food Chemistry, 2007, 102, 669-675)

P29 F. Kinoo and P. Ramasami "Performance of Theoretical Methods and Basis sets on the Molecular Structure, Atomisation and Ionisation energies, Electron affinity, and Vibrational Spectrum of Silylene" (Silicon Chemistry, 2007, 3, 251-257)

P30 P. Ramasami "Gas Phase Study of the Trans and Gauche Rotamers of 1,2-Dicyanoethane, Novel 1,2-Dicyanodisilane and Cyano(cyanomethyl)silane by *Ab initio* and Density Functional Methods" (Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 752-726)

P31 P. Ramasami "Theoretical Gas Phase Study of the Gauche and Trans Conformers of 1-Bromo-2-chloroethane and Solvent Effects" (Lecture Notes in Computer Science. 2007, 4488, 296-303)

P32 P. Ramasami "Theoretical Gas Phase Study of the Gauche and Trans Conformers of 1-Bromo-2-iodoethane and Solvent Effects" (Solution Chemistry, 2007, 36, 901-911)

P33 P. Ramasami "Density Functional Study of the Molecular Structures, Infrared and Raman Spectra of Carbon Suboxide, its Sulfur and Selenium Analogues"(Molecular Physics, 2007, 105, 1067 - 1072)

P34 H. Ashish and P. Ramasami "Rotational Barrier and Thermodynamical Parameters of Furfural, Thiofurfural, and Selenofurfural in the Gas and Solution Phases: Theoretical Study Based on Density Functional Theory Method" (Molecular Physics, 2008, 106, 175-185)

P35 P. Ramasami "DFT Study of the Molecular Structures, Infrared and Raman spectra of 1,5-Dichloropenta-1,4-diyn-3-one, 1,5-Dibromopenta-1,4-diyn-3-one, 1,5-Diiodopenta-1,4-diyn-3-one, their Sulfur, and Selenium Analogues"(Journal of Sulfur Chemistry, 2008, 29, 475-488)

P36 F. Kinoo and P. Ramasami "Molecular Structure, Atomisation Energy, Ionisation Energy, Electron Affinity, and Vibrational Spectrum of SiX_2 (X=F, Cl, Br, I) by Theoretical Methods" (Main Group Chemistry, 2008, 7, 57-64)

P37 R. Sreeruttun, P. Ramasami, C. Wannere, A. Andrew and H. Schaefer "α and β-Phenylethynyl Radicals and their Isomers o-, m and p-Ethynylphenyl: Structures, Energetics, and Electron Affinities" (Journal of Physical Chemistry, 2008, 112, 2838-2845)

P38 P. Ramasami "First Principle Gas Phase Study of the Trans and Gauche Rotamers of 1,2-Diisocyanoethane, 1,2-Diisocyanodisilane and Isocyano(isocyanomethyl)silane" (Lecture Notes in Computer Science, 2008, 5102, 344-352) (This is a conference proceedings)

P39 N. Seeburrun, E. F. Archibong and P. Ramasami "Structures and Electron Detachment Energies of $Ga_2S_3^-$ and $Ga_3S_2^-$" (Chemical Physics Letters, 2008, 467, 23-27)

P40 N. Seeburrun, P. Gohee, H. H. Abdallah, L. Kanime, E. F. Archibong and P. Ramasami "Electronic Structures of Al_4As, Ga_4As and their Anions" (Chemical Physics Letters, 2009, 472, 35-38)

P41 H. H. Abdallah and P. Ramasami "First Principle Study of the Anti- and Syn-Conformers of Thiophene-2-carbonyl Fluoride and Selenophene-2-carbonyl Fluoride in the Gas and Solution Phases" (Lecture Notes in Computer Science, 2009, 5545, 114-121) (This is a conference proceedings)

P42 L. Rhyman, H. H. Abdallah and P. Ramasami "Theoretical Study of the Structures, Conformations and Spectroscopic Properties of 2-Formylthiophene N-acetylhydrazone and 2-Thiophenecarboxaldehyde 2-thienylhydrazone" (Heteroatom Chemistry, 2009, 20, 144-150)

