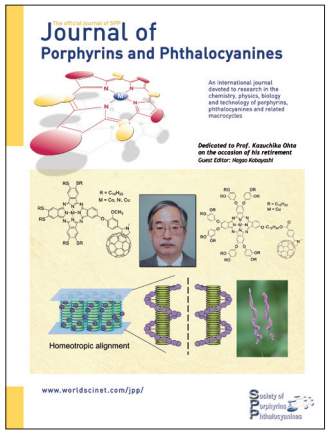
Journal of Porphyrins and Phthalocyanines
J. Porphyrins Phthalocyanines 2018; **22**: 1–290

CONTENTS

Journal of Porphyrins & Phthalocyanines
http://www.u-bourgogne.fr/jpp/

About the Cover



Guest Editor: Nagao Kobayashi

This issue of JPP is dedicated to P**rofessor Kazuchika Ohta** on the occasion of his retirement in the end of March 2018. It consists of 28 original research papers presented by his colleagues and friends. Professor Ohta is a very ingenious scientist. He developed a new field of metal-containing liquid crystals, namely metallomesogens in 1978. His continual creativity has brought about a number of phthalocyanine-based liquid crystals with original molecular and phase structures showing unique properties. The cover picture shows the spiranthes-like supramolecular structure of some selected phthalocyanine-fullerene dyads that were designed and characterized by Professor Ohta. From precise analysis of the SAXS and CD spectra, he established the helical structure of fullerenes in the Col_{ho} mesophase. Fullerenes pile up in left-handed and right-handed helicity in a ratio of 50:50. This helical structure resembles spiranthes flower. The helical stacking of C_{60} moieties is very favorable as an electron carrier path.

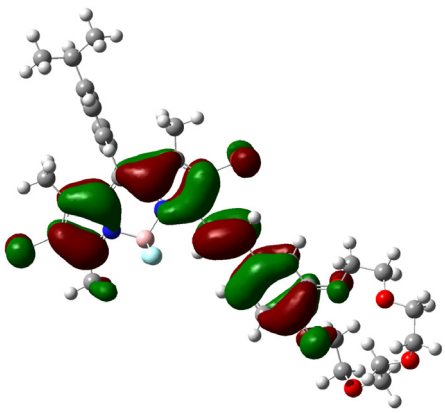
Articles

pp. 1–9

Photophysical properties of a novel styryl-BODIPY with a fused crown ether moiety

Justin Stone, John Mack*, Tebello Nyokong, Mutsumi Kimura and Nagao Kobayashi*

The synthesis and characterization of a crown-ether-substituted 3-styrylBODIPY dye with a 4-isopropylphenyl group at the *meso*-position is reported.

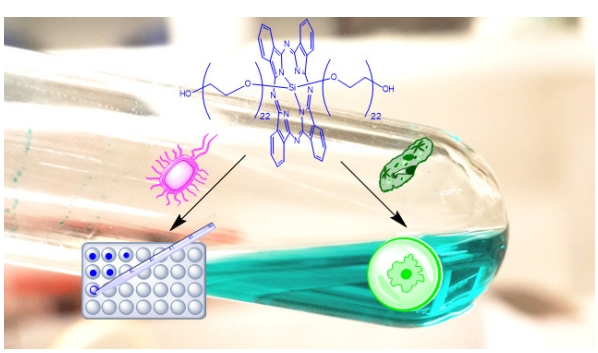


pp. 10–24

A novel of PEG-conjugated phthalocyanine and evaluation of its photocytotoxicity and antibacterial properties for photodynamic therapy

Canan Uslan, Naciye Durmuş İşleyen, Yetkin Öztürk, Burcu Turanlı Yıldız, Z. Petek Çakar, Meltem Göksel, Mahmut Durmuş, Yeşim Hepuzer Gürsel and B. Şebnem Sesalan*

A new PEG-conjugated silicon(IV) phthalocyanine axially substituted with poly(ethylene glycol) (PEG 1000) chains was synthesized and characterized. Its photophysical, photochemical properties and its photocytotoxicity were also investigated by applying it on HeLa and HuH-7 tumor cells. The antibacterial activity against Gram-negative (*Escherichia coli*) bacterium was also tested.

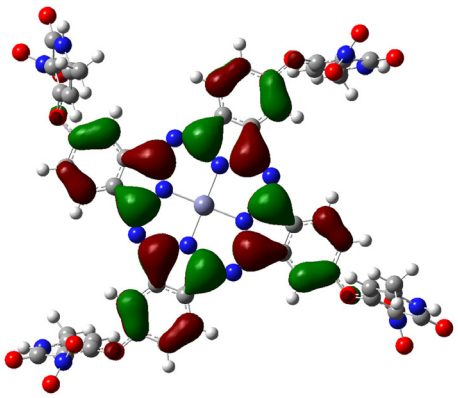


pp. 25–31

Pyridone substituted phthalocyanines: Photophysicochemical properties and TD-DFT calculations

Şaziye Abdurrahmanoğlu*, Mevlüde Canlıca, John Mack and Tebello Nyokong*

A 4-(6-methyl-3-nitro-2-oxo-1,2-dihydropyridin-4-yloxy)phthalonitrile has been used to prepare a novel Zn(II) phthalocyanine with four peripheral pyridone substituents and the photophysicochemical properties of the product were analyzed.

