The 15th International Conference of Physical Chemistry

CONFERENCE PROGRAM

ROMPHYSCHEM 15

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ROMANIAN ACADEMY
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organizers

"Ilie Murgulescu" Institute of Physical Chemistry Bucharest
Department of Physical Chemistry, Faculty of Chemistry,
ALPHA Association

ANCS
AUTORITATEA NATIONALA PENTRU CERCETARE STIINTIFICA

S6-P21	Spectral and biological evaluation of some mesoporphyrinic complexes *Rica Boscencu, Radu-Petre Socoteanu, Mihaela Ilie, Anabela Sousa Oliveira, Carolina Constantin, Georgiana Vasiliu, Veronica Nacea and Luis Filipe Vieira Ferreira*
S6-P22	Magnetic automatic extraction and purification for human DNA *Alexandru Ioan Chivulescu, Mihaela Filip, Melania-Liliana Arsene, Maria Luiza Jecu and Mihaela Badea - Doni*
S6-P23	Relationships between buffer capacities of chemical components in heterogeneous natural systems *Oxana Spinu and Igor Povar*
S6-P24	Examining the redox activity of the ambiental particulate matter (PM_{10} and $PM_{2.5}$) in Craiova urban area during 2012 and statistically analyzing OC and EC graphs by using a charge-transfer reaction of dithiothreitol catalyzed by 9,10-phenanthraquinone *Liana-Simona Sbîrnă, Sebastian Sbîrnă and Cristian Codreşi*
S6-P25	Ordering of entire molecules in monolayers of GPIs fragments *Cristina Stefaniu, Ivan Vilotijevic, Mark Santer, Daniel Varón Silva, Gerald Brezesinski and Peter H. Seeberger*
S6-P26	Hydrothermally prepared biochars from potato and potato peels as green approach: The effect of activation route on drug adsorption capacity *George Kyzas and Eleni Deliyanni*
S6-P27	Evidences for differences in biogenic amines content from several Romanian red and white wines using HPLC *Florian Harja, Michaela Dina Stănescu and Eleonora Mihaela Ungureanu*
S6-P28	Removal of Pb^{2+} from aqueous solutions by slovak bentonites *Zuzana Melichová, Ladislav Hromada and Andrea Luptáková*
S6-P29	Metal content in moss samples from copper old mining areas Ľubietová, Staré Hory and Špania Dolina, central Slovakia *Zuzana Melichová, Anna Petrášová, Ingrid Turisová and Iveta Nagyová*
S6-P30	Solidification study of a PCM composite system PEG 6000-Epoxy into a spherical cell *Petrică Mircea Pavel, Mariella Constantinescu and Elena Maria Anghel*

Workshop 8 - Sol-gel science and applications.

S8-P01	The influence of Co dopant on TiO_2 structure of sol-gel nanopowders *Maria Crişan, Adelina Ianculescu, Mălina Răileanu, Dorel Crişan, Nicolae Drăgan, Simona Şomăcescu, Petre Osiceanu, Nicolae Stănică and Ligia Todan*
S8-P02	The role of Fe dopant on TiO_2 structure of sol-gel nanopowders *Dorel Crişan, Nicolae Drăgan, Maria Crişan, Mălina Răileanu, Adelina Ianculescu, Petre Osiceanu, Simona Şomăcescu, Nicolae Stănică and Cristina Stan*
S8-P03	Effects of Ni dopant on TiO_2 structure of sol-gel nanopowders *Mălina Răileanu, Maria Crişan, Adelina Ianculescu, Dorel Crişan, Nicolae Drăgan, Ligia Todan, Petre Osiceanu, Simona Şomăcescu and Nicolae Stănică*
S8-P04	Nanosized oxide powders in the MgO-TiO_2 binary system obtained by sol-gel method *Ligia Todan, Dana Culiță, Silviu Preda, Cristian Andronescu, Cornel Munteanu, Tiberiu Dăscălescu and Maria Zaharescu*
S8-P05	Sol-gel processes in SiO_2-P_2O_5 system studied by NMR spectroscopy *Alina Nicolescu, Ligia Todan, Calin Deleanu and Maria Zaharescu*
S8-P06	Modeling of some parameters of interest in the sol-gel process *Adrian Beteringhe, Maria Zaharescu and Virgil Bădescu*
S8-P07	Thin silica layers doped with GeO_2 for Bragg waveguides *Ivo Barton, Jan Mrazek and Vlastimil Matejec*
S8-P08	Sol-gel ITO films for solar cell applications *Luminita Predoana, Silviu Preda, Adriana Rusu, Madalina Nicolescu, Mihai Anastasescu, Jose Calderon Moreno, Mariuca Gartner and Maria Zaharescu*
S8-P09	Synthesis of zeolite NaA with facets by the sol-gel technology *Dimitar Georgiev and Tsvetan Dimitrov*