P43 P. Ramasami "Structure and Vibrational Spectroscopic Parameters of Selenoxopropanedinitrile and Selenoxosilanedicarbonitrile. Theoretical Study Based on Density Functional Theory Method" (Heteroatom Chemistry, 2009, 20, 208-217)

P44 P. Ramasami "Theoretical Study of 2-Selenophenecarboaldehyde in the Gas and Solution Phases: Rotational Barrier, Energy Difference and Thermodynamic Parameters" (Journal of Molecular Structure THEOCHEM, 2009, 907, 57-61)

P45 A. Bundhun, P. Ramasami and H. F. Schaefer "Germylene Energetics: Electron Affinities and Singlet−Triplet Gaps of GeX_2 and GeXY Species (X, Y = H, CH_3, SiH_3, GeH_3, F, Cl, Br, I)" (Journal of Physical Chemistry, 2009, 113, 8080-8090)

P46 H. H. Abdallah and P. Ramasami "Rotational Barrier, Energy difference and Thermodynamic Parameters of 2-Furoylfluoride and its Sulfur and Selenium Analogues in the Gas and Solution Phases: A Theoretical Study" (Journal of Molecular Structure THEOCHEM, 2009, 913, 157-161)

P47 E. F. Archibong, N. Seeburrun and P. Ramasami "Geometric and Electronic Structure of AlO_4 and AlO_4^-" (Chemical Physics Letter, 2009, 481, 169-172)

P48 L. Rhyman, H. H. Abdallah and P. Ramasami "Theoretical Study of the Structural, Spectroscopic and Energetic Properties of Difluoro(germylthio)phosphine and Difluoro(germylseleno)phosphine in the Gas Phase" (Polyhedron, 2010, 29, 220-225)

P49 P. Ramasami and T. A. Ford "An *Ab initio* Molecular Orbital Study of the Complexes Formed Between Silicon Tetrafluoride and some Lewis Bases" (Journal of Molecular Structure THEOCHEM, 2010, 940, 50-55)

P50 L. Rhyman, H. H. Abdallah and P. Ramasami "Quantum Mechanical Study of the Structure and Spectroscopic Characterisation of the Novel Trisilylsilylcyanide and Trigermylgermylcyanide in the Gas Phase (Polyhedron, 2010, 29, 1168-1174)

P51 A. Bundhun, P. Blowers, P. Ramasami and H. F. Schaefer "Quantum Mechanical Modeling for the GeX_2/GeHX + GeH_4 Reactions (X = H, F, Cl, and Br)" (Journal of Physical Chemistry, 2010, 114, 4210-4223)

P52 A. Bundhun and P. Ramasami "Density Functional Theory Study of the Carbon Chains C_nX, C_nX^+ and C_nX^- (X = O and Se; n = 1–10)" (European Physical Journal D, 2010, 57, 355-364)

P53 P. Ramasami “First Principle Study of the Trans and Gauche Rotamers of 1,2-Dihalogenodisilanes ($XSiH_2SiH_2X$; X = F, Cl, Br, I) in Vacuum” (Procedia Computer Science Series, 2010, 1, 1133-1140) (This is a conference proceedings)

P54 P. Ramasami and T. Ford “*Ab Initio* Studies of the Vibrational Spectra of Some Hydrogen-bonded Complexes of Fluoroacetylene” (Canadian Journal of Chemistry, 2010, 88, 716-724

P55 A. Bundhun, H. H Abdallah, P. Ramasami and H. F Schaefer "Germylenes: Structures, Electron Affinities, and Singlet-Triplet Gaps of the Conventional $XGeCY_3$ (X = H, F, Cl, Br, and I; Y = F and Cl) Species and the Unexpected Cyclic $XGeCY_3$ (Y = Br and I) Systems" (Journal of Physical Chemistry A, 2010, 114, 13198-13212)

P56 L. Rhyman, H. H. Abdallah, S. Jhaumeer-Laulloo, L. R. Domingo, J. A. Joule and P. Ramasami “The 1,3-Dipolar Cycloaddition of 1*H*-Pyridinium-3-olate and 1-Methylpyridinium-3-olate with Methyl Acrylate: A Density Functional Theory Study” (Tetrahedron, 2010, 66, 9187-9193)