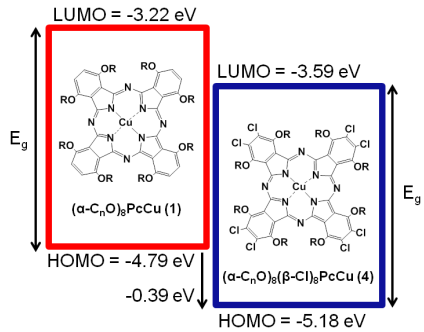


pp. 32–45

Discotic liquid crystals of transition metal complexes, 55: Novel chlorine-substituted phthalocyanine derivatives showing mesomorphism and low HOMO energy level

Masashi Yatabe, Akio Kajitani, Mikio Yasutake and Kazuchika Ohta*

Two series of PcCu compounds, $(\alpha\text{-}C_nO)_8$PcCu (**1a–1d**) and $(\alpha\text{-}C_nO)_8(\beta\text{-Cl})_8$PcCu (**4a–4d**) [$n$ = 6 (**a**), 8 (**b**), 10 (**c**) and 12 (**d**)], were successfully synthesized. Among them, the derivatives **4c–4d** exhibit a $Col_{ro}(P2m)$ mesophase. The derivatives **4a–4d** showed a Q band in the near-infrared region and lower HOMO levels than conventional PcCu derivatives.

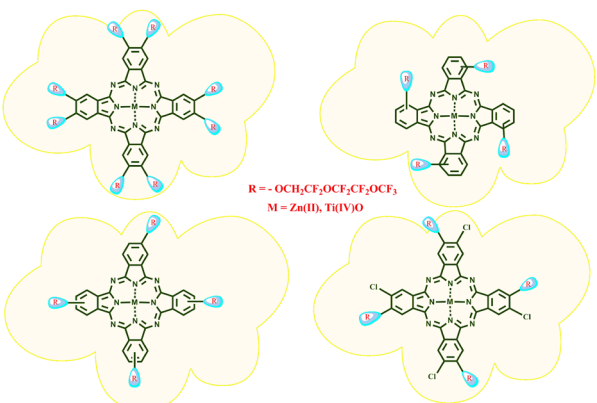


pp. 46–55

Photophysical and photochemical properties of fluoroether-substituted zinc(II) and titanium(IV) phthalocyanines

İlke Gürol*, Gülay Gümüş, Deniz Kutlu Tarakci, Ömer Güngör, Mahmut Durmuş and Vefa Ahsen

The synthesis and characterization of novel zinc(II) (**1a–4a**) and oxotitanium(IV) (**1b–4b**) phthalocyanine derivatives bearing 1H,1H-nonafluoro-3,6-dioxaheptan-1-ol groups were described for the first time. The influence of the number of the substituted groups (tetra or octa), position of the substituents (peripheral or non-peripheral) and the nature of the central metal atom (zinc or titanium) on the photophysical and photochemical properties of these phthalocyanines were investigated.

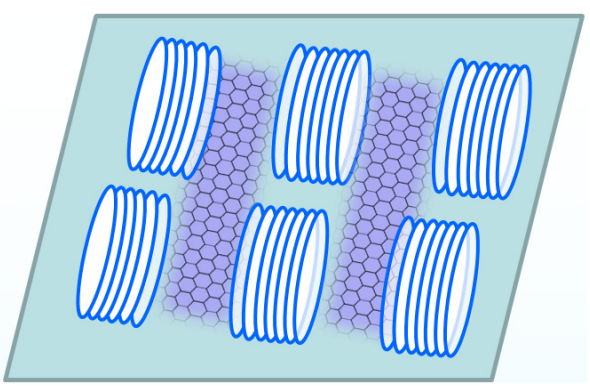


pp. 56–63

Pyrene containing liquid crystalline asymmetric phthalocyanines and their composite materials with single-walled carbon nanotubes

Esra Nur Kaya, Maxim S. Polyakov, Tamara V. Basova*, Mahmut Durmuş and Aseel Hassan

Liquid crystalline asymmetrically substituted phthalocyanines MPc (M=Cu, Co, 2H) bearing one pyrene and six polyoxy groups and their composite materials with single-walled carbon nanotubes was investigated. The incorporation of small amount of SWCNT (0.1–1 wt.%) does not alter the MPc mesophases significantly. The structural features and the sensor response of MPc/SWCNT composite thin films to ammonia vapor (10–50 ppm) was studied and compared with those of the films of pure MPc derivatives.

