2016

Chemistry Abstracts

Forth Annual International Conference on Chemistry 18-21 July 2016, Athens, Greece

Edited by Gregory T. Papanikos

THE ATHENS INSTITUTE FOR EDUCATION AND RESEARCH

Chemistry Abstracts

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Athens, Greece

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TABLE OF CONTENTS

(In Alphabetical Order by Author's Family name)

Preface

This abstract book includes all the abstracts of the papers presented at the 4th Annual International Conference on Chemistry, 18-21 July 2016, Athens, Greece, organized by the Athens Institute for Education and Research. In total, there were 11 papers and 12 presenters, coming from 9 different countries (Azerbaijan, Canada, China, Egypt, Mexico, Morocco, Poland and USA). The conference was organized into ten sessions that included areas such as Environmental Issues, Organic Chemistry & Biochemistry, New Ideas and Methods in Education and other related fields. As it is the publication policy of the Institute, the papers presented in this conference will be considered for publication in one of the books of ATINER.

The Institute was established in 1995 as an independent academic organization with the mission to become a forum where academics and researchers from all over the world could meet in Athens and exchange ideas on their research and consider the future developments of their fields of study. Our mission is to make ATHENS a place where academics and researchers from all over the world meet to discuss the developments of their discipline and present their work. To serve this purpose, conferences are organized along the lines of well established and well defined scientific disciplines. In addition, interdisciplinary conferences are also organized because they serve the mission statement of the Institute. Since 1995, ATINER has organized more than 150 international conferences and has published over 100 books. Academically, the Institute is organized into six research divisions and twenty-seven research units. Each research unit organizes at least one annual conference and undertakes various small and large research projects.

I would like to thank all the participants, the members of the organizing and academic committee and most importantly the administration staff of ATINER for putting this conference together.

Gregory T. Papanikos
President

FINAL CONFERENCE PROGRAM
4th Annual International Conference on Physics
18-21 July 2016, Athens, Greece

Conference Venue: Titania Hotel, 52 Panepistimiou Street, 10678 Athens, Greece

Monday 18 July 2016
(all sessions include 10 minutes break)

08:00-08:30 Registration and Refreshments

08:30-09:00 Welcome & Opening Address (ROOM A--10th Floor)

- Gregory T. Papanikos, President, ATINER.
- George Poulos, Vice-President of Research, ATINER & Emeritus Professor, University of South Africa, South Africa.

09:00-10:30 Session I (ROOM B-10th Floor): Environmental Issues

Chair: Ethel Petrou, Academic Member, ATINER & Professor and Chair, Department of Physics, Erie Community College-South, State University of New York, USA.

1. Jagannathan Sankar, Distinguished Professor, North Carolina A&T State University, USA. Revolutionizing Metallic Biomaterials for Biodegradable Implants – A Global Status.
2. Marwa Elkady, Associate Professor, Egypt-Japan University of Science and Technology, Egypt & Hassan Shokry Ahmed, Assistant Professor, City of Scientific Researches and Technological Applications, Egypt. Nano-Tube Zirconium Tungesto-Vanadate as Cation Exchanger for Lead Decontamination from Polluted Wastewater.
3. *Burhan Davarcioglu, Associate Professor, Aksaray University, Turkey. Adaptation to Climate Change and Eco-Efficiency (Cleaner Production) for More Effective Environmental Management in Industry.

10:30-12:00 Session II (ROOM C-10th Floor): Organic Chemistry & Biochemistry

Chair: Marwa Elkady, Associate Professor, Egypt-Japan University of Science and Technology, Egypt.

1. Dimitris Argyropoulos, Finland Distinguished Professor, North Carolina State University, USA, C. Cui, North Carolina State University, USA, R. Sun, North Carolina State University, USA, S. Sen, North Carolina State University, USA & H. Sadeghifar, North Carolina State University, USA. Homogeneous Technical Lignins as Phenolic Precursors to Heat Stable Polymers and Carbon Fibers.
2. *Ryszard Ostaszewski, Professor and Head of The Scientific Group, Institute of Organic Chemistry Polish Academy of Sciences, Poland. The Studies on Enzymatic Kinetic Resolution of Selected Unsaturated Carboxylic Acids.
3. *Khadija Mammadyarova, Ph.D. Student, Azerbaijan National Academy of Sciences, Azerbaijan. Anti-wear Properties of Amino Derivatives.
4. Anouar Alami, Head, Department of Chemistry, Sidi Mohamed Ben Abdellah University, Morocco. Heterocyclic Compounds: Synthesis, Characterization, Electrochemical Study, Study and Prediction of Biological Activity.

