

REVUE ROUMAINE DE CHIMIE (ROMANIAN JOURNAL OF CHEMISTRY)

Tome 52, N^{os} 8-9

Août-Septembre 2007

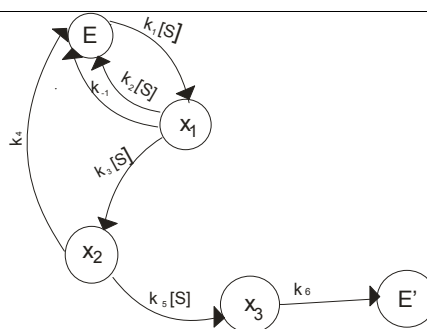
Professor Victor-Emanuel Sahini
List of publications

Rev. Roum. Chim., 2007, 52(8-9), 701-711

PAPERS

Adina RĂDUCAN, Dumitru OANCEA and
Eugen SEGAL

Models for irreversible inactivation in the enzymatic decomposition of hydrogen peroxide and their kinetic treatment by means of graphs

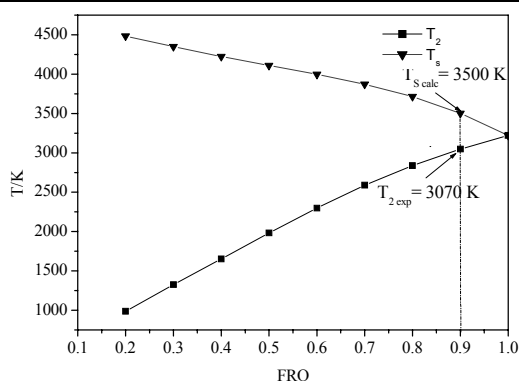


Rev. Roum. Chim., 2007, 52(8-9), 713-717

Key words: catalase inactivation, kinetic modelling, graph theory.

Mihaela PUIU, Valentin MUNTEAN and
Dumitru OANCEA

Modeling kinetic limitations of acetylene detonation

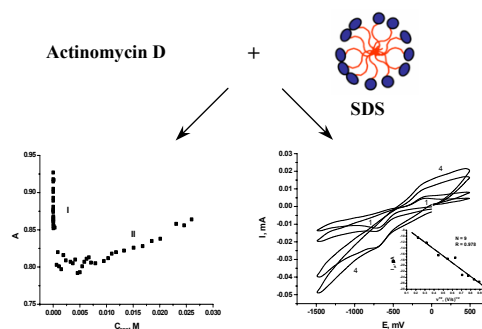


Rev. Roum. Chim., 2007, 52(8-9), 719-724

Key words: acetylene detonation, Chapman-Jouguet model, ZND model.

Mirela ENACHE, Daniela BULCU,
Iuliana ȘERBĂNESCU and
Elena VOLANSCHI

Interaction of actinomycin D with anionic surfactant, sodium dodecyl sulphate: spectral and electrochemical investigations

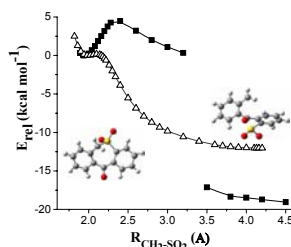


Rev. Roum. Chim., 2007, 52(8-9), 725-731

Key words: anticancer drugs, actinomycin D, surfactant, spectral and electrochemical methods.

**Aurica VĂRLAN, Sorana IONESCU,
Soong-Hyuck SUH and
Mihaela HILLEBRAND**

Modelling of the electrochemical reduction behaviour of some dibenz[b,e]-thiepinosulphones by the DFT method

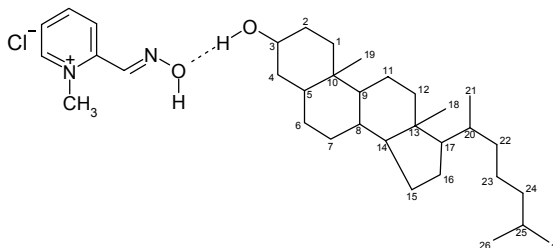


Rev. Roum. Chim., 2007, 52(8-9), 733-737

Key words: thiepinosulphones, reduction behaviour, DFT.

**Valentina CHIOSA, Mihaela MANEA,
Ioana STĂNCULESCU and
Cristina MANDRAVEL**

IR spectral study on nature of 2-pyridine aldoxime methyl chloride interaction with some sterols. II. Cholesterol

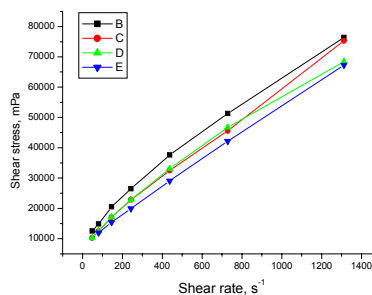


Key words: FTIR spectral study, 2-pyridine aldoxime methyl chloride, cholinesterase reactivator, cholesterol, hydrogen bonded complex.

