

**Programme of the ICPAC 2014**  
*Crystallising Ideas: The Role of  
Chemistry*

**23-27 June 2014**  
**Mauritius**

## Detailed Programme

23<sup>rd</sup> June 2014

<b>08.00-09.45</b>	<b>Registration</b>
<b>Opening Ceremony and Keynote Address</b>	
<b>Venue: Imperial</b>	
<b>Chairperson: H. Li Kam Wah</b>	
<b>10.00-10.10</b>	<i>Welcome Address by Chairman of ICPAC 2014</i> Prof P. Ramasami
<b>10.10-10.15</b>	<i>Address by Vice-Chancellor of the University of Mauritius</i> Prof R. Mohee
<b>10.15-10.30</b>	<i>Address by Minister of Tertiary Education, Science, Research &amp; Technology</i> Dr The Honourable Rajeshwar Jeetah
<b>10.30-11.00</b>	<b>Tea/Coffee Break</b>
<b>11.00-12.00</b>	<i>Keynote Address by the Deputy Director-General of OPCW</i> <i>Working for Security and Prosperity: The OPCW's Deepening Partnerships with Science</i> Amb Grace Asirwatham
<b>12.00-12.10</b>	<b>Group Photo</b>
<b>12.10-13.00</b>	<b>Lunch</b>

<b>Venue: Imperial</b>	
<b>Plenary Lecture</b>	
<b>Chairperson: A. Klamt</b>	
<b>13.00-14.00</b>	PL-1: S. Coles <i>Chemical Insights from Systematic Structural Studies</i>
<b>Invited Lectures</b>	
<b>14.00-14.40</b>	I-1: P. de Kock <i>Publishing Scientific Research with Springer</i>
<b>14.40-15.20</b>	I-2: A. Gurib-Fakim <i>Bioresources of Africa – Yesterday’s Traditions and Tomorrow’s Promise of Healing and Well-Being</i>
<b>15.20-15.40</b>	<b>Tea/Coffee Break</b>
<b>Venue: Imperial</b>	
<b>Chairperson: A. Deshpande</b>	
<b>15.40-16.20</b>	I-3: A. Klamt, J. Reinisch and F. Eckert <i>COSMO Polarization Charge Densities Provide New Insights to Hydrogen Bond, Enthalpy and Entropy</i>
<b>16.20-17.00</b>	I-4: R. Somanah <i>Astrochemistry: Detection of Prebiotic Molecules in Space using the Atacama Large Millimeter Array Telescope (ALMA) and the Very Large Array (VLA), Green Bank (GBT), the Australia Telescope Compact Array (ATCA) and the Square Kilometer Array (SKA) Radio Telescopes</i>
<b>17.00-17.40</b>	I-5: S. Saumtally and G. Umrit <i>Research and Development in Agricultural Chemistry for the Advancement and Sustainability of the Sugarcane Industry in Mauritius</i>
<b>19.00-21.00</b>	Welcome Reception Pearl Beach Resort & Spa, Flic-en-Flac <i>Dinner and Musical Entertainment</i>

24<sup>th</sup> June 2014

<b>Venue: Imperial A</b>	
<b>Plenary Lecture</b>	
<b>Chairperson: A. A. Adeniyi</b>	
<b>09.00-10.00</b>	PL-2: T. Gerber <i>Rhenium and Technetium: Coordination Chemistry and Radiopharmacy</i>
<b>Invited Lecture</b>	
<b>10.00-10.40</b>	I-6: J.-R. Hwu, K.-S. Chuang, Y. C. Hsu and S.-C. Tsay <i>Synthesis of Functionalized Indoles and Benzo[b]furans as Electroluminescent Materials</i>
<b>10.40-11.00</b>	<b>Tea/Coffee Break</b>
<b>Parallel Oral Sessions</b>	
<b>Venue: Imperial A</b>	
<b>Inorganic Chemistry</b>	
<b>Chairperson: M. Gupta Bhowon</b>	
<b>11.00-11.20</b>	O-2: K. H. Thebo, A. A. Thebo and H. A. Shad <i>Thermal Investigation of Synthesized Binuclear Copper(II) Complexes of Dicarboxylic Acids and N-Heterocyclic Amines</i>
<b>11.20-11.40</b>	O-4: H. A. Mohamad and B. M. H. Ammen <i>Synthesis and Characterization of Co(II), Ni(II) and Cu(II) Complexes with Thio-1,3,4-Oxadiazole Derivatives</i>
<b>11.40-12.00</b>	O-8: S. Hadi, H. Afriyani, W. D. Anggraini, H. I. Qudus and T. Suhartati <i>Some Organotin(IV) Nitrobenzoates as Corrosion Inhibitor for Mild Steel in DMSO-HCl</i>
<b>12.00-12.20</b>	O-11: W. Purcell, M. Nete and J. T. Nel <i>(Ta/Nb)<sub>2</sub>O<sub>5</sub> as Models for Tantalite Beneficiation</i>
<b>Venue: Imperial B</b>	
<b>Symposium: Computational Chemistry and its Applications</b>	
<b>Chairperson: L. Rhyman</b>	
<b>11.00-11.20</b>	S-2: S. Abdalla and R. F. Fink <i>Analyzing Interaction Energy in Polycyclic Aromatic Hydrocarbon (PAH) Dimers</i>
<b>11.20-11.40</b>	S-3: Y. Umar and J. Tijani <i>Theoretical Investigation of the Internal Rotations and Vibrational Spectra of 2-, 3- and 4-Formyl Pyridine in the Gas and Solution Phases</i>
<b>11.40-12.00</b>	S-4: S. Dhail <i>Correlation of the Experimental and Theoretical Study of some Novel 2-Phenazinamine Derivatives in terms of the Semi-Empirical and Hartree-Fock Method</i>