P57 B. Bhonoah, A. Ghoorun, H. H. Abdallah, P. Ramasami "Theoretical Study of the Gauche and Trans Conformers of SiH_2X-CH_2X, SiH2F-CH2Y and SiH_2Y-CH_2F (X=F, Cl, Br, I and Y=Cl, Br, I) in the Gas and Solution Phases" (Journal of Solution Chemistry, 2011, 40, 430-436)

P58 L. Rhyman, H. H. Abdallah and P. Ramasami "Quantum Mechanical Study of the Syn-Anti Isomerisation of 2-Tellurophenecarboaldehyde: Vive La Différence" (Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 2011, 78, 258-263)

P59 E. F. Archibong and P. Ramasami "On the Molecular and Electronic Structure of GaO_4" (Computational and Theoretical Chemistry, 2011, 964, 324-328)

P60 N. Seeburrun, H. H. Abdallah, E. F. Archibong and P. Ramasami "Geometries and Electronic Structures of Ga_2Se_3, Ga_3Se_2 and their Anions. Theoretical insights" (European Physical Journal D, 2011, 63, 351-358)

P61 L. Rhyman and P. Ramasami "Molecular Structures and Vibrational Spectra of Roesky's Ketone, its Isomers and their Novel Sulfur and Selenium Analogues: An Insight using Density Functional Theory" (Pakistan Journal of Chemistry, 2011, 1, 48-59) (Invited paper)

P62 L. Rhyman, H. H. Abdallah, S. Jhaumeer-Laulloo, L. R. Domingo, J. A. Joule and P. Ramasami "1,3-Dipolar Cycloaddition of 1H-Pyrazinium-3-olate and N1- and C-Methyl Substituted Pyrazinium-3-olates with Methyl acrylate: A Density Functional Theory Study" (Tetrahedron, 2011, 67, 8383-8391)

P63 L. Rhyman, S. Jhaumeer-Laulloo, L. R. Domingo, J. A. Joule and P. Ramasami "Computational Assessment of 1,3-Dipolar Cycloaddition of Nitrile Oxides with Ethene and [60]Fullerene" (Heterocycles, 2012, 84, 719-735) (Invited paper)

P64 P. Ramasami and T. Ford "An initio Studies of the Properties of Some Halogen-Bonded Complexes of Ammonia, Water, Phosphine and Hydrogen Sulphide" (Computational and Theoretical Chemistry, 2012, 990, 227-235)

P65 N. Jaufeerally, H. H. Abdallah, P. Ramasami and H. F Schaefer "Telluroformaldehyde and its Derivatives: Structures, Ionization Potentials, Electron Affinities and Singlet-Triplet Gaps of the X_2CTe and XYCTe (X,Y=H, F, Cl, Br, I and CN) Species" (Theoretical Chemistry Accounts, 2012, 131, 1127-1149)

P66 A. Bundhun, P. Ramasami, P. Gaspar and H. F Schaefer "Stannylenes: Structures, Electron Affinities, Ionization Energies and Singlet-Triplet Gaps of SnX_2/SnXY and XSnR/SnR_2/RSnR' Species (X; Y = H, F, Cl, Br, I, and R; R′ = CH_3, SiH_3, GeH_3, SnH_3)" (Inorganic Chemistry, 2012, 51, 851-863)

P67 S. Beccaceci, N. Armata, S. J. Ogden, J. M. Dyke, L. Rhyman and P. Ramasami "A Study of the Atmospherically Important Reactions of I_2 and ICl with Dimethylsulphide (DMS) using Infrared Matrix Isolation Spectroscopy and Electronic Structure Computations" (Physical Chemistry Chemical Physics, 2012, 14, 2399-2407)

P68 M. Soopramanien, N. Seeburrun, H. H. Abdallah, E. F. Archibong and P. Ramasami "Ga_2Te_3 and Ga_3Te_2 Clusters: Understanding their Structures, Vibrational and Energetic Features using Ab initio Methods" (Journal of Material Science, 2012, 47, 4332-4341)

P69 N. Seeburrun, H. H. Abdallah and P. Ramasami "From Matrix Isolation to Computational Investigation: A Closer Look at Digallium Tetraoxide, Ga_2O_4" (Journal of Physical Chemistry A, 2012, 116, 3215-3223)