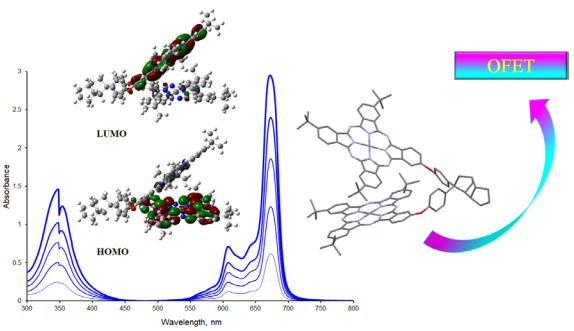


pp. 64–76

Structural, spectroscopic and passivation properties of a novel binuclear clamshell-type zinc(II) phthalocyanine as gate dielectric for OFET

Sebile Işık Büyükekşi, Ahmet Altındal, Nursel Açar and Abdurrahman Şengül*

A new clamshell-type binuclear zinc phthalocyanine (**2**) was synthesized and characterized by microanalysis, ^{1}H NMR, ^{13}C DEPT NMR, ^{1}H–^{1}H COSY NMR, HR MALDI TOF MS, UV-vis and fluorescence spectrophotometers. The electronic structure and the nature of the excited states in **2** were correlated with the results obtained by DFT and TDDFT calculations. The performance of **2** as gate dielectric in an organic field effect transistor was investigated and a field effect mobility value of 6.4×10^{-3} cm^2/V s was obtained.

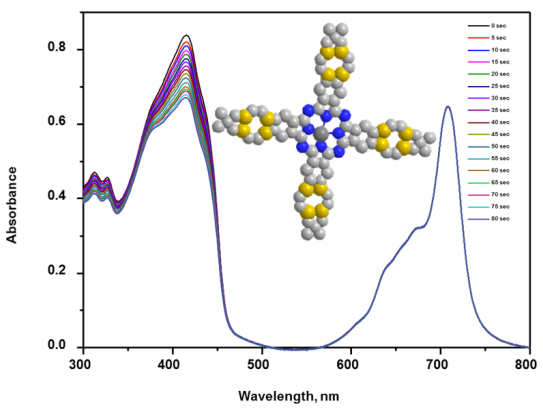


pp. 77–87

Synthesis, characterization, photophysicochemical properties and theoretical study of novel zinc phthalocyanine containing four tetrathia macrocycles

Mohamad Albakour, Gülenay Tunç, Büşra Akyol, Sinem Tuncel Kostakoğlu, Savaş Berber, Özer Bekaroğlu and Ayşe Gül Gürek*

In this study, Zn(II) phthalocyanine bearing 13-membered tetrathia macrocycles was synthesized; the photophysical, photochemical and electrochemical properties were investigated.

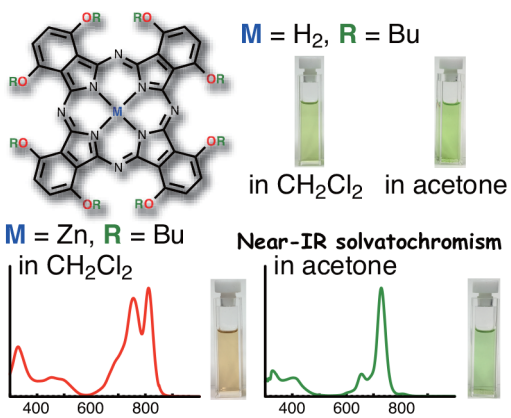


pp. 88–94

Changes of phthalocyanine visible color caused by near-IR solvatochromism

Taniyuki Furuyama*, Shiori Uchiyama, Takayuki Iwamoto, Hajime Maeda and Masahito Segi

We show that the Zn complex of 1,4,8,11,15,18,22,28-octakis(butoxy)phthalocyanine exhibits solvatochromism and characterize the corresponding visible color changes. Although the variation of the solvent-dependent position of the Q band is relatively small (~100 nm), the solution colors change from red to yellow and green depending on the composition of the solvent mixture. Substituents on oxygen atoms were shown to influence phthalocyanine aggregation and thus affect near-IR absorption, with the observed near-IR solvatochromism.