12.00-12.20	S-5: D. B. Khadka <i>Optical Model Calculation of the Total Penning Ionization Cross Sections of Ne(<sup>3</sup>P<sub>1</sub>) by O<sub>2</sub></i>
12.20-13.20	<b>Lunch</b>
<b>Venue: Imperial A</b>	
<b>Inorganic Chemistry</b>	
<b>Chairperson: T. Gerber</b>	
13.20-13.40	O-21: V. Abeyawarathan, G. Bradtmöller, C. Dietz, M. Gock, L. Iovkova-Berends, T. Zöllner and K. Jurkschat <i>Alkanolamines and their Tin Derivatives: How Industrial Applications Stimulate Academic Research and vice versa</i>
13.40-14.00	O-32: S. Perveen, S. Mustafa, M. A. Masiak, A. Khan, K. M. Khan, M. I. Choudhary, M. Latif, L. Iqbal and T. H. Usmani <i>Synthesis of 1,3-Disubstituted Urea Derivatives as Potent <math>\alpha</math>-Chymotrypsin Inhibitors and Immunomodulators</i>
14.00-14.20	O-37: A. Najafi and R. Takjoo <i>Structural Study of New Isothiosemicarbazone Uranium and Copper Complexes</i>
14.20-14.40	O-41: F. Özen, K. Koran, M. Arslan and A. O. Görgülü <i>Fluorescence Properties of New Synthesized Dihydroxycoumarin and Related Compounds</i>
14.40-15.00	O-49: S. Moosun, S. Coles, L. H. Blair, S. Jhaumeer-Laulloo and M. Gupta Bhowon <i>Different Crystal Geometries of Copper(II) Complexes of Mono and Dithiodibenzoic Acid</i>
<b>Venue: Imperial B</b>	
<b>Symposium: Computational Chemistry and its Applications</b>	
<b>Chairperson: Y. Umar</b>	
13.20-13.40	S-6: H. Bhakhoa, L. Rhyman, P. Ramasami and J. M. Dyke <i>The Cousin of Crown Ether: A Theoretical Approach</i>
13.40-14.00	S-7: J. Z. A. Laloo, L. Rhyman, P. Ramasami, A. de Cózar and F. M. Bickelhaupt <i>Theoretical Study of S<sub>N</sub>2 Reactions</i>
14.00-14.20	S-8: K. Bahadoor, L. Rhyman and P. Ramasami <i>Density Functional Theory Study of Methanethiol and Organic Molecules</i>
14.20-14.40	S-9: I. M. Domah, L. Rhyman and P. Ramasami <i>Theoretical Study of DMSe with CF<sub>3</sub>X (X = Cl, Br or I)</i>
14.40-15.00	S-10: D. Kodi Ramanah, L. Rhyman, R. Somanah and P. Ramasami <i>Ab initio Studies on Molecules of Astrochemical Interest</i>
15.00-15.20	<b>Tea/Coffee break</b>