13:30-14:30 Lunch

14:30-16:00 Session III (ROOM B-10th Floor): New Ideas and Methods in Education

Chair: *Avinash Sharma, Professor and Director, GGS Indraprastha University, India.

1. *Bala Maheswaran, Professor, Northeastern University, USA. Assessment and Analysis of a New Teaching and Learning Approach via Mastering Technique.
2. Mina Katramatou, Associate Professor, Kent State University, USA. Winds of Change in Undergraduate Physics Programs in the USA.
3. Nassim Haramein, Director of Research, Hawaii Institute for Unified Physics, USA & Amira Val Baker, Research Scientist, Hawaii Institute for Unified Physics, USA and University of Malaya, Malaysia. The Electron and the Holographic Mass.

16:00-18:00 Session IV (ROOM B-10th Floor): A Round-Table Discussion on *Teaching and Researching Sciences (Physics and Chemistry) in a Global World*

Chair: Ethel Petrou, Academic Member, ATINER & Professor and Chair, Department of Physics, Erie Community College-South, State University of New York, USA.

1. Dr **Jagannathan Sankar**, Distinguished Professor, North Carolina A&T State University, USA.
2. Dr **Edward Lee-Ruff**, Professor, York University, Canada.
3. Dr **Nassim Haramein**, Director, Hawaii Institute for Unified Physics, USA
4. Dr **Avinash Sharma**, Professor & Director, GGS Indraprastha University, India.
5. Dr **Batric Pesic**, Professor, University of Idaho, USA.
6. Dr **Anouar Alami**, Professor & Head of Department of Chemistry, Sidi Mohamed Ben Abdellah University, Morocco.

21:00-23:00 Greek Night and Dinner (Details during registration)

Tuesday 19 July 2016

08:00-11:00 Educational and Cultural Urban Walk Around Modern and Ancient Athens (Details during registration)

11:00-13:00 Session V (ROOM B-10th Floor): Applied Chemistry & Applied Physics

Chair: *Bala Maheswaran, Professor, Northeastern University, USA.

1. *Haiduke Sarafian, Professor, The Pennsylvania State University, USA. Vibrating Inductor and an RL(t) Network.
2. *Edward Lee-Ruff, Professor, York University/Chemistry, Canada. Photochemical Generation of 9-Fluorenyl Radicals.
3. Batric Pesic, Professor, University of Idaho, USA. Transport of Chloride Ions Evaluation through Modulated Concrete Microstructures.
4. Gregory Boutis, Associate Professor, The City University of New York, USA. 13C, 2H NMR Studies of Structural and Dynamical Modifications of Cholesterol Exposed Porcine Aortic Elastin.
5. Jorge Rosenblatt, Professor Emeritus, Institut National de Sciences Appliquées, France. Inequality and Indistinguishability in Statistical Econophysics.

13:00-14:00 Lunch

14:00-16:00 Session VI (ROOM C-10th Floor): Special Topics

Chair: *Edward Lee-Ruff, Professor, York University/Chemistry, Canada.

1. Jun Peng, Professor, Northeast Normal University, China. Tri-vanadium Substituted Keggin Tungstosilicate Microtubes: Synthesis and Characterization.
2. Hassan Shokry Ahmed, Assistant Professor, City of Scientific Researches and Technological Applications, Egypt, Abdel-Hady Kashyout, Head, City of Scientific Researches and Technological Applications, Egypt, Iman Morsi, Professor, Arab Academy for Science, Technology and Maritime Transport, Egypt, Abdelmenem Nasser, Professor, Arab Academy for Science, Technology and Maritime Transport, Egypt & Ibrahim Ali, Specialist, Arab Academy for Science, Technology and Maritime Transport, Egypt. Fabrication of High Sensitive ZnO Gas Sensor for LPG Gas Detection.
3. Maria Elena Campos-Aldrete, Researcher, ENCB - Instituto Politécnico Nacional, Mexico. Modulator Effect of the Nitro Group over Imidazo [1,2] Piridines Activity.