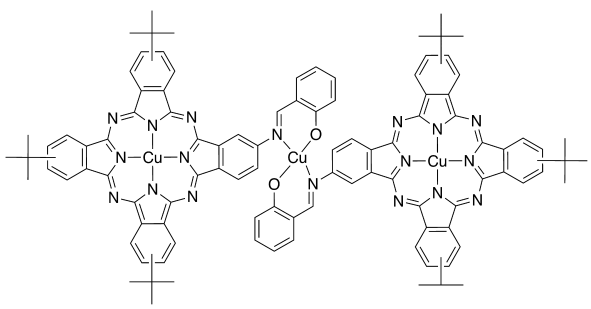


pp. 95–101

Synthesis and properties of a trinuclear copper(II) complex of a ligand with phthalocyanine and Schiff-base coordination sites

Makoto Handa*, Kenichi Kanagawa, Natsumi Yano, Haruki Yairi, Airi Okuno, Minoru Mitsumi and Yusuke Kataoka

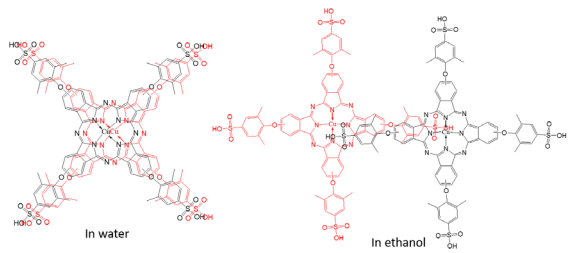
A trinuclear copper(II) phthalocyanine complex was synthesized by chelate coordination of the peripherally introduced Schiff-base nitrogen and phenoxide oxygen on the Cu(pc) core to a copper(II) ion. The magnetic, spectral and electrochemical properties were investigated for the trinuclear complex.



CONTENTS

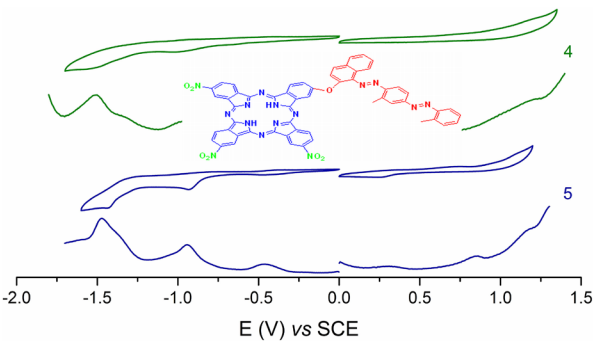
pp. 102–111
Solvent effects on molecular aggregation of highly water-soluble phthalocyanines
Hiroaki Isago* and Harumi Fujita

Solvent effects on molecular aggregation behaviors of highly water-soluble phthalocyanines have been investigated by concentration studies on optical absorption and magnetic circular dichroism spectra in water, ethanol, and their mixed solvent systems.



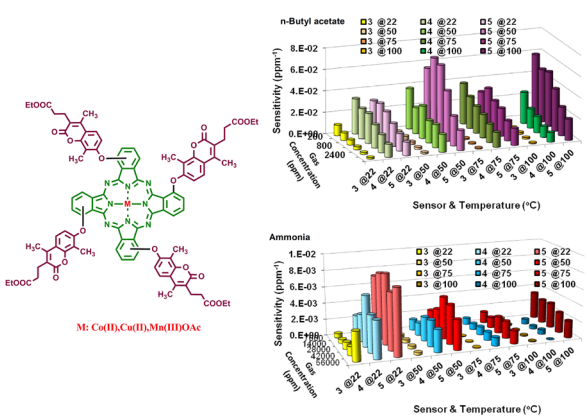
pp. 112–120
Synthesis, photophysical and electrochemical properties of novel unsymmetrical phthalocyanines with a Sudan IV moiety
İbrahim Özçeşmeci, Pınar Büyük, Ilgın Nar and Ahmet Gül*

The synthesis of novel, A_3B type unsymmetrical metal-free and metallo phthalocyanines bearing one aza dye group Sudan IV and three nitro terminal moieties was achieved by cyclotetramerization of novel 4-((1-((E)-(2-methyl-4-((E)-*o*-tolyldiazenyl)phenyl)diazenyl) naphthalen-2-yl)oxy)phthalonitrile and 4-nitrophthalonitrile. The aggregation properties of the compounds were investigated. General trends were also studied for fluorescence quantum yields and lifetimes of these phthalocyanine compounds. In-depth investigation of the electrochemical properties showed that nitro groups extended the reduction potentials.