## Parallel Oral Sessions

### Venue: Imperial A Organic Chemistry

**Chairperson: S. Jhaumeer-Laulloo**

- 15.20-15.40** O-5: S. Hameed, Z. Iqbal, J. Iqbal and I. Z. Qureshi  
*Arylsulfonylspirobicyclohydantoin: Aldose Reductase Inhibitors as well as Antidiabetic Agents*
- 15.40-16.00** O-47: N. Joondan, P. Caumul and S. Jhaumeer-Laulloo  
*Effect of Quaternary Ammonium Moiety on the Antibacterial Properties of L-Phenylalanine Amphiphiles*
- 16.00-16.20** O-15: M. M. Naseer and S. Hameed  
*Giant Molecular Cages: Synthesis and Efficient Surface Functionalization*
- 16.20-16.40** O-25: M. M. Maluleka and M. J. Mphahlele  
*Novel Polysubstituted Pyrazolo[4,3-c]quinolines and Thieno[3,2-c]quinoline-2-carboxylates Derived from 6,8-Dibromo-4-chloroquinoline-3-carbaldehyde*
- 16.40-17.00** O-30: M. Isaac  
*Critical Study of Natural Products Biosynthesis*
- 17.00-17.20** O-34: B. Barton, M. R. Caira, E. C. Hosten, C. W. McClelland and S. Weitz  
*TETROL, a Novel Chiral Host Compound: Preferred Guests, Structures and Stabilities*

### Venue: Imperial B

#### Symposium: Computational Chemistry and its Applications

**Chairperson: S. Abdalla**

- 15.20-15.40** S-11: S. U. A. Ramjauny, N. Jaufeerally, L. Rhyman and P. Ramasami  
*CBS Approach to Solve the Schrödinger Equation: An Application to the [HSSeBr] Species*
- 15.40-16.00** S-12: P. Surajbali, L. Rhyman, R. Somanah and P. Ramasami  
*A Density Functional Theory Study on Molecules of Astrochemical Interest: Cyanoetheneselenol*
- 16.00-16.20** S-13: N. D. Zeadally, L. Rhyman and P. Ramasami  
*Theoretical Investigation of a Series of N-Heterocyclic Carbene Silver(I) Complexes*

<b>Polymer Chemistry</b>	
<b>16.20-16.40</b>	O-24: O. Watanabe <i>Photo-Induced Deformation and Immobilization Processes using an Azopolymer for Optical and Medical Applications</i>
<b>Biophysical Chemistry</b>	
<b>16.40-17.00</b>	O-9: A. Tokmakov <i>Bioinformatics Analysis of Cell-Free Protein Synthesis</i>
<b>17.00-17.20</b>	O-16: S. D. Yuwono, R. Heru, Nugroho and S. Hadi <i>Purification of Lactic Acid from Cassava Bagasse Fermentation using Ion Exchange</i>
<b>Venue: Imperial C</b>	
<b>Environmental Chemistry</b>	
<b>Chairperson: M. J. Mphahlele</b>	
<b>15.20-15.40</b>	O-10: S. B. Jonnalagadda <i>Dechlorination and Mineralisation of Non-Biodegradable Organics in Aqueous Systems</i>
<b>15.40-16.00</b>	O-12: A. A. Adeniyi, K. Yusuf, O. Okedeyi and M. Sowemimo <i>Polycyclic Aromatic Hydrocarbons and Health Risk Assessment of Selected Household Borehole Water of Lagos-Ogun Axis, Nigeria</i>
<b>16.00-16.20</b>	O-23: O. S. I. Fayomi, A. P. I. Popoola and V. Tau <i>Anti-Corrosion Characteristic of Green Extract Inhibitor Performance on Aluminum in Aggressive Environment</i>
<b>16.20-16.40</b>	O-27: K. K. Deshmukh <i>Chemistry of Groundwater near Municipal Solid Waste Dumping Yard and its Environmental Impact at Sangamner Ahmednagar, Maharashtra, India</i>
<b>16.40-17.00</b>	O-31: V. Dookhun and R. Clift <i>Assessing Suitability of Environmental Models for Predicting Concentration of Mercury in Air, Water and Soil as Part of an Environmental Risk Assessment</i>
<b>Chemical Education</b>	
<b>17.00-17.20</b>	O-46: A. Rest, J. Ogunde, A. Omolo and K. Wilkinson <i>Installing Solar Classrooms - Enhancing Science Education in Developing Countries</i>
<b>19.00-21.00</b>	Conference Banquet Aanari Hotel & Spa, Flic-en-Flac

**25<sup>th</sup> June 2014**

<b>Conference Tour</b>	
<b>09.00-17.00</b>	<i>Colourful South</i>

26<sup>th</sup> June 2014

Venue: Imperial A

Workshop: COSMO-RS: From Quantum Chemistry to Fluid Phase  
Thermodynamics and Drug Design

Chairperson: A. Klamt

08.40-10.40 *COSMO-RS: From Quantum Chemistry to Fluid Phase  
Thermodynamics and Drug Design*

