

## ISSUE CONTENTS LIST WITH GRAPHICAL ABSTRACTS

### RESEARCH PAPER

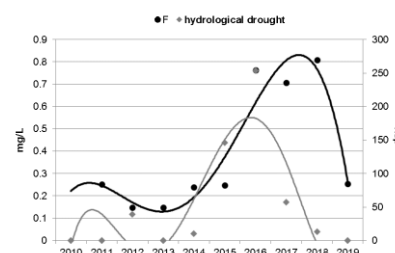
### ECOLOGICAL CHEMISTRY

7

#### FLUORIDE TRENDS IN THE DNIESTER RIVER AND DUBASARI RESERVOIR OVER 2011-2024 PERIOD

Nina Bagrin, Elena Zubcov, Lucia Biletschi, Natalia Borodin

Concentrations of fluoride ions in the Dniester river and Dubasari reservoir, located on the territory of the Republic of Moldova, were analysed for 2011–2024. They ranged 0.05–1.07 mg/L, with higher values during low-water periods. Despite seasonal sampling, no clear dynamics were observed, due to altered hydrological regime. Fluoride levels were lower than the World Health Organization for drinking water.



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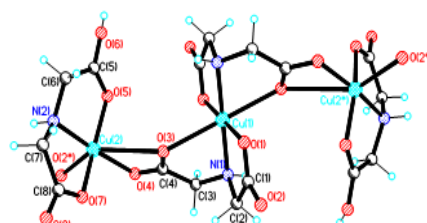
### INORGANIC AND COORDINATION CHEMISTRY

15

#### DESIGN, SYNTHESIS, AND STRUCTURAL STUDY OF MONO- AND POLYNUCLEAR Cu(II) IMINODIACETATE COMPLEXES

Dumitru Ureche, Pavlina Bourosh, Ion Bulhac

The synthesis of three structurally distinct copper(II) coordination compounds with iminodiacetic acid ( $H_2IDA$ ) as ligand was achieved by varying the reaction pH. Under neutral conditions (pH 6–6.5), compound **1** formed as a two-dimensional ionic coordination polymer,  $\{[NH_2(CH_3)_2]_2[Cu_3(IDA)_4] \cdot 1.75H_2O\}_n$ , consisting of layered  $[Cu_3(IDA)_4]^{2-}_n$  anions stabilized by hydrogen-bonding networks. Under basic conditions (pH 8–8.5), compound **2** was obtained as a neutral 2D molecular polymer,  $\{[Cu_3(IDA)_2(IDAH)_2] \cdot 5H_2O\}_n$ , built from trinuclear copper units bridged by bi- and monodeprotonated ligands. Under acidic conditions (pH 3), compound **3**,  $((CH_3)_2OH)_2[Cu(IDA)_2] \cdot [Cu(IDAH)_2]$ , was isolated as an ionic structure containing neutral and anionic mononuclear complexes charge-balanced by protonated dimethylether cations.



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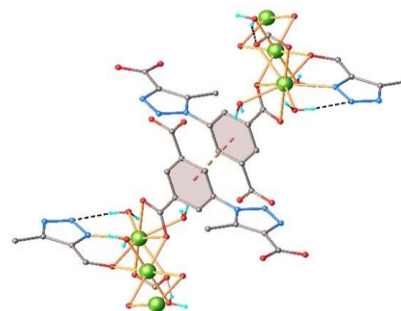
### INORGANIC AND COORDINATION CHEMISTRY

25

#### SOLVOTHERMAL SYNTHESIS, CRYSTAL STRUCTURE AND PHOTOLUMINESCENCE OF Cd(II) COORDINATION POLYMER DERIVED FROM A 1,2,3-TRIAZOLE-BASED TRICARBOXYLATE LIGAND