Rev. Roum. Chim., 2007, 52(8-9), 739-743

**Minodora LECA, Lelian CIOROIANU,
Gabriela CIOROIANU, Gabriela DAMIAN,
Cătălina COSTEA and Ana Maria MATEI**

Aqueous ecological intumescent fire retardant coatings for multifunctional applications. 1. Preparation and characterization

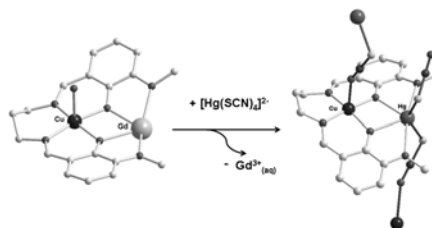


Key words: intumescent fire retardant coatings, passive fire protection, expanding indices, char aspect, rheological behaviour

Rev. Roum. Chim., 2007, 52(8-9), 745-752

**Ruxandra GHEORGHE,
Jean-Pierre COSTES, Sergiu SHOVA and
Marius ANDRUH**

Unexpected replacement of Gd(III) and Hg(II) from an oxygen binding set leading to a heterometallic Cu(II)-Hg(II) 1-D coordination polymer

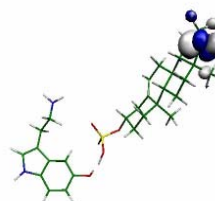


Key words: mixed metal Gd(III)/Hg(II) complexes; coordination polymers; thiocyanato bridges

Rev. Roum. Chim., 2007, 52(8-9), 753-758

**Josette WEINBERG, Dan A. LERNER and
Constantin BĂLĂCEANU-STOLNICI**

Theoretical study of DHEAS: the electronic properties of a complex between DHEAS and serotonin by comparative calculations HF and DFT

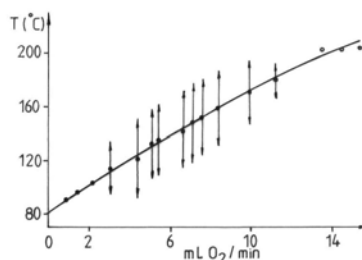


Rev. Roum. Chim., 2007, 52(8-9), 759-764

Key words: DHEAS, Serotonin, *Ab initio*, DFT, NBO

Niculae I. IONESCU, Monica CĂLDĂRARU,
Cristian HORNOIU and Cornel MUNTEANU

Overall activation energy of methanol oxidation
in oscillatory regime

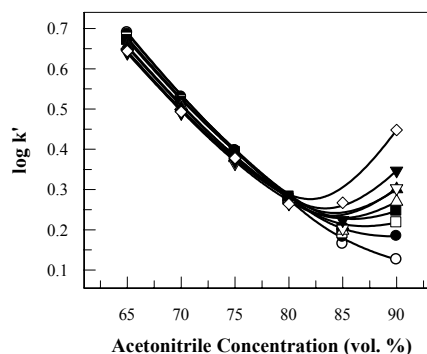


Rev. Roum. Chim., 2007, 52(8-9), 765-769

Key words: Oscillations activation energy, methanol oxidation.

Marieta BALCAN, Dan F. ANGHEL,
Dan Donescu and Valerică RAICU

The retention behavior of ethoxylated nonionic
surfactants in reversed-phase high performance
liquid chromatographic systems

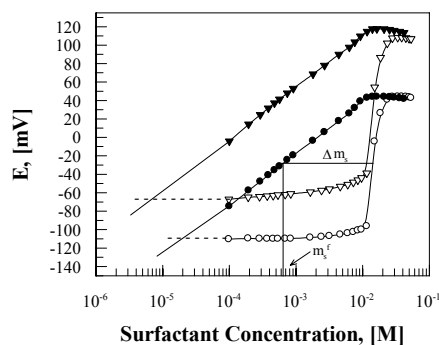


Rev. Roum. Chim., 2007, 52(8-9), 771-780

Key words: nonionic ethoxylated surfactants, reversed-phase liquid
chromatography, hydro-organic mobile phase, molar refraction,
dielectric constant.

