X Jornadas CICECO
CICECO Meeting

Book of Abstracts

Universidade de Aveiro, 18-19 April 2013

X CICECO Meeting - Schedule

April 18^{th}

09:00	REGISTRATION
09:45	OPENING
	SESSION 1 - Chair: Ana Barros
10:00	Mário Vaz - LABIOMEP, Faculdade de Engenharia, Universidade do Porto
	Experimentation in Biomechanics: potential and applications
10:30	Carla Vilela
	Synthesis of New Vegetable Oil-based Polymeric Materials
10:50	Igor Marques
	Anion transmembrane transport mediated by synthetic molecules: molecular modelling insights
11:10	Mariana Sardo
	High-resolution solid-state NMR: from small molecules to materials
11:30	Luis Amaral
	Grain boundary and interfaces in the design of the electrical response of functional oxides
	SESSION 2 - Chair: Vítor Amaral
14:00	João Paulo Farinha - Departamento de Química, Inst. Superior Técnico, Lisboa
	Highly fluorescent materials
14:30	Cátia Teixeira
	Computer-aided starving of parasites: What can we learn from QM/MM MD studies?
14:50	Rui M.A Domingues
	Triterpenic acids production by supercritical fluid extraction integrated in a Eucalyptus wood pulp mill
15:10	Eddy M. Domingues
	Relationships between composition, microstructure and proton conductivity in acid functionalised organosilicas and their Nafion composites
15:30	Eduardo Silva
	Diamond Microelectrodes for Corrosion Studies
15:50	COFFEE BREAK - POSTER SESSION
	SESSION 3 - Chair: Paula Vilarinho
17:00	Henrique Gomes - Faculdade de Ciências e Tecnologia, Universidade do Algarve
	Bioelectronic devices to communicate with living cells: Applications in medicine and biosensing
17:30	Bárbara Ferreira
	Copper and Iron complexes with anti-tumoral properties
17:50	João Nuno Gonçalves
	Ab-initio modelling of multiferroic materials
18:10	Mohamed Taha
	Finding 'Organic-phase biological buffers' for biocatalysis in organic media using a new class of Ionic Liquids
18:30	Ana L. Daniel da Silva
	Hydrogel nanocomposites for photothermally enhanced drug release
18:50	POSTER AWARDS announcement

20:00 DINNER at Hotel Imperial

April 19^{th}

	SESSION *materials and society* - Chair: João Rocha
09:00	opening
09:15	Nuno Camarneiro - Physics Engineer, writer, Leya Prize
	The Matter Of Fiction
10:15	Vítor Figueiredo and Carlos Gil - Martifer Group
	Martifer: land, sea and sky
11:15	Fernando Merino - Innovation Manager, ERT Têxtil Portugal
	The technological innovation on the automotive sector as an entrepreneurial boosting factor on the textile industry
12:15	closing

Invited Lectures

Mário Vaz - LABIOMEP, Faculdade de Engenharia, Universidade do Porto
Experimentation in Biomechanics: potential and applications

João Paulo Farinha - Departamento de Química, Inst. Superior Técnico, Lisboa
Highly fluorescent materials

Henrique Gomes - Faculdade de Ciências e Tecnologia, Universidade do Algarve
Bioelectronic devices to communicate with living cells: Applications in medicine and biosensing

Nuno Camarneiro - Physics Engineer, writer, Leya Prize
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Vítor Figueiredo and Carlos Gil - Martifer Group
Martifer: land, sea and sky

Fernando Merino - Innovation Manager, ERT Têxtil Portugal
The technological innovation on the automotive sector as an entrepreneurial boosting factor on the textile industry

Oral Presentations

O1 Carla Vilela
Synthesis of New Vegetable Oil-based Polymeric Materials

O2 Igor Marques
Anion transmembrane transport mediated by synthetic molecules: molecular modelling insights

O3 Mariana Sardo
High-resolution solid-state NMR: from small molecules to materials

O4 Luis Amaral
Grain boundary and interfaces in the design of the electrical response of functional oxides

O5 Cátia Teixeira
Computer-aided starving of parasites: What can we learn from QM/MM MD studies?