Viorina Gorinchoy, Sergiu Shova, Olga Kulikova, Gheorghe Roman, Vasile Lozan

A new cadmium(II) polymeric complex was synthesized under solvothermal conditions by the reaction of 5-(4-carboxy-5-methyl-1H-1,2,3-triazol-1-yl)isophthalic acid ( $H_3L$ ) with cadmium nitrate tetrahydrate in a mixture of *N,N*-dimethylacetamide and water. The polymeric complex is an infinite 2D coordination polymer with the general formula  $\{[Cd_3L_2(H_2O)_6] \cdot 2H_2O\}_n$ . The two-dimensional coordination polymer  $\{[Cd_3L_2(H_2O)_6]\}_n$  presents p–p stacking interactions between benzene rings of adjacent 2D coordination polymers, which contribute along with numerous O–H...O H-bonds to the assembly of a 3D supramolecular assembly. The intense photoluminescence emission of cadmium(II) complex is observed in the blue-violet region of the spectrum.



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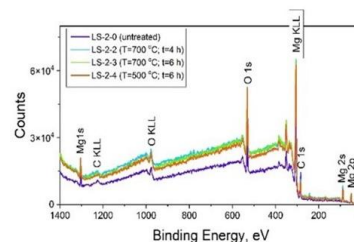
### INORGANIC AND COORDINATION CHEMISTRY

33

#### COMPARATIVE STUDY OF MgO NANOPARTICLES SYNTHESIZED IN THE PRESENCE OF SODIUM DODECYL SULPHATE AND ALOE VERA

Mariana Diru, Ion Lungu, Tamara Potlog

Two methods for synthesizing MgO nanoparticles using sodium lauryl sulphate and Aloe Vera extract as dispersing agents are described. Varying dispersing agent quantities and calcination temperatures were applied. The morphology and size were characterized using SEM-EDX and XRD, confirming successful synthesis and structure of the MgO nanoparticles.



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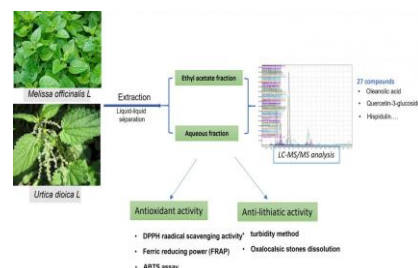
NATURAL PRODUCT CHEMISTRY AND SYNTHESIS

45

**CHEMICAL COMPOSITION AND BIOLOGICAL EVALUATION OF TRADITIONAL ALGERIAN PLANTS MELISSA OFFICINALIS L. AND URTICA DIOICA L.**

Dahia Meridja, Kamel Belhamel, Mohamed Harrat, Chiraz Belhamel, Mohamed Yousfi

*Melissa officinalis* L. and *Urtica dioica* L. were evaluated for their phytochemical composition and antioxidant and anti-lithiatic activities. LC-MS/MS analysis showed that *M. officinalis* contained a more diverse profile, especially flavonoids and phenolic acids enriched in the ethyl acetate fraction, while *U. dioica* demonstrated a simpler composition dominated by myricetin, riboflavin, sinapic acid, catechin, and  $\beta$ -carotene in its aqueous fraction. *M. officinalis* ethyl acetate extract showed the strongest antioxidant capacity in DPPH, ABTS, and FRAP assays. Its aqueous extract also exhibited notable anti-lithiatic activity, inhibiting calcium oxalate crystal formation by 87.12% at 2 mg/mL.