Hydrothermally prepared biochars from potato and potato peels as green approach: The effect of activation route on drug adsorption capacity

George Z. Kyzas and Eleni A. Deliyanni

Laboratory of General & Inorganic Chemical Technology, Aristotle University of Thessaloniki, Greece

In the present study, activated carbons (ACs) were hydrothermally prepared with an environmental friendly preparation route after pyrolysis from biomass (specifically from potato peels and potato starch). The prepared biochars were activated with potassium hydroxide (chemical activities). Biochars were impregnated with aqueous solutions of potassium hydroxide following a variant of the incipient wetness method. Activation was carried out under nitrogen flow by heating to 873 K. Biochars were also activated with aqueous solutions of potassium hydroxide at room temperature for reasons of comparison. The porous texture of the obtained ACs was characterized by physical adsorptions of N_2 at 77 K. The preparation route had a strong impact on the pore structure of ACs. In addition, surface chemistry was also affected by the preparation and activation process. The adsorbent materials were also characterized by Scanning Electron Microscopy (SEM) and Fourier Transform Infrared (FTIR) spectroscopy. The prepared activated carbons were used as adsorbents for the removal of the Pramipexole, a drug agonist for Parkinson disease, from aqueous solutions. Batch experiments were performed to investigate the effect of physico-chemical parameters, such as pHpzc, ionic strength, adsorbent dose, contact time, initial drug concentration and temperature. The kinetics of adsorption were studied by applying the pseudo-first order, pseudo-second order and intraparticle diffusion models. Equilibrium data were analyzed using Langmuir and Freundlich isotherm models. The thermodynamic parameters such as the change of enthalpy (ΔH^0), entropy (ΔS^0) and Gibb's free energy (ΔG^0) of adsorption systems were also determined and evaluated.

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Abstract

In the present study, activated carbons (ACs) were hydrothermally prepared with an environmental friendly preparation route after pyrolysis from biomass (specifically from potato peels and potato starch). The prepared biochars were activated with potassium hydroxide (chemical activities). Biochars were impregnated with aqueous solutions of potassium hydroxide following a variant of the incipient wetness method. Activation was carried out under nitrogen flow by heating to 873 K. Biochars were also activated with aqueous solutions of potassium hydroxide at room temperature for reasons of comparison. The porous texture of the obtained ACs was characterized by physical adsorptions of N_2 at 77 K. The preparation route had a strong impact on the pore structure of ACs. In addition, surface chemistry was also affected by the preparation and activation process. The adsorbent materials were also characterized by Scanning Electron Microscopy (SEM) and Fourier Transform Infrared (FTIR) spectroscopy. The prepared activated carbons were used as adsorbents for the removal of the Pramipexole, a drug agonist for Parkinson disease, from aqueous solutions. Batch experiments were performed to investigate the effect of physico-chemical parameters, such as pHpzc, ionic strength, adsorbent dose, contact time, initial drug concentration and temperature. The kinetics of adsorption were studied by applying the pseudo-first order, pseudo-second order and intraparticle diffusion models. Equilibrium data were analyzed using Langmuir and Freundlich isotherm models. The thermodynamic parameters such as the change of enthalpy (ΔH0), entropy (ΔS0) and Gibb's free energy (ΔG0) of adsorption systems were also determined and evaluated.