Dan F. ANGHEL, Doina M. MIHAI,
Gabriela STÎNGĂ, Alina IOVESCU,
Adriana BĂRAN and Regine Von KLITZING

A study upon interaction of dodecylpyridinium
chloride with sodium dextran sulfate

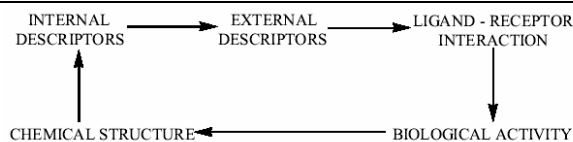


Rev. Roum. Chim., 2007, 52(8-9), 781-787

Key words: cationic surfactant, surfactant-polymer interaction, solid-state
surfactant-selective electrode.

Paul Gabriel ANOICA, Emilia AMZOI and
Costinel I. LEPĂDATU

The hierarchy of the molecular descriptors and
the ligand-receptor interaction



Rev. Roum. Chim., 2007, 52(8-9), 789-793

Key words: QSAR, electronegativity, hardness, OMO – UMO quantum
states, fingerprint descriptors, CADD.

Viorel CHIHAIA, Godehard SUTMANN,
Chang-Sup LEE and Soong-Hyuck SUH

Divergence-free description for molecular
rotation in Cartesian coordinates: the axis-rotation
formula and some its applications to
computational chemistry

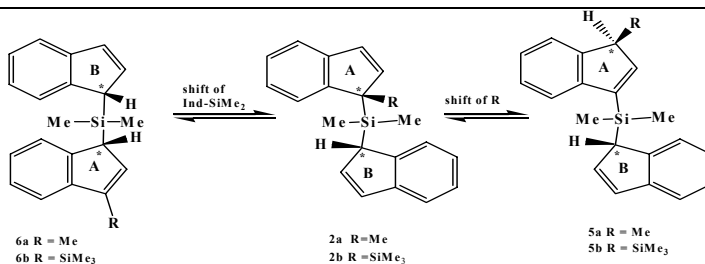
$$R_n^\varphi = \cos \varphi I + (1 - \cos \varphi) \hat{n}(\hat{n} \cdot I) + \sin \varphi \hat{n} \times I$$

Rev. Roum. Chim., 2007, 52(8-9), 795-808

Key words: axis-rotation formula; rigid-body system; axis-rotation operator;
symmetry operator.

Gabriela NEMEȘ,
Lumița SILAGHI-DUMITRSCU,
Ioan SILAGHI-DUMITRSCU, Jean
ESCUDE, Henri RANAIVONJATOVO and
Julio ZUKERMAN-SCHPECTOR

Silatropic migration in
 (1-trimethylsilylindenyl)(indenyl) dimethylsilane,
 bis(1-trimethylsilylindenyl)dimethylsilane and
 related compounds

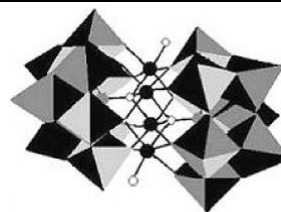


Key words: bis(indenyl)silane, silatropic migration, molecular structure, B3LYP/6-31G(d) DFT calculations, AM1 semiempirical calculations.

Rev. Roum. Chim., **2007**, 52(8-9), 809-816

Dan RUSU, Cora CRĂCIUN, Mariana RUSU,
Adrian PĂTRUȚ and Leontin DAVID

Complexes of the trilacunary Keggin
 arseno(V)polyoxotungstate with iron(III),
 cobalt(II) and nickel(II)

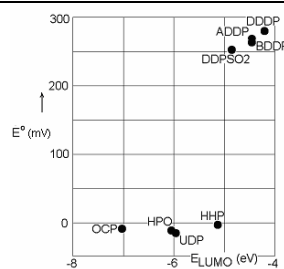


Key words: polyoxometalate, metal cluster, FT-IR spectroscopy, EPR spectroscopy, paramagnetism

Rev. Roum. Chim., **2007**, 52(8-9), 817-821

Ossi HOROVITZ, Delia GLIGOR and
Ionel Cătălin POPESCU

Correlations between electrochemical activity of
 phenothiazine derivatives modified graphite
 electrodes and some structural and molecular
 characteristics

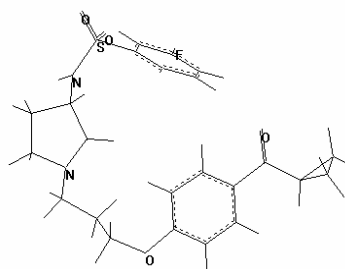


Key words: phenothiazine derivatives, modified electrodes, MO calculations.