O6 Rui M.A Domingues
Triterpenic acids production by supercritical fluid extraction integrated in a Eucalyptus wood pulp mill

O7 Eddy M. Domingues
Relationships between composition, microstructure and proton conductivity in acid functionalised organosilicas and their Nafion composites

O8 Eduardo Silva
Diamond Microelectrodes for Corrosion Studies

O9 Bárbara Ferreira
Copper and Iron complexes with anti-tumoral properties

O10 João Nuno Gonçalves
Ab-initio modelling of multiferroic materials

O11 Mohamed Taha
Finding 'Organic-phase biological buffers' for biocatalysis in organic media using a new class of Ionic Liquids

O12 Ana L. Daniel da Silva
Hydrogel nanocomposites for photothermally enhanced drug release

List of Posters

P1	Abel Fenta	Hyperfine Techniques Studies of Graphene Layers Using Isolated Ad-Atom Probes
P2	Alexandre Bastos	The oddities of micro-potentiometric measurements in corrosion
P3	Alexey Dronov	Controllable growth of highly ordered titanium oxide nanotube arrays
P4	Ali Baghizadeh	EELS study of multiferroic Lu_{2-x} Mn_x O_3 compound
P5	Aliaksandr Zhaludkevic	$CuGaS_2$ -$CuGaO_2$ Chalcopyrite-Delafossite System: Phase Formation at High-Pressure High-Temperature Conditions
P6	Ana Brandão	A potential hydrogen permeation membrane from $(SrLa)(NbV)O_4$ -based composite
P7	Ana Filipa Cláudio	Assessment of solubility behavior of phenolic compounds and alkaloids in ionic liquids aqueous solutions
P8	Ana Gil	Metabolic response of lettuce to different growth conditions and exposure to pesticide Mancozeb assessed by ^{1}H NMR Spectroscopy
P9	Ana Gomes	Tris(pyrazolyl)methane Molybdenum Tricarbonyl Complexes as Catalyst Precursors for Olefin Epoxidation
P10	Ana Inês Rondão	Ageing of ceria-based composite electrolytes
P11	Ana Margarida Silva	In Vitro Surface Reactivity of Powder and Bulk TiO_2 -P_2O_5 -CaO Glasses
P12	Ana Rosa Silva	Asymmetric benzoylation of hydrobenzoin by copper(II) bis(oxazoline) anchored onto ordered mesoporous silicas and their carbon replicas
P13	Ana Rute Ferreira	Desulfurization of fuels through selective extraction using ionic liquids in membrane contactors
P14	Ana Xavier	Catalytic activity of fungal laccase in ionic liquids
P15	André Oliveira	Electrochemical corrosion study of Al_90Si_10 and Al_50Si_10 Zn_40 metallic alloys
P16	Andreia F Sousa	From PET to renewable-based PEF: synthesis and characterisation of PET-ran-PEF copolymers
P17	Angela Pereira	Green vegetable oil solvents in nanoparticle synthesis
P18	Belinda Soares	Valorization of biomass residues via acid liquefaction using polyhydric alcohols
P19	Bernd Schröder	Physico-Chemical Property Prediction and Environmental Fate Modelling of N-acyl-chalcogenourea Derivatives
P20	Carla Pereira	Synthesis of Tetra-Phosphonated Porphyrins for the Preparation of Metal-Organic Frameworks
P21	Catarina Seiça Neves	Removal and recovery of ionic liquids from contaminated water streams using aluminium salts
P22	Catia Soares	Relevance of the ceramic oxide content on composite membrane performance
P23	Claudia Bispo	Advanced solid state NMR studies in the comprehension of the catalytic activity of propylsulfonic acid-fuctionalized periodic mesoporous benzenesilicas
P24	Cristina Fernandes	Selective laser sintering of WC powders sputter-coated with stainless steel
P25	Daniela Firmino	Fast microwave-assisted syntheses of lanthanide metal phosphonates
P26	Daniela Tavares	Surface Modified Magnetite Sorbents for Water Purification Technologies
P27	Diogo Queiros	PHA Production by Mixed Cultures: A Way to Valorize Industrial Waste
P28	Diogo Almeida	PU/ZnO nanocomposites for drug delivery applications
P29	Elena Zdrachek	Sodium- and Chloride-Selective Microelectrodes Optimized for Corrosion Studies
P30	Erika Davim	Glass and glass-ceramic scaffolds: a biocompatibility study
P31	Fabio Silva	Release behaviour of Ag(I) in synthetic silver/cellulose nanocomposites
P32	Fanian Shi	Multifunctional Porous RE^{3+} - Furan-2,5-Dicarboxylate Metal Organic Frameworks
P33	Filipa Sousa	Encapsulation of essential oils in SiO_2 microcapsules and release behavior of volatile compounds
P34	Filipe Davim	Structural studies of Ba-B-Si-Zn glasses
P35	Francisco A. Da Silva	Improvements on modelling supercritical fluid extraction curves
P36	Francisco Loureiro	Chemical stability of oxide matrices with alkali carbonate electrolytes for intermediate temperature applications
P37	Gerard Novell-Leruth	DFT study of the condensation of silicates on the surface of a surfactant micelle
P38	German Perez-Sanchez	Coarse-Grained Molecular Dynamics Simulations for Self-Assembly of Silicate/Surfactant Mesostructures
P39	Guilherme J. Maximo	Fatty Acid Based Protic Ionic Liquids: Phase Equilibrium and Physicochemical Characterization
P40	Hugo F. D. Almeida	Effect of the cation symmetry on the surface tension of bis[(trifluoromethyl)sulfonyl]imide-based ionic liquids
P41	Imran Khan	Vapor-Liquid Equilibria Measurements of Ionic liquid and modeling with COSMO-RS
P42	Iola Duarte	Metabolic Response of A549 Lung Cells to Cisplatin and Ionizing Radiation Assessed by ^{1}H NMR Spectroscopy
P43	Isa Branco	Kelvin Probe Force Microscopy of Boron-Doped Diamond Electrodes
P44	Isabel Boal Palheiros	Recycling and reusing ionic liquids in the back extraction of gallic acid using aqueous two-phase systems
P45	Joana Barata	Synthesis and Characterization of Hybrid corrole-Au nanoparticles