10.40-11.00 Tea/Coffee Break

11.00-12.20 *COSMO-RS: From Quantum Chemistry to Fluid Phase  
Thermodynamics and Drug Design*

Parallel Oral Sessions

Venue: Imperial B

Material Science

Chairperson: I. Moreira

08.40-09.00 O-13: J. V. Grazulevicius  
*Organic Electroactive Materials for Electroluminescent Devices*

09.00-09.20 O-17: M. Malíková, J. Rychlý, L. Matisová-Rychlá, K. Csomorová,  
I. Janigová and H.-W. Wilde  
*Study of Degradation of Stabilised Polyurethane Films by  
Chemiluminescence*

09.20-09.40 O-20: R. Bissessur, D. J. A. Cameron and D. C. Dahn  
*Polymer Nanocomposites Based on Graphite*

09.40-10.00 O-22: B. S. Martincigh  
*Nanomaterials for Wastewater Treatment*

10.00-10.20 O-26: O. S. I. Fayomi, A. P. I. Popoola and O. M. Popoola  
*The Study of the Microstructure and Interfacial Reaction of Binary  
Composite Coating*

10.20-10.40 O-39: S. Aouad, W. Daaboul, S. Hany, B. El Khoury, J. El Nakat,  
E. Abi Aad and A. Aboukais  
*Tuning CeO<sub>2</sub> for the Catalytic Oxidation of Propylene Correlating  
between PhysicoChemical Properties and Catalytic Performance*

10.40-11.00 Tea/Coffee Break

Medicinal Chemistry

Chairperson: R. Bissessur

11.00-11.20 O-14: F. A. Audhal, F. A. Sattar, M. A. K. Malghani and S. A.  
Sattar  
*Antiviral Potential of Medicinal Plants of Balochistan, Pakistan*



<b>11.20-11.40</b>	O-28: S. J. Lee, T. Yi, J. Lee, S. U. Song and S. W. Kwon <i>LC-QTOFMS Based Lipidomic Interpretation of Aging for Human Clonal Mesenchymal Stem Cells</i>
<b>11.40-12.00</b>	O-29: J. Zhao, Y. J. Shin, M. W. Nam, K. M. Jeong, Y. Jin, Y. H. Jung, C. G. Jang and J. Lee <i>Metabolomic Investigation of a Mouse Model for Depression Treated with Popular Antidepressants</i>
<b>12.00-12.20</b>	<i>Video Projection on the International Year of Crystallography</i>
<b>12.20-13.20</b>	<b>Lunch</b>
<b>Venue: Imperial A</b>	
<b>Plenary Lecture</b>	
<b>Chairperson: S. Hadi</b>	
<b>13.20-14.20</b>	PL-3: L. S. Chua <i>Phytochemical Profiling of Herbal Plants by LC-MS/MS</i>
<b>Invited Lecture</b>	
<b>14.20-15.00</b>	I-7: H. G. Visser, A. Roodt, A. Brink, M. Schutte and N. Cloete <i>When Basic Chemistry Meets Industrial Requirements: Examples from Catalysis and Radiopharmacy</i>
<b>15.00-15.20</b>	<b>Tea/Coffee Break</b>
<b>Venue: Imperial B</b>	
<b>15.20-17.30</b>	<b>Poster Session</b>
<b>19.00-21.00</b>	Participants' Night Pearl Beach Resort & Spa, Flic-en-Flac <i>Dinner and Musical Entertainment</i>

27<sup>th</sup> June 2014

<b>Venue: Imperial A</b>	
<b>Plenary Lecture</b>	
<b>Chairperson: F. A. Siddiqui</b>	
<b>09.00-10.00</b>	PL-4: A. Gauvin-Bialecki, M. Aknin, Y. Kashman, E. Gros, A. Al-Mourabit and B. Illien <i>Bioactive Molecules of Marine Invertebrates from South-West Indian Ocean: Status and Perspectives</i>
<b>Invited Lecture</b>	
<b>10.00-10.40</b>	I-8: N. Sekar <i>Red Emitting Coumarin: Design and Synthesis</i>
<b>10.40-11.00</b>	<b>Tea/Coffee Break</b>
<b>Parallel Oral Sessions</b>	
<b>Venue: Imperial A</b>	
<b>Analytical Chemistry</b>	
<b>Chairperson: N. Sekar</b>	
<b>11.00-11.20</b>	O-18: C. G. Mahajan and S. Bagade <i>Method Development and Cleaning Validation of Rosuvastatin Calcium by Swab Technique</i>
<b>11.20-11.40</b>	O-19: H. Kehrig, T. Seixas and I. Moreira <i>Accumulation of Trace Elements and Methylmercury by the Liver of Dolphins from the Brazilian Coast</i>
<b>11.40-12.00</b>	O-40: A. Jafar Ahamed, K. Loganathan, S. Ananthakrishnan and K. Manikandan <i>Physicochemical and Microbiological Studies of Soils in Amaravathi River Bed Area, Karur District, Tamil Nadu, India</i>
<b>12.00-12.20</b>	O-48: S. S. Deshpande, H. Shah and A. Khandhar <i>Simultaneous Estimation of Silodosin and Dutasteride in Solid Dosage Form by RP-HPLC using Wavelength Gradient Programming</i>
<b>Venue: Imperial B</b>	
<b>Medicinal Chemistry</b>	
<b>Chairperson: K. Jurkschat</b>	
<b>11.00-11.20</b>	O-1: S. H. Soidrou, A. Farah, B. Satrani, M. Ghanmi, S. O. S. Hassane, R. Fouad and D. Bousta <i>Chemical Composition, Antioxidant and Antimicrobial Activity of Essential Oils Isolated from Two Piper Species Collected in Comoros</i>