Rev. Roum. Chim., **2007**, 52(8-9), 823-828

Maria MRACEC, Ana BOROTA,
Ramona RAD, Liliana OSTOPOVICI and
Mircea MRACEC

QSAR analysis of a series of non-imidazolic
 derivatives acting on the histamine H3 receptor

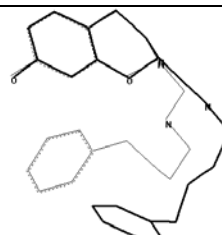


Key words: QSAR, MLR, AM1, H3 histamine receptor, disubstituted pyrrolidinic derivatives.

Rev. Roum. Chim., **2007**, 52(8-9), 829-835

Liliana OSTOPOVICI, Ramona RAD,
Ana BOROTA, Maria MRACEC and
Mircea MRACEC

Conformational analysis with AMBER and AM1
 methods of a partial agonist, (R)-2-[(4-phenyl-
 butylamino)-methyl]-chroman-7-ol active on the
 dopaminic D2 receptor

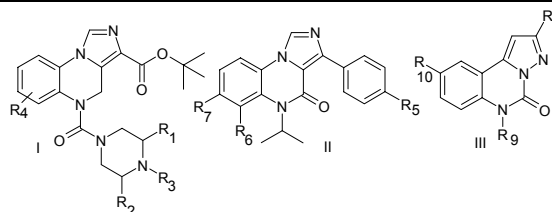


Rev. Roum. Chim., **2007**, 52(8-9), 837-844

Key words: conformational analysis, D2 receptor, AM1 rotation barrier.

**Ramona RAD, Maria MRACEC,
Liliana OSTOPOVICI, Ana BOROTA and
Mircea MRACEC**

QSAR study for a series of imidazo[1,5-*a*]-
quinoxaline and pyrazolo[1,5-*c*]quinazoline
derivatives acting on GABA_A/benzodiazepine
receptor

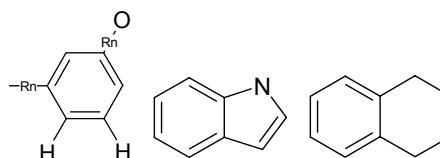


Rev. Roum. Chim., 2007, 52(8-9), 845-851

Key words: GABA_A/benzodiazepine receptor, quinoxaline and quinazoline
derivatives, MTD, MLR.

**Ramona RAD, Maria MRACEC,
Mircea MRACEC and Tudor OPREA**

The privilege structures hypothesis for G protein-
coupled receptors – some preliminary results

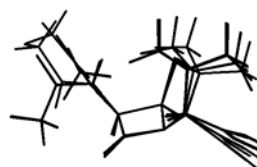


Rev. Roum. Chim., 2007, 52(8-9), 853-858

Key words: cheminformatics, drug design, database, GPCR, privileged
structures.

**Mihaela SCHULTZ, Maria MRACEC,
Eugen SISU and Mircea MRACEC**

AM1 conformational analysis of the (3*S*,5*R*,6*R*)-
6-acetylamidodopenicillanic acid

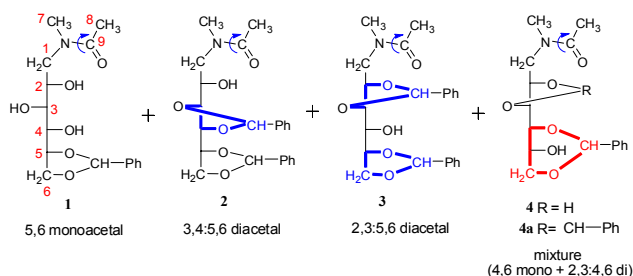


Rev. Roum. Chim., 2007, 52(8-9), 859-867

Key words: (3*S*,5*R*,6*R*)-6-acetylamidodopenicillanic acid, conformational
analysis, steric and electronic properties, AM1.

**Cristian NEANU, Anca LASCU, and
Carol CSUNDERLIK**

Synthesis of benzylidene acetals of *N*-acetyl-*N*-
methyl glucamine

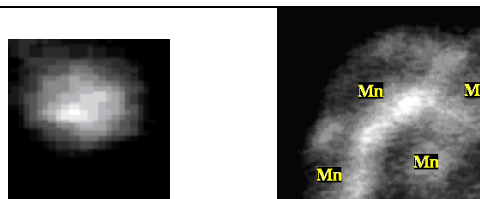


Rev. Roum. Chim., 2007, 52(8-9), 869-874

Key words: aminoalditols, pseudoceramides, flash chromatography,
glucosamine.