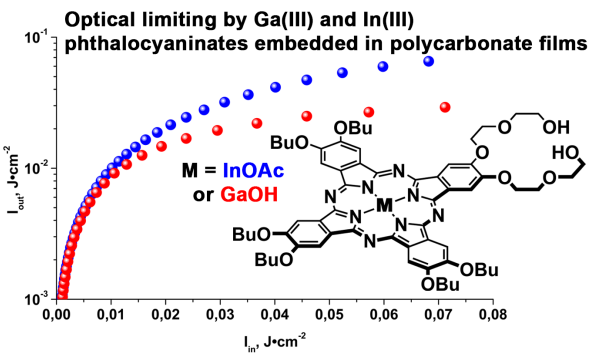
pp. 121–136
Electrical and gas sensing properties of novel cobalt(II), copper(II), manganese(III) phthalocyanines carrying ethyl 7-oxy-4,8-dimethylcoumarin-3-propanoate moieties
Baybars Köksoy, Meryem Aygün, Aylin Çapkin, Fatih Dumludağ* and Mustafa Bulut*

Co(II), Cu(II), Mn(III)OAc phthalocyanines bearing four ethyl 7-oxy-4,8-dimethylcoumarin-3-propanoate moieties were prepared and characterized. DC and AC (40–10^5 Hz) electrical properties of the films of metallophthalocyanines were investigated in the temperature range of 295–523 K. Impedance spectroscopy measurements revealed that bulk resistance decreases with increasing temperature indicating semiconductor property. Their gas sensing properties were also investigated for the vapors of VOCs, *n*-butyl acetate (200–3200 ppm) and ammonia (7000–56000 ppm) between temperatures 25–100 °C.



pp. 137–148
Photophysics and NLO properties of Ga(III) and In(III) phthalocyaninates bearing diethyleneglycol chains
Muthumuni Managa, Samson Khene, Jonathan Britton, Alexander G. Martynov, Yulia G. Gorbunova*, Aslan Yu. Tsivadze and Tebello Nyokong*

This paper reports the synthesis, photophysical and nonlinear optical properties of Ga(III) and In(III) complexes with low symmetry phthalocyanine bearing diethyleneglycol chains. The NLO parameters of In(III) complex exhibited the strongest nonlinear optical behavior in comparison with Ga(III) in solution and reverse tendency when embedded in poly(bisphenol A carbonate) thin films. DFT calculations were used to rationalize these results.

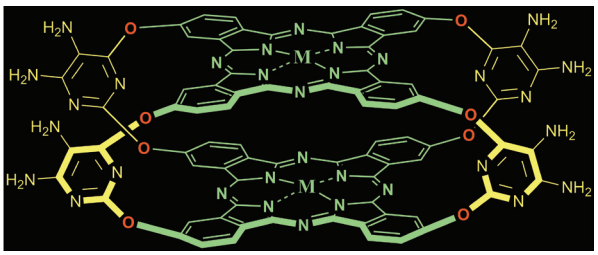


pp. 149–156

Synthesis, characterization and OFET property of four diaminouracil bridged novel ball-type phthalocyanines

Ayşegül Yazıcı, Ayşe Avcı, Ahmet Altındal, Bekir Salih and Özer Bekaroğlu*

OFET devices with top gate structure were fabricated using the new ball-type metallo bisphthalocyanines as the active material. The devices characterized by means of their output and transfer characteristics and it was found that OFET devices exhibit *p*-type behavior.

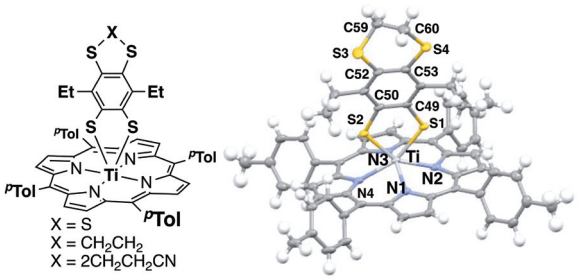


pp. 157–164

Preparation, structure, and electrochemistry of porphyrinato titanium (IV) benzenedithiolates with a trithiole ring, a dithiin ring, and two 2-cyanoethylthio groups

Takeshi Kimura*, Yusuke Muraoka, Kaori Amano, Toshiyuki Fujio, Takao Nishikawa, Tsukasa Nakahodo and Hisashi Fujihara

The reaction of tetra(*p*-tolyl)porphyrinato titanium (IV) oxide with dimercaptobenzo[1,2,3]trithiole, dimercaptobenzo[1,4]dithiin, and dimercapto-1,2-bis(2-cyanoethylthio)benzene produced the corresponding titanium (IV) complexes bearing a trithiole ring, a dithiin ring, and two 2-cyanoethylthio groups, respectively.

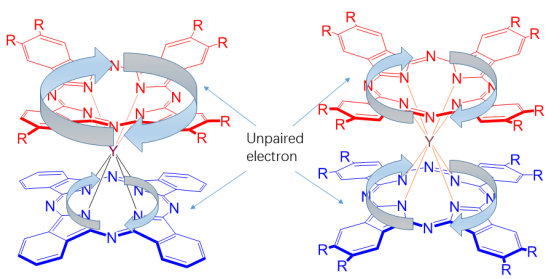


pp. 165–172

Distribution of the unpaired electron in neutral bis(phthalocyaninato) yttrium double-deckers: An experimental and theoretical combinative investigation

Xin Chen, Yuxiang Chen, Ming Bai*, Chiming Wang, Dongdong Qi*, Qingyun Liu, Meixing Xu and Jianzhuang Jiang

The distribution of the unpaired electron is affected by the peripheral substituents. The electron-donating substituents attract the unpaired electrons concentrated on the substituted side.