RESEARCH PAPER

NATURAL PRODUCT CHEMISTRY AND SYNTHESIS

56

**SPECTROCHEMICAL CHARACTERIZATION OF LIPID FRACTION IN SUNFLOWER POLLEN**

Maria Duca, Alexandru Ciocarlan, Ana Mutu, Steliana Clapco

Lipid fractions from *Helianthus annuus* L. pollen collected across three Moldovan agroclimatic zones were analyzed via GC-MS after Soxhlet extraction, saponification, and methylation. Chromatographic profiling resolved >40 constituents, including: Polyunsaturated fatty acid esters (e.g., methyl linolenate, a  $\omega$ -3 precursor); Diterpenoid derivatives (methyl labdatrien-19-oate); Oxygenated sterols (lanostan-3-one); Lipophilic vitamins ( $\alpha$ -tocopherol, retinol derivatives). Chemometric analysis revealed climate-induced shifts in metabolite profiles, with heat and drought favoring terpenoid accumulation. Results highlight sunflower pollen as a structurally rich source of bioactive lipids with nutraceutical potential.



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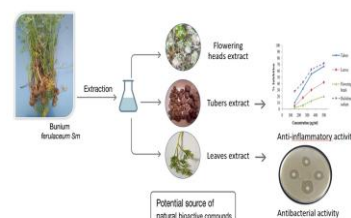
NATURAL PRODUCT CHEMISTRY AND SYNTHESIS

65

**PHYTOCHEMICAL ANALYSIS AND BIOACTIVITIES OF DIFFERENT ORGANS OF BUNUM FERULACEUM SM.**

Achraf Khaldi, Abdelkader Elhadj Berrezig, Amina Mazeri, Kheira Mehdi, Rahima Hadjer Gouabi

Hydro-methanolic extracts of *Bunium ferulaceum* leaves, flowering heads, and tubers show organ-dependent phytochemical variation. Leaves are richest in phenolics and flavonoids, while tubers contain the highest triterpene levels. Polyphenol content correlates strongly with antibacterial activity, whereas triterpenes are tightly linked to anti-inflammatory effects. These complementary chemical-biological relationships highlight the plant's multifunctional pharmacological potential, supporting further isolation and mechanistic studies.



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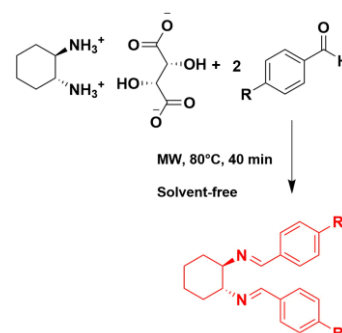
ORGANIC CHEMISTRY

72

**INFLUENCE OF AROMATIC SUBSTITUENTS ON THE SYNTHESIS OF SCHIFF BASES DERIVED FROM TRANS-(R,R)-DIAMINOCYCLOHEXANE: A SPECTROPHOTOMETRIC AND DFT B3LYP STUDY**

Lili Dahiana Becerra, Carlos Coy-Barrera, Diego Quiroga

In this work, the synthesis of Schiff bases derived from trans-(R,R)-diaminocyclohexane by microwave irradiation (MW) is presented. The reaction yields varied between 31% and 69%, being influenced by the electronic nature of the substituents (H, Cl, Br, NO<sub>2</sub>, MeO, t-BuO, BnO, and 4-(4-Me)PhO) and the reaction temperature. The spectrophotometric properties of the products were investigated by UV-Vis spectrophotometry, revealing bathochromic and hypso-chromic effects attributable to the different substituent groups. These effects were interpreted by DFT calculations with the B3LYP functional at the 6-311G(d,p) level. The results suggest that the electronic properties of the substituents in the para position have a significant impact on the spectroscopic characteristics of the Schiff bases.



RESEARCH PAPER

PHYSICAL CHEMISTRY AND CHEMICAL PHYSICS

84

**EMPLOYMENT OF IN SILICO IN PREDICTION OF FURAN DERIVATIVES AS EFFICIENT CORROSION INHIBITORS FOR MILD STEEL IN ACIDIC MEDIA**

Maimoonah Khalid Qasim, Rabah Ali Khalil

The contribution of in silico analysis in the development of corrosion inhibitors field by predicting adequate new molecules that could be employed for this purpose. QSAR analysis of already published experimental results of corrosion inhibition efficiency (IE%) of mild steel in acidic media for eighteen furan derivatives was performed.