21:00-22:30 Dinner (Details during registration)

Wednesday 20 July 2016
Cruise: (Details during registration)

Thursday 21 July 2016
Delphi Visit: (Details during registration)

Hassan Shokry Ahmed
Assistant Professor, City of Scientific Researches and Technological Applications, Egypt
Abdel-Hady Kashyout
Head, City of Scientific Researches and Technological Applications, Egypt
Iman Morsi
Professor, Arab Academy for Science, Technology and Maritime Transport, Egypt
Abdelmenem Nasser
Professor, Arab Academy for Science, Technology and Maritime Transport, Egypt
&
Ibrahim Ali
Specialist, Arab Academy for Science, Technology and Maritime Transport, Egypt

Fabrication of High Sensitive ZnO Gas Sensor for LPG Gas Detection

The fabricated In-doped ZnO gas sensors with different ratio (1, 5 and 10 %) were successfully synthesized via sol gel technique. ZnO is a sensitive material to different kind's gases especially to Liquefied Petroleum Gas (LPG). The morphological structures of the prepared ZnO were revealed using scanning electron microscope (SEM). X-ray diffraction (XRD) patterns exhibited a highly crystallized wurtzite structure and used for identifying phase structure and chemical state of both ZnO and ZnO doped with In. The gas sensitivity and voltage are measured as a function of temperature for the fabricated In-doped and un-doped ZnO gas sensor devices for LPG gas. The maximum sensitivity is recorded at Zn/In = 95:5 is 111%. This concentration has a good voltage variation. By increasing the load resistances the voltage will decreases. The fabricated gas sensor is used with Arduino kit to make it as an audible gas detector.

Anouar Alami
Head, Department of Chemistry, Sidi Mohamed Ben Abdellah University, Morocco

Heterocyclic Compounds: Synthesis, Characterization, Electrochemical Study, Study and Prediction of Biological Activity

The chemistry of the heterocycles constitutes one of the research themes very studied and developed in organic synthesis. The interest of the heterocyclic compounds is explained, inter alia, by their many applications in the pharmacological, agro-chemical and electrochemical field.

The development of new ways of synthesis making it possible to functionalize these heterocycles remains a major target. A share of the activity of our laboratory is thus directed as well towards the preparation of new spiro-heterocyclic structures, derived from the isothiochomanone, the tétralones or the aurones and thioaurones, as towards the synthesis of new heterocyclic compounds, precursory or derived from amino acids mono, bi and triheterocyclic carboxylic and phosphonic. The other hand, undoubtedly most significant, is to carry out an electrochemical study and biological tests of the synthesized products. Thus we present in this conference our recent research tasks in this field. The research orientations chosen are the following:

- Elaboration of new spiro-heterocyclic compounds, study and prediction of their pharmacological activities.
- Synthesis and study of the corrosion inhibitor power of some derivatives of tetrazole, synthesis of derivatives of heterocyclic carboxylic amino acids likely to present biological and electrochemical properties interesting.

Dimitris Argyropoulos
Finland Distinguished Professor, North Carolina State University, USA
C. Cui
North Carolina State University, USA
R. Sun
North Carolina State University, USA
S. Sen
North Carolina State University, USA
&
H. Sadeghifar
North Carolina State University, USA

Homogeneous Technical Lignins as Phenolic Precursors to Heat Stable Polymers and Carbon Fibers

Most efforts to utilize lignin have been limited by various factors that impart in it characteristics that define it as an unreliable precursor to polymer production. This is because lignin (and more specifically technical lignin) offers relatively unpredictable polymerization characteristics, is of low molecular weight offering materials of no mechanical integrity , is highly functional & reactive causing gel formation and is highly heterogeneous and of variable nature depending on the details of the pulping process. Consequently, if one is to create new opportunities for softwood kraft lignin in markets of value added polymer products one needs to thoroughly address these limitations. The work of our group has focused at creating new opportunities for softwood kraft lignin in markets that include value added polymers. During this presentation we will describe our systematic efforts in the following areas aimed at actualizing our objectives:

a. Refining technical kraft lignin so as to expose its potential as a source for reactive polyphenols of well-defined molecular weight polymers and oligomers. More specifically, we have demonstrated that a continuum of narrow fractions can be isolated from softwood kraft lignin, common to a variety of such sources irrespective of the manufacturing details of the pulping process. Such consistently homogeneous lignin streams from LignoboostR lignins offer significant commercial ramifications.
b. Creating heat stable kraft lignin copolymers with heat stabilities approaching 300 0C.
c. Creating new thermoplastic lignin polymers and precursors to carbon fibers by applying propargylation derivatization chemistry followed by thermal treatments, offering a versatile novel route for the eventual chain extension & utilization of technical lignins with a significant amount of molecular control.