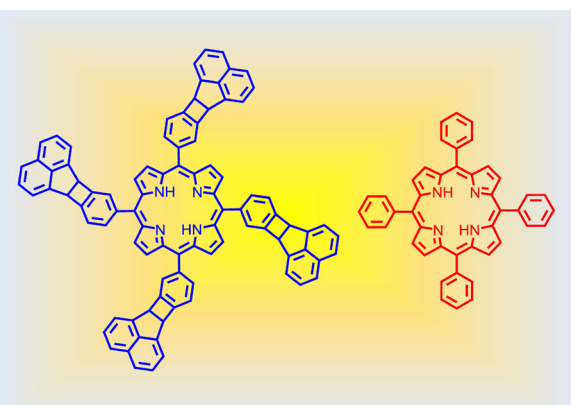


pp. 173–180

Synthesis and characterization of a new *meso*-tetra-di-hydrobenzocyclobutacenaphthylene free-base porphyrin

Ümit İşci, Sevinc Zehra Topal, Emel Önal, İsmail Fidan, Savaş Berber, Vefa Ahsen, Concepción Parejo, Ángela Sastre-Santos* and Fabienne Dumoulin*

A *meso*-tetra-6b,10b-dihydrobenzo[j]cyclobut[a]acenaphthylene-free base porphyrin was synthesized. It retains the same photophysical, photochemical and electrochemical properties than free base *meso*-tetraphenylporphyrin.



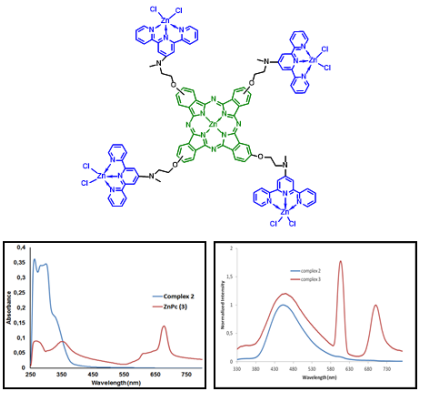
CONTENTS

pp. 181–188

Five-nuclear phthalocyanine complex bearing terpyridine zinc complex: Synthesis, and photophysicochemical studies

Pinar Sen*, S. Zeki Yildiz, Göknur Yasa Atmaca and Ali Erdoğmuş*

New terpyridine-Zn(II) complexes substituted Zinc-Pc was synthesized as new functionalized materials and characterized by using different spectroscopic methods such as FT-IR, UV-vis, and ^{1}H-NMR, ^{13}C-NMR, elemental analysis and mass. Spectral, photophysical (fluorescence quantum yields and lifetimes) and photochemical (singlet oxygen production and photodegradation under light irradiation) properties of newly synthesized phthalocyanine (**3**) as five nuclear phthalocyanine were investigated in DMSO solutions.

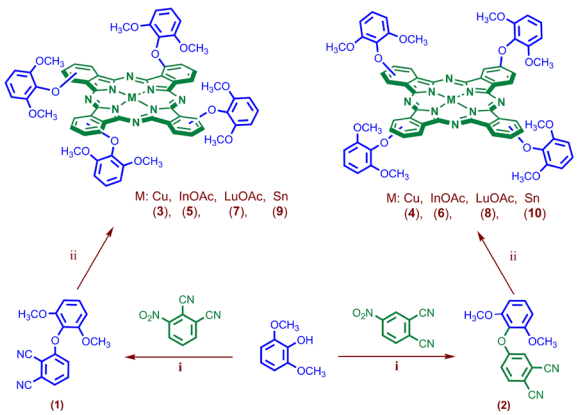


pp. 189–197

Toluene vapor sensing characteristics of novel copper(II), indium(III), mono-lutetium(III) and tin(IV) phthalocyanines substituted with 2,6-dimethoxyphenoxy bioactive moieties

Mehmet Pişkin, Nursel Can, Zafer Odabaş* and Ahmet Altındal*

The effects of the substituent's positions on the toluene vapor detection capabilities of copper(II), indium(OAc), mono-lutetium(OAc) and tin(IV) phthalocyanines substituted with 2,6-dimethoxyphenol bioactive groups were investigated. Adsorption data were analysed by using first order and Elovich equations in order to investigate the adsorption kinetics. It was found that the kinetics of the toluene adsorption strongly depends on the position of the substituent groups.