Drugs/Pharmaceuticals in wastewaters

Pharmaceuticals are of scientific and public concern as newly recognized classes of environmental pollutants and are receiving considerable attention with respect to their environmental fate and toxicological properties over the last 15 years. Many of these pharmaceutical compounds, which often are pharmacologically active or endocrine modulating across multiple levels of biological organization, are not completely removed by wastewater treatment plants (WWTPs) and municipal effluents as well as effluents from hospitals and pharmaceutical manufacturing facilities have been identified as important sources. Consequently, a vast number of these compounds have been detected in WWTP effluents, surface waters and, less frequently, in ground and drinking water all over the world. The above considerations reflect the need for the complete removal of pharmaceuticals and their transformation products (TPs) from aquatic systems to avoid their potential toxicity and other possible dangerous health effects. As conventional water and wastewater treatment processes are unable to act as a reliable barrier towards some recalcitrant pharmaceutical compounds, it is necessary to introduce and apply specific treatment methodologies for pharmaceutical wastewaters, especially for those generated from pharmaceutical industry in which large volumes of wastewater are produced with specific nature and high pharmaceutical loading.

Removal of pharmaceuticals by adsorption is one of the most promising techniques, due to its convenience once applied into current water treatment processes. Up to now, activated carbon and other inorganic materials such as zeolites are among the most commonly used effective adsorptive materials that have been tested for the treatment of wastewaters.

Hydrothermally prepared biochars from potato peels as green adsorbents

Prior to the use, the potato peel was repeatedly washed with distilled water in order to remove dust and other inorganic impurities, then oven-dried for 24 h at 393 K to reduce the moisture content. Samples of potato peels were cut into small pieces and dried at 105 °C for 12 hours. Then the samples were ground into powdered form and sieved to get the proper size (particle size between 1 mm to 500 μm) for uniform activation.

The dried mixtures were then transferred into capped crucibles and kept inside the muffle furnace for pyrolysis at 600 °C for 2 hours under self-burn atmosphere. The crucibles were then cooled at room temperature, and the content inside was ground into a uniform particle size (particle size <180 μm). The hydrochars were denoted as (char).

Preparation of hydrothermal carbons

The hydrocarbonization process (HTC) of the precursors was carried out in a 0.120 L stainless steel autoclave (Berghof, Germany) using a volume of 0.1 L of deionized water and 5 g of biomass. The mixture was sealed into a Teflon vessel and then inserted in the autoclave, which was subjected to 150 or/and 200 °C for 2 h. The autoclave was cooled down to room temperature and then the hydrochar was collected and washed with distilled water. The hydrochar was then dried in an oven (100 °C) and the solid yield determined by weight. The hydrochars were denoted as Pot-Hyd (150 °C)

Activation at room temperature

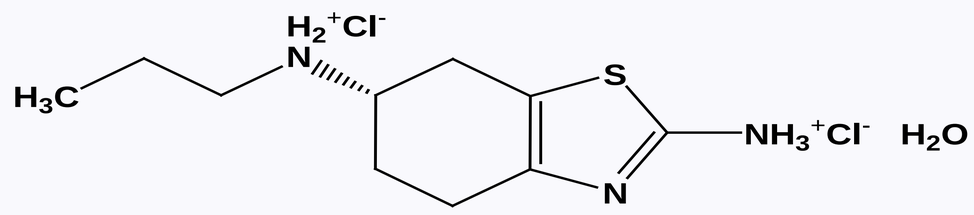
A known weight of the sample was dipped into the solution of activating agent, KOH, keeping the impregnation mass ratio equal to 1, under stirring at room temperature for 2 hours. Uniform particles of activated carbon were washed with excess demineralized water to remove the excess activating agents, and by-products that may have form during activation on the surface of activated carbon. The samples were then dried in the oven at 105 °C for 12 hours for complete removal of the absorbed water. The activated carbon were labeled here as Pot-Hyd (KOH 25 °C).

Activation by pyrolysis

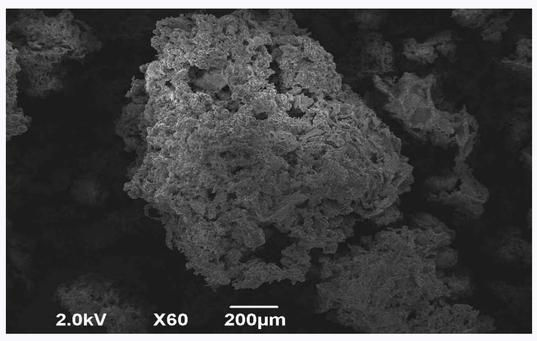
A known weight of the sample was dipped into the solution of activating agent, KOH, keeping the impregnation mass ratio equal to 1, under stirring at room temperature for 2 hours. The samples were then filtered and put for pyrolysis. Pyrolysis treatments (activations) were carried out in a vertical tubular reactor made of quartz in furnace CarboliteTM, using in all cases 25 g of impregnated and dried material. All treatments were done at a constant heating rate of 10K/min and with a nitrogen (99%) flow of 30 STP cm^3/min, which was kept during heating and cooling. An activation temperature of 823K and a soaking time of 2 h were used. After cooling, the solid pyrolysis residue to room temperature it was washed with distilled water. The resulting ACs was dried at 383K for 24 h in a vacuum furnace. The activated carbon were labeled here as Pot-Hyd (KOH 600 °C).