P70 R. Takjoo, R. Centore, L. Rhyman and Ponnadurai Ramasami "Nickel(II) and Copper(II) Complexes of Allyl 2-(thiophen-2-ylmethylene)hydrazinecarbodithioate: Synthesis, X-ray crystal structures and Theoretical study (Journal of Coordination Chemistry, 2012, 65, 1569-1579)

P71 L. Rhyman, S. Jhaumeer-Laulloo, L. R. Domingo, J. A. Joule and P. Ramasami "Regio- and Stereoselectivity of the 1,3-Dipolar Cycloaddition of Pyridinium-3-olates and Pyrazinium-3-olates with Methyl Methacrylate: A Density Functional Theory Exploration" (Current Organic Chemistry, 2012, 16, 1711-1722)

P72 P. Ramasami and T. Ford "Ab initio Studies of some Hydrogen-bonded Complexes of Fluoroform-Evidence for Blue-shifted Behavior" (Journal of Molecular

Structure, 2012, 1023, 163-169)

P73 L. Rhyman, N. Armata, P. Ramasami and John M. Dyke "A Study of the Atmospherically Important Reactions Between Dimethyl Selenide (DMSe) and X_2 (X_2 = Cl_2, Br_2 and I_2) with Ab Initio Calculations" (Journal of Physical Chemistry, 2012, 116, 5595-5603)

P74 A. Bundhun, H. H. Abdallah, P. Ramasami, P. Gaspar and H. F Schaefer "Dicyanogermylenes: A Tale of their Isomers and Interconversions" (Inorganic Chemistry, 2012, 51, 12152-12164)

P75 L. Rhyman, L. R. Domingo, J. A. Sáez, J. A. Joule and P. Ramasami "A DFT Analysis of the Lewis Acid Catalyzed Reaction between Methyl Glyoxylate Oxime and Cyclopentadiene. 1,3-Dipolar Cycloaddition versus hetero-Diels-Alder Reaction." (RSC Advances, 2013, 3, 447-457)

P76 W. Hermoso, N. Jaufeerally, P. Ramasami and F. Ornellas "Exploring New Species on the [H, S, Se, Cl] Potential Energy Surface" (International Journal of Quantum Chemistry, 2013, 113, 112-118)

P77 K. R. Phatangare,V. D. Gupta, A. B. Tathe, Vikas S. Padalkar, Vikas S. Patil, P. Ramasami and N. Sekar "ESIPT Inspired Fluorescent 2-(4-benzo[d]oxazol-2-yl)naphtho[1,2-d]oxazol-2-yl)phenol: Synthesis and DFT Based Approach to Photophysical Properties" (Tetrahedron, 2013,69, 1767-1777)

P78 A. Bundhun, P. Ramasami, J. S. Murray and P. Politzer "Trends in σ-Hole Strengths and Interactions of F_3MX Molecules (M = C, Si, Ge and X = F, Cl, Br, I)" (Journal of Molecular Modeling, Accepted, 2013)

P79 V. D. Gupta, A. B. Tathe, V. S. Padalkar, V. S. Patil, K. R. Phatangare,P. G. Umape, P. Ramasami and N. Sekar "TDDFT Investigation of the Electronic Structures and Photophysical Properties of Fluorescent Extended Styryl Push-Pull Chromophores Containing Carbazole Unit" (Journal of Fluorescence, Accepted, 2013)

P80 N. Seeburrun, H. H. Abdallah, E. F. Archibong and P. Ramasami "Unveiling the Structural and Electronic Properties of the Neutral and Anionic Gallium Sulfide clusters" (Dalton Transactions, Submitted, 2013)

P81 P. Gohee, H. H. Abdallah, E. F. Archibong, P. Ramasami "First Principles Gas Phase Study of the Structures, Energetics and Spectroscopic Parameters of Aluminium Antimonide, Al_xSb_y (x+y = 3,5), Nanoclusters)" (European Physical Journal D, Submitted, 2013)

P82 N Jaufeerally, H. H. Abdallah and P. Ramasami "Novel Silanetellurones: Structures, Ionization Potentials, Electron Affinities, Singlet-Triplet Splittings and

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