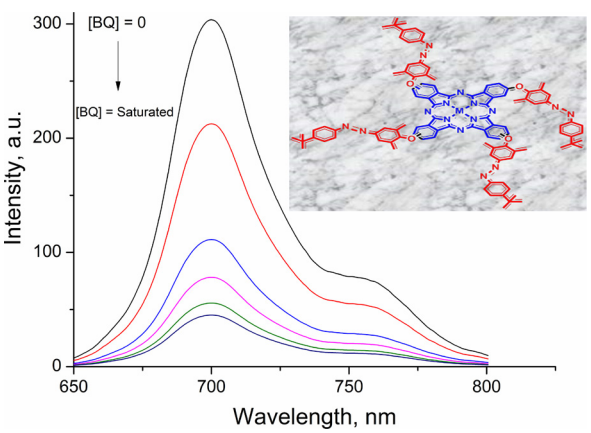


pp. 198–206

Novel phthalocyanines containing azo chromophores; synthesis, characterization, photophysical, and electrochemical properties

Ebru Özkan Garip, Mukaddes Özçeşmeci, Ilgın Nar, İbrahim Özçeşmeci and Esin Hamuryudan*

A series of novel metal-free and zinc (II), copper (II), cobalt (II), and manganese (III) phthalocyanine complexes bearing peripheral 2,6-dimethyl-4-(4-*tert*-butyl-phenylazo)phenoxy units have been synthesized. The structures of these new compounds were characterized by using elemental analyses, proton and carbon nuclear magnetic resonance, fourier transform infrared spectroscopy, ultraviolet–visible spectroscopy and mass spectrometry. The photophysical properties of metal-free and zinc(II) phthalocyanines were studied in tetrahydrofuran. The electrochemical properties of the phthalocyanine complexes were investigated by cyclic and square wave voltammetry.

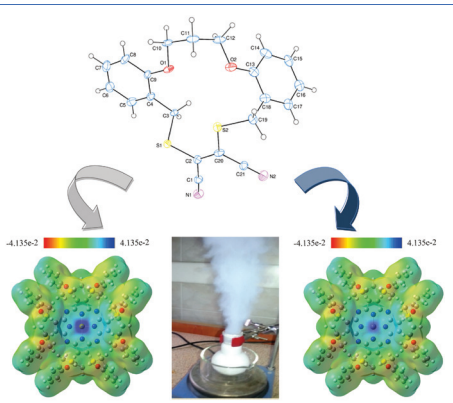


pp. 207–220

Synthesis, characterization and computational investigation of novel metalloporphyrazines containing 15-membered O_2S_2-donor macrocyclic moieties

Yasemin Baygu, Burak Yıldız, İzzet Kara, Hakan Dal and Yaşar Gök*

Synthesis, crystal structure and computational investigation of metalloporphyrazines containing 15-membered O_2S_2 macrocyclic moieties are presented.

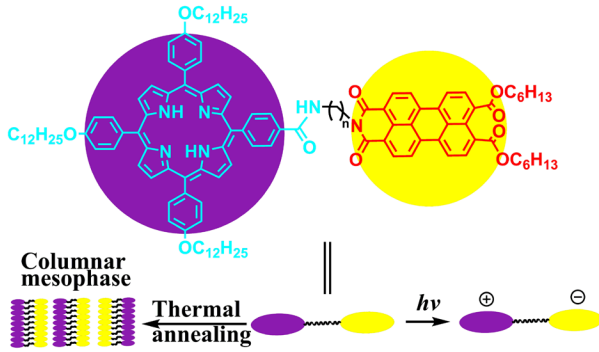


pp. 221–232

Mesogenic complementary absorbing dyads based on porphyrin and perylene units

Xiangfei Kong, Hongkang Gong, Shengping Dai, Wei Yao, Linping Mu*, Shufen Zhang and Guixia Wang*

Donor–accepter dyads consisting of a porphyrin unit, which is linked to a perylene unit by a flexible aliphatic bridge, have been synthesized and characterized. These dyads have broad optical absorption in the ultraviolet and visible regions. Due to photo-induced electronic transfer, the charge-separated states of the dyad molecules formed when photo-excited. In addition, they have columnar liquid-crystal phase and tend to form the face-on alignment on the glass substrates when cooled from the isotropic liquid.

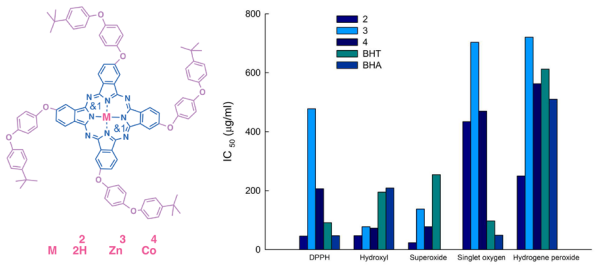


pp. 233–242

Antioxidant activities of the new tetrasubstituted metal-free, Zn(II) and Co(II) monophthalocyanines

Nazlı Söylemez, Ebru Yabaş*, Serap Şahin Bölükbaşı and Mustafa Sülü

New tetrasubstituted metal-free, zinc(II) and cobalt(II) phthalocyanines have been synthesized and characterized. Antioxidant activities and aggregation behaviors of these compounds have been investigated.