11.20-11.40	O-33: N. Shafi, F. A. Siddiqui, N. Sher and H. Naseem <i>Simultaneous Determination of Piracetam and Levetiracetam in Pharmaceuticals, in Human Serum and Urine: Application in Stability Studies</i>
11.40-12.00	O-35: H. Naseem, N. Mushtaq and N. Shafi <i>Synthesis and Analgesic Evaluation of Piperidine Derivatives</i>
12.00-12.20	O-36: P. S. Kharkar <i>Mining Chemical Space in Search of Constitutional Isomers: An Innovative Approach to Drug Discovery</i>
12.20-13.20	<b>Lunch</b>
<b>Venue: Imperial A</b>	
<b>Plenary Lecture</b>	
<b>Chairperson: M. Malíková</b>	
13.20-14.20	PL-5: F. R. van Heerden <i>Challenges and Opportunities in Natural Product Chemistry</i>
<b>Parallel Oral Sessions</b>	
<b>Venue: Imperial A</b>	
<b>Chemical Physics</b>	
<b>Chairperson: H. A. Mohamad</b>	
14.20-14.40	O-3: C. K. Quah, H.-K. Fun and L.-H. Ong <i>Temperature-Dependent Phase Transition Studies in Molecular Crystals: First Order Landau Phenomenological Theory Approach</i>
14.40-15.00	O-6: C. S. Chidan Kumar, H.-K. Fun, S. Chandraju and C. K. Quah <i>Synthesis and Conformational Analysis of 4-Bromophenacyl Benzoates</i>
<b>Agricultural Chemistry</b>	
<b>Chairperson: H.-K. Fun</b>	
15.00-15.20	O-7: A. Rambabu, M. Krishna Murthy, B. Hari Babu and G. V. Subbaraju <i>Optimized Synthesis of 4',5,7-Trimethyl Apigenin</i>
15.20-15.40	O-42: G. Umrit, S. Ganeshan, A. Saumtally, K. Mulleegadoo and Y. Motee <i>Production of Bioplastics from Sugarcane Trash</i>

<b>Venue: Imperial B Medicinal Chemistry</b>	
<b>Chairperson: R. Takjoo</b>	
<b>14.20-14.40</b>	O-38: P. C. Acharya, P. S. Kharkar and R. Bansal <i>Hybrids of Steroid and Nitrogen Mustard as Antileukemic Agents: Design, Synthesis, Biological Evaluation and in silico Inverse Screening</i>
<b>14.40-15.00</b>	O-43: N. Hasan, N. Sher, F. A. Siddiqui, M. Ahmad, N. Shafi, A. A. Sial and M. T. Baig <i>A New Stability RP-HPLC Method for Quantitative Determination of Cefazoline Sodium in Pharmaceutical Formulations and Human Serum</i>
<b>15.00-15.20</b>	O-45: F. A. Siddiqui, N. Sher and N. Shafi <i>Simultaneous Determination of Diltiazem, Captopril, Lisinopril and Enalapril: Their Application to Pharmacokinetics</i>
<b>Applied Chemistry</b>	
<b>15.20-15.40</b>	O-50: J. C. Ngila and R. M. Nthumbi <i>Dechlorination of Pesticides using Catalytic Bimetallic Nanoparticles on Mixed Metal Oxide Matrix Impended on Electrospun Nanofiber Support</i>
<b>15.40-16.00</b>	<b>Tea/Coffee Break</b>
<b>Venue: Imperial A</b>	
<b>16.00-16.30</b>	<b>Closing Ceremony</b> <b>Chairperson: P. Ramasami</b>