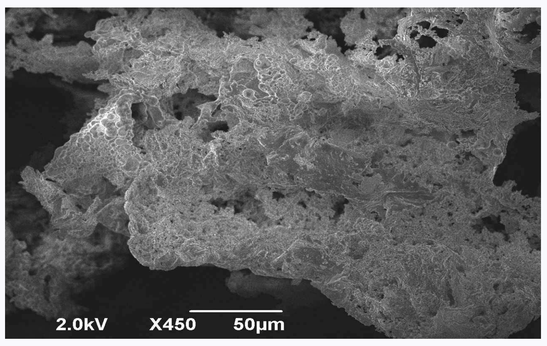
Pramipexole as drug model pollutant

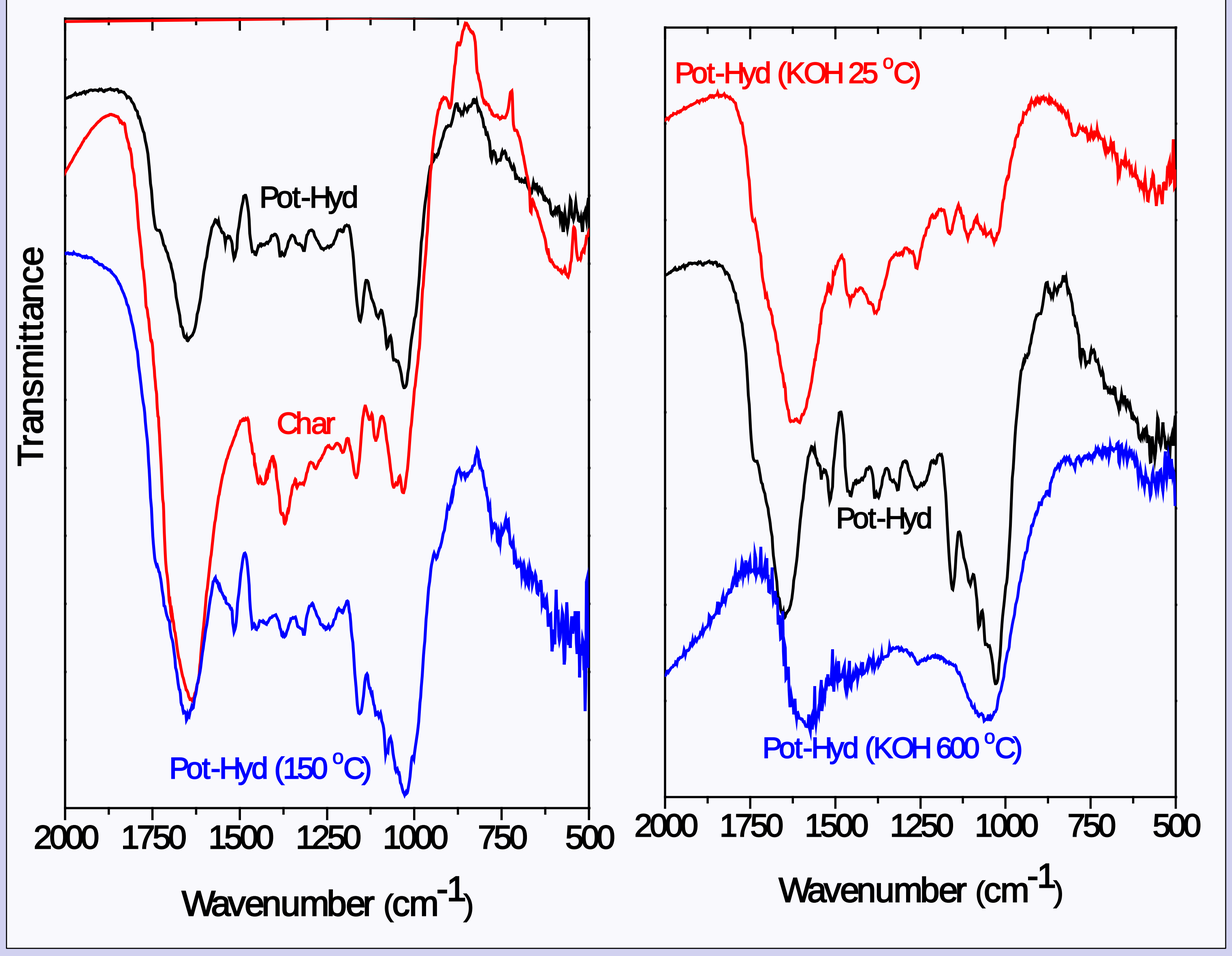
Pramipexole (denoted as PMR) initially introduced for treatment of the signs and symptoms of idiopathic Parkinson's disease and recently approved in US and Europe also for the treatment of idiopathic restless legs syndrome in adults. It is being used widely all over the world for its unique pharmaceutical activity and on the basis of recent drug usage trends; it seems likely that the use of this recently available non–ergot dopamine agonist will continue to increase in the immediate future, as primary care physicians (PCP) become more familiar with it. Some pharmaceutical industries and hospitals are discharging PRM in their effluents resulting into the contamination of our natural water resources. Therefore, treatment of wastewater by high polluted levels of PRM is required and urgent needed.