Gregory Boutis
Associate Professor, The City University of New York, USA

13C, 2H NMR Studies of Structural and Dynamical Modifications of Cholesterol Exposed Porcine Aortic Elastin

Elastin is a protein of the extracellular matrix that contributes significantly to the elasticity and extensibility of connective tissues, including arteries. In this study we examine dynamical and structural modifications of porcine aortic elastin exposed to cholesterol by ^{13}C and ^{2}H NMR spectroscopic and relaxation methodologies. Results from macroscopic measurements are also presented and reveal that cholesterol treatment causes a decrease in the stiffness of tissue along the circumferential and longitudinal directions. Applying 2D T_1-T_2 NMR techniques, we measured the correlation time, distribution, and population of water in cholesterol treated samples. The measured correlation times of tumbling motion of water were similar; however, there were differences between the relative populations of water which correlate with macroscopic changes in the swelling of the tissue following cholesterol exposure. ^{13}C magic-angle-spinning NMR methods were applied to investigate structural and dynamical modifications after cholesterol treatment. These measurements indicate that cholesterol treated aortic elastin cross polarizes less than the control samples. The measured correlation times of the tumbling motion of the ^{13}C-^{1}H internuclear vectors in the cholesterol treated sample are smaller than in untreated samples pointing to increased mobility. Simulations on a short elastin repeat VPGVG in the presence of cholesterol are used to investigate the energetic (dU/dr) and entropic (-TdS/dr) contributions to the retractive force, in comparison to the same peptide in water. Peptide stiffness reduces for the peptide in cholesterol in comparison to the peptide in water due to a decrease in the entropic force, in qualitative agreement with macroscopic stress-strain measurements.

Maria Elena Campos-Aldrete
Researcher, ENCB - Instituto Politécnico Nacional, Mexico

Modulator Effect of the Nitro Group over Imidazo [1,2] Piridines Activity

In order to increase the probability of obtaining pharmacologically succesful molecules, a variety of methodologies have been developed involved their design and syntheses. Molecular modelling is an example of those methodologies.

In the present investigation, three derivatives of pyrido (1',2':1,2) imidazo[5,4-d]-1,2,3-triazinones were synthesized and evaluated in relation to a possible antineoplasic activity.

To optimize the pharmacological response, a structural study on molecules showing anticancer activity was carried out. Temozolomide, a drug used in the treatment of brain tumors was chosen as a reference model to select suitable structural variations in order to optimize the pharmacological response. Data bases such as Molinspiration, Actelion and PC Spartan Pro program were used to compare proporties such as pharmacophore groups recognition involved in antineoplasic activity, Log P, Lipinski rule, toxicology and electronic density.

Structural changes were performed on the imidazo[1,2-a]pyridine nucleus to furnish compounds related to Temozolomide. After permforming a retrosynthetic analysis, the imidazo[1,2-a]pyridine-ethyl carboxylate was nitrated at position 3, followed by treatment with amines to get the corresponding amides. Reduction of the nitro group followed by cyclization delivered the desired pyridoimidazotriazinone. This synthetic route provided six novel pyridotriazinones.

Three selected pyrido(1',2':1,2)imidazo[5,4-d]-1,2,3-triazinonas (R= H, isopropyl and cyclopropyl) were prepared and purified to get sufficient amount to evaluate their biological activity as potential antineoplasic drugs. Compounds were characterized by conventional spectroscopic means, IR, NMR.

The glioma model (C6) was used to perform the anticancer assay in vitro of selected compounds at several doses (0,1,10,100,500,1000 μM) to obtain a response profile at 24 h of treatment and in comparison with Temozolomide. The most active compound turned out to be the imidazopyridinetriazinone with substituent H (CI50= 284μM), whereas the least active was the one with cyclopropyl substituent (310μM, c.f. temozolomide, 310μM). Overall these results suggest further investigation on these compounds as candidate drugs for cancer treatment.