**Geta DAVID, Bogdan C. SIMIONESCU and
Cristofor I. SIMIONESCU**

Synthesis of polymer supported–transition metal
catalysts for olefin epoxidation

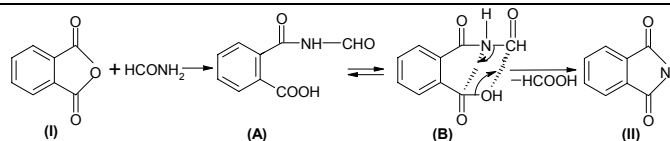


Rev. Roum. Chim., 2007, 52(8-9), 875-882

Key words: metal-polymer, polymer supported manganese catalyst,
molecular imprinting polymers

**Constantin I. CHIRIAC,
Marioara NECHIFOR and Fulga TANASĂ**

Formamide, a novel challenging reagent for the
direct synthesis of non-*N*-substituted cyclic
imides

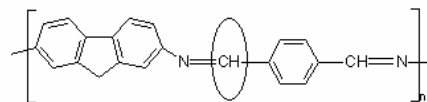


Rev. Roum. Chim., 2007, 52(8-9), 883-886

Key words: formamide, direct synthesis, cyclic imides

Aurica FARCAȘ and Valeria HARABAGIU

Synthesis and characterization of a new conjugated polyazomethine

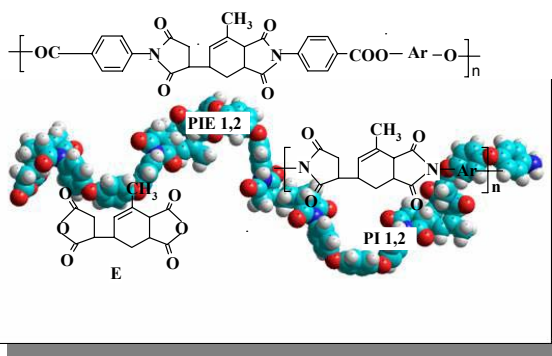


Rev. Roum. Chim., 2007, 52(8-9), 887-890

Key words: Schiff base, rotaxane architecture, supramolecular chemistry, β -cyclodextrin

Camelia HULUBEI, Elena HAMCIUC and Maria BRUMĂ

New imide type polymers based on Epiclon

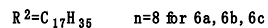
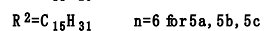
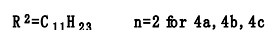
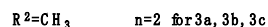
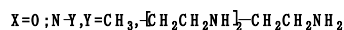
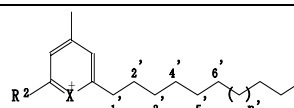


Rev. Roum. Chim., 2007, 52(8-9), 891-898

Key words: alicyclic dianhydride, epiclon, thermostable polymers, solubility.

Mariana Viorica BOGĂȚIAN, Mircea VÎNĂTORU, Gheorghe BOGĂȚIAN, Demetra NUȚĂ, Filip CHIRALEU, Valentin CĂMPEANU and Călin DELEANU

Pyrylium salts with long alkyl substituents and derived pyridinium salts having a terminal free amino group

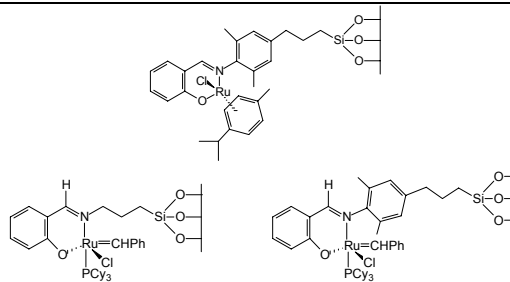


Rev. Roum. Chim., 2007, 52(8-9), 899-904

Key words: pyrylium perchlorates, pyridinium salts, CMC

Valerian DRĂGUȚAN and Francis VERPOORT

Immobilized ruthenium complexes bearing N,O-bidentate ligands

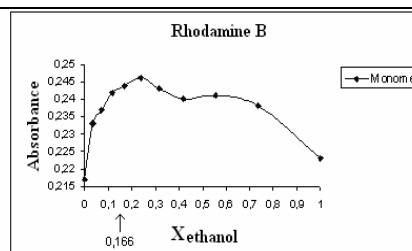


Key words: N,O-bidentate ligands, immobilized Ru complexes, Schiff-base, ring-closing metathesis, Kharasch addition, enol-ester, atom transfer radical polymerization.

Rev. Roum. Chim., 2007, 52(8-9), 905-915

Violeta PURCAR, Dan DONESCU, Marius GHIUREA, Cristina Lavinia NISTOR and Cristian PETCU

Silver nanodispersions in organic-inorganic filmogene hybrids



Rev. Roum. Chim., 2007, 52(8-9), 917-925

Key words: sol-gel process, cationic dyes, colloidal silver, hybrid materials, nanoparticles