No.	Name	Chemical Structure	IE% (a)	IE% (b)	IE% (c)	IE% (d)
1	2,5-bis(4-methylphenyl)furan		6.51	17	-0.020	94.47
2	2,5-bis(4-methylphenyl)furan		4.58	18	-0.045	93.75
3	2,5-bis(4-methylphenyl)furan		7.10	19	-0.010	95.00
4	2,5-bis(4-methylphenyl)furan		4.10	16	-0.040	94.00
5	2,5-bis(4-methylphenyl)furan		4.10	16	-0.040	94.00
6	2,5-bis(4-methylphenyl)furan		4.10	16	-0.040	94.00
7	2,5-bis(4-methylphenyl)furan		4.10	16	-0.040	94.00
8	2,5-bis(4-methylphenyl)furan		4.10	16	-0.040	94.00
9	2,5-bis(4-methylphenyl)furan		4.10	16	-0.040	94.00
10	2,5-bis(4-methylphenyl)furan		4.10	16	-0.040	94.00
11	2,5-bis(4-methylphenyl)furan		4.10	16	-0.040	94.00
12	2,5-bis(4-methylphenyl)furan		4.10	16	-0.040	94.00

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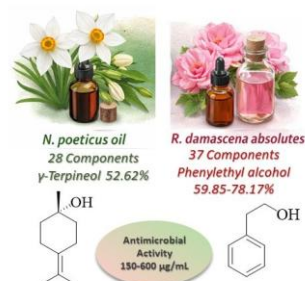
NATURAL PRODUCT CHEMISTRY AND SYNTHESIS

94

**CHEMICAL COMPOSITION AND ANTIMICROBIAL ACTIVITY OF ESSENTIAL OIL FROM NARCISSUS (NARCISSUS POETICUS L.) AND ABSOLUTE FROM FOUR ROSE (ROSA DAMASCENA MILL.) CULTIVARS**

Alexandru Ciocarlan, Ion Dragalin, Violeta Popescu, Lidia Lungu, Lucian Lupascu, Aculina Aricu, Tatiana Calugaru-Spataru, Zinaida Balmus, Dmitrii Grozdov, Pavel Nekhoroshkov, Inga Zinicovscaia

The chemical composition and antimicrobial activity of *Narcissus poeticus* L. essential oil and *Rosa damascena* Mill. absolutes of Moldovan origin were studied. Using GC-MS analysis 28 constituents of *N. poeticus* essential oil and 37 of *R. damascena* absolutes were identified. The  $\gamma$ -terpineol (52.62%) was the main component of *N. poeticus* oil, while the phenylethyl alcohol predominated in *R. damascena* absolutes (59.85–78.17%). Both products exhibited strong *in vitro* antibacterial and antifungal activity against four bacterial strains and two fungal species, with effective concentrations of 150–300  $\mu\text{g/mL}$  and 300–600  $\mu\text{g/mL}$ , respectively.



REVIEW

PHYSICAL CHEMISTRY AND CHEMICAL PHYSICS

101

**ELECTRONIC STRUCTURE AND PROPERTIES OF TRANSITION METAL COMPOUNDS. THEORY AND APPLICATIONS, THIRD EDITION BY ISAAC B. BERSUKER, YANG LIU**

Gheorghe Duca and Marius Andruh

The volume Electronic Structure and Properties of Transition Metal Compounds. Theory and Applications, now in its third edition, is one of the most comprehensive and modern works dedicated to the theory of the electronic structure of transition metal compounds. The lead author, Acad. Isaac B. Bersuker, renowned for his contributions to the theory of the Jahn–Teller effect and vibronics, collaborated in this edition with Dr. Yang Liu, a specialist from the Harbin Institute of Technology, China, thus adding an updated and international perspective to the field.

INSTRUCTIONS FOR AUTHORS