Physico-Chemical Property Prediction and Environmental Fate Modelling of *N*-acyl-chalcogenourea Derivatives

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***Abstract* — (Subcooled) vapour pressures, aqueous solubilities, Henry constants, log KOW and log KOC partition constants have been estimated for a set of N-acyl-chalcogenourea derivatives using several prediction methods (COSMO-RS in its COSMOtherm implementation, SPARC as well as EPA's EPIsuite). The data are discussed in terms of substituent effects: how do subtle changes in the chemical composition influence basic physico-chemical properties and hence, the environmental fate of the title compounds?**

I. INTRODUCTION

N-acyl-chalcogenourea derivatives [1] are fairly stable substances, containing important structural features encountered in pesticide chemistry (see figure 1), e.g. in fungicidal thiourea derivatives. They might serve as model compounds for the study of substituent effects on environmentally important partition properties. Information on environmental and toxicological effects are scarce; the same holds for accurate physico-chemical property data, most prominent vapour pressure, aqueous solubility and log KOW data, which belong to the fundamental parameters for predicting transport, distribution and fate of organic substances in the environment. Here, modern in-silico prediction methods may supply missing data with reasonable accuracy, addressing the urgent data needs related to partition coefficients of polar organic chemicals.

II. METHODS

COSMO-RS, the conductor-like screening model for realistic solvation [2-3], combines quantum chemistry, dielectric continuum models, electrostatics surface interactions and statistical thermodynamics and can predict thermodynamic properties of neutral and charged molecules in liquid phase. The method is based on a very small number of adjustable parameters only, which are completely independent of any molecular or structural information.

As complementary methods, the online calculator SPARC [4] and individual models of US EPA's EPIsuite [5] are used, as well.

III. RESULTS AND DISCUSSION

The performance of several physico-chemical property estimation approaches applied on the title compounds is discussed; quantum-chemical based methods are thought to be advantageous over classical group contribution methods in cases of substances for which no such contributions could be established, yet.

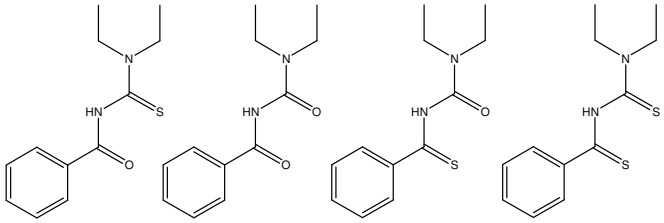

Fig. 1. Examples of N-acyl-chalcogenourea derivatives

The results are placed in environmental partitioning space maps, thus visualizing the estimated equilibrium prediction in the respective environmental compartments as well as quality and magnitude of substituent effects.

ACKNOWLEDGMENTS

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[2] [2] A. Klamt, COSMO-RS: From quantum chemistry to fluid phase thermodynamics and drug design, Elsevier, Amsterdam, 2005.
[3] [3] F. Eckert, A. Klamt, Fast Solvent Screening via Quantum Chemistry: COSMO-RS Approach, AIChE J. 48 (2002) 369-385.
[4] [4] SPARC (October 2011 release w4.6.1691-s4.6.1687) (http://ibmlc2.chem.uga.edu/sparc/)
[5] [5] EPI Suite, US EPA, 2011. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.1. United States Environmental Protection Agency, Washington, DC, USA.