Characterization (SEM, FTIR)







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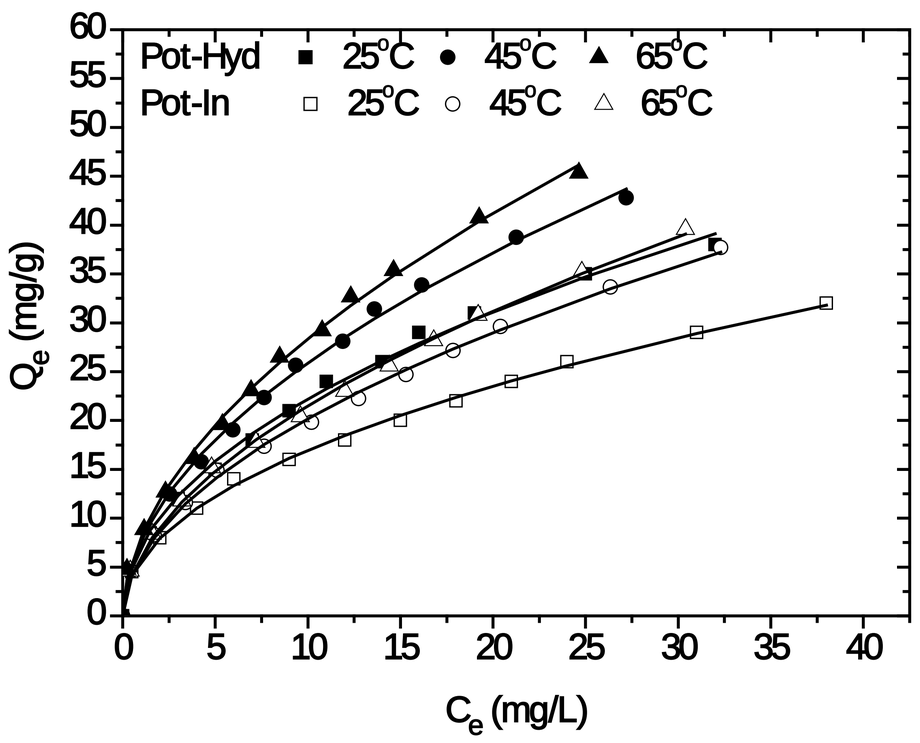

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Certificate of Attendance

This is to confirm that PhD Researcher

George KYZAS

from

Laboratory of General & Inorganic Chemical Technology, Aristotle University of Thessaloniki, Greece

presented the scientific contribution

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authors:

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as poster presentation

at

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"Ilie Murgulescu"
Institute of
Physical Chemistry
- Bucharest -

University of
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Dept. of
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