Marwa Elkady
Associate Professor, Egypt-Japan University of Science and Technology, Egypt
&
Hassan Shokry Ahmed
Assistant Professor, City of Scientific Researches and Technological Applications, Egypt

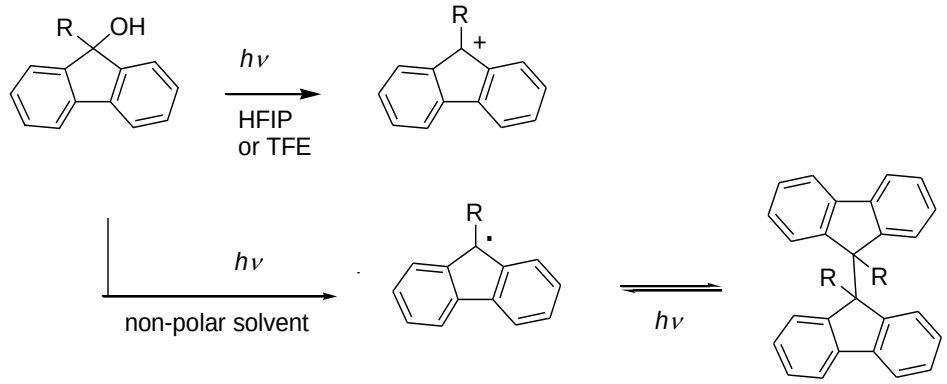
Nano-Tube Zirconium Tungesto-Vanadate as Cation Exchanger for Lead Decontamination from Polluted Wastewater

A unique zirconium tungesto-vanadate cation exchange material was architecture at the hollow nanotube morphological structure using microwave technique in presence of poly vinyl alcohol as stabilizing agent. The prepared cation exchanger was characterized using different physical and chemical techniques. The material characterized by its high surface area that equivalent 640 m2/g. The material assigned as an efficient cation exchanger, where, it possess 4.8 meq/g ion exchange capacity. X-ray diffraction pattern explored its pure crystalline structure. Scanning electron microscope identifies the average aspect ratio of the architecture zirconium tungesto-vanadate nano-tubes as 6.5. The efficiency of the prepared material for lead ions sorption from aqueous solutions was examined using batch technique. The material poses 97.2% lead ion decontamination within 90 minutes.

Edward Lee-Ruff
Professor, York University/Chemistry, Canada

Photochemical Generation of 9-Fluorenyl Radicals

A series of 9*H*-fluorenols and 9*H*, 9′H-bifluorenyls were irradiated in non-polar solvents giving photoproducts derived from their corresponding 9*H*-fluorenyl radicals. These transient species were directly observed by laser flash photolysis and their uv/visible spectra compared to their corresponding cations. Theoretical calculations (DFT calculations) of these intermediates indicate their destabilizing nature in similar fashion to the antiaromatic character of the corresponding cations. The theoretical spectra are compared with the experimental showing the same trends of shift with substituent effects.



Khadija Mammadyarova
Ph.D. Student, Azerbaijan National Academy of Sciences, Azerbaijan

Anti-wear Properties of Amino Derivatives

Due to the harsh operating conditions of Industrial equipment operating under heavy loads for their lubrication only usage of additive based lubrication oil is required. Despite the many studies and synthesis on anti-wear additives there is still the need in new quality additives to be taken.

AKI -1, AKI-2, AKI-3 amino derivatives have been synthesized by us. These additives have detergent, anticorrosion and antioxidant properties and have also been studied for their anti-wear properties.

It is shown that increasing the concentration of oil in synthesized amino derivatives also increases their anti-wear properties.

The additives significantly reduce the corrosion caused by oil friction on the surfaces and also increases the duration of the operations.

Thus, the AKI-1, AKI-2, AKI-3 additives have high anti-wear properties.

Ryszard Ostaszewski
Professor and Head of The Scientific Group, Institute of Organic Chemistry Polish Academy of Sciences, Poland

The Studies on Enzymatic Kinetic Resolution of Selected Unsaturated Carboxylic Acids

Chiral, β,γ-Unsaturated carboxylic acids derivatives are important intermediates in the synthesis of many biologically active compounds; for example anti-microtubule agents [1], Bisnorvernolepin [2] and Vineomycinone B2 [3].