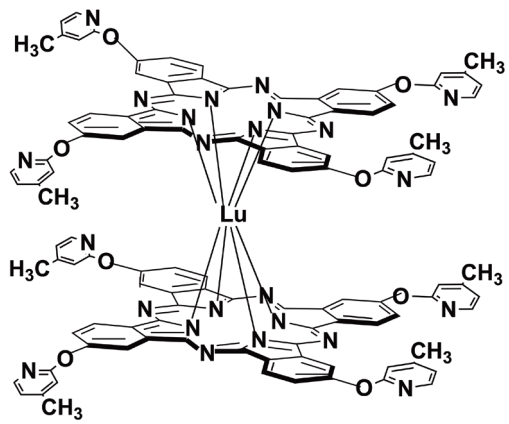


pp. 243–249

Synthesis, characterization and electrochemical properties of novel pyridine phthalocyanine derivatives

Büşra Mızrak, Efe Baturhan Orman, Şaziye Abdurrahmanoğlu* and Ali Rıza Özkaya*

In this study, the novel Zn(II), metal-free and sandwich-type Lu(Pc)2 phthalocyanines containing tetra pyridine substituted at peripheral position were synthesized. All the new compounds have been characterized by FT-IR and UV-vis spectroscopies, ^{1}H-NMR, MALDI-MS and elemental analysis. The electrochemical and spectroelectrochemical properties of all novel metallo and metal free phthalocyanine compounds were also investigated by voltammetric and *in situ* spectroelectrochemical measurements on Pt in dimethylsulfoxide/tetrabutylammonium perchlorate.

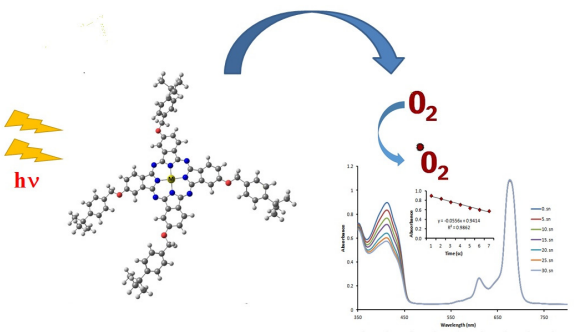


pp. 250–265

Synthesis, characterization of new phthalocyanines and investigation of photophysical, photochemical properties and theoretical studies

Ömer Tayfuroğlu, Fatma Aytan Kılıçarslan, Göknur Yasa Atmaca and Ali Erdoğmuş*

Phthalocyanine derivatives comprise the second generation of photosensitizer molecules employed in photodynamic therapy.

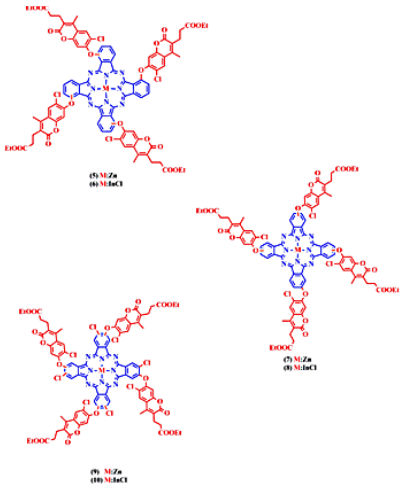


pp. 266–278

Zinc(II) and chloroindium(III) phthalocyanines bearing ethyl 7-oxy-6-chloro-4-methylcoumarin-3-propanoate groups: Synthesis, characterization and investigation of their photophysicochemical properties

Halid Kuruca, Baybars Köksoy, Begümhan Karapınar, Mahmut Durmuş and Mustafa Bulut*

The novel ethyl 7-oxy-6-chloro-4-methylcoumarin-3-propanoate substituted zinc(II) and cloroindium(III) phthalocyanines were synthesized and characterized by using different spectroscopic methods such as ^{1}H NMR, FT-IR, UV-vis, mass spectroscopy. The photophysical and photochemical properties as fluorescence lifetime, fluorescence, singlet oxygen and photodegredation quantum yields were investigated. The fluorescence quenching behavior of these phthalocyanines were also investigated using 1,4-benzoquinone as a quencher.



pp. 279–290

Novel peripherally and non-peripherally 6-oxyflavone substituted metal-free, zinc(II) and cobalt(II) phthalocyanines: Electrochemical and *in situ* spectroelectrochemical properties

Ahmet Arıbal