Recently we have performed studies on enzymatic kinetic resolution based on esterification of carboxylic acids with orthoestres, used as a donor of alkoxy group [4,5]. As a compound for our studies, we choose 2-benzyl-2-methylbut-3-enic acid, which contains stereogenic quaternary carbon center. This compound is a substrate for the synthesis of irreversible inhibitors of a carboxypeptidase A, a representative zinc-containing proteolytic enzyme [6]. 2-Benzyl-2-methylbut-3-enic acid was synthesized in 4-step synthesis, containing enzymatic hydrolysis of benzylmethylmalonic dimethylester [6]. We propose short, two step synthesis of optically active 2-benzyl-2-methylbut-3-enic acid from commercially available tiglic acid. The results of optimization of the kinetic resolution of 2-benzyl-2-methylbut-3-enic acid, containing enzyme screening, influence of solvent and reaction conditions will be demonstrated.[7]

Batric Pesic
Professor, University of Idaho, USA

Transport of Chloride Ions Evaluation through Modulated Concrete Microstructures

It is known that properties of concrete, including the transport of moisture, depend on its microstructure, which can be modulated by chemical and mineral additives, termed as admixtures. In the previous study, the effect of admixtures, such as glycerol as a nanoviscosity modifier, was evaluated indirectly by measuring the corrosion rate of reinforcement steel. However, it was found that this method (corrosion) could be biased due to the effects of admixtures on corrosion inhibition per se. Therefore, there was a need to evaluate the concrete permeability by direct transport through its matrix. This was done in a new experimental design, which allows direct measurement of chloride concentration change with time. A concrete with particular admixture, and of disks geometry, separates two compartments. A ponding compartment serves as a supplier of chloride ions, which upon transport through the concrete matrix are received by a pure water compartment. Chloride concentration in initially pure water compartment is measured with time using ion chromatography. Therefore, the rate of chloride ion concentration change enables its correlation to the corrosion rate of embedded steel as an indirect method for measurement of concrete permeability to moisture and chloride ions. In the similar experimental design, utilizing electrochemical impedance spectrometry (EIS), the ohmic resistance of concrete matrix as a function of moisture and chloride ions was evaluated, and again correlated to the corrosion of reinforcement steel.

Jun Peng
Professor, Northeast Normal University, China

Tri-vanadium Substituted Keggin Tungstosilicate Microtubes: Synthesis and Characterization

Polyoxometalate nano- and micro-tubes have both the advantages of polyoxometalates and the structure of tubes. Recently, saturated POM microtubes and mono-substituted POM microtubes have been reported. However, there are few reports about the research on tubular structures of multiple substituted POMs. It is known that if three vanadium atoms replace the tungsten atoms in a Keggin 12-W cluster, redox properties and catalytic behavior of the POMs could change. Here, we raise a template-free synthesis of tri-vanadium substituted Keggin tungstosilicate microtubes from tri-vacant $[SiW_9O_{34}]^{10-}$. The obtained microtubes were characterized by FT-IR, TG, CV and SEM. The formation mechanism has been discussed. And the catalytic performance in desulfurization of fuel has been explored.

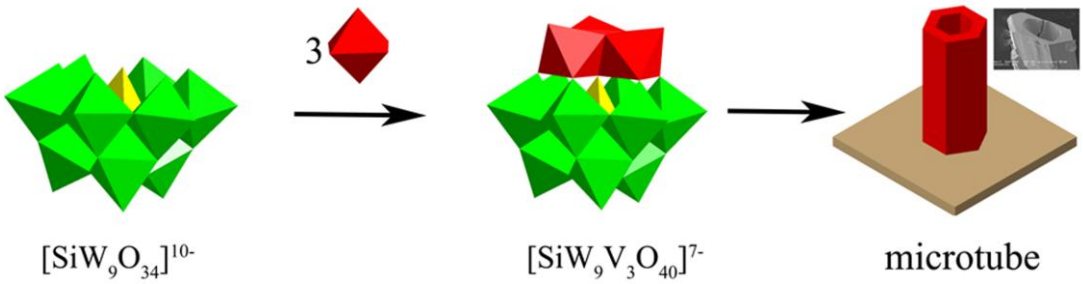


Fig.1 Mechanism for Formation of $SiMo_3V_9$ microtubes

Acknowledgements
We thank the National Natural Science Foundation of China (Grant 21373044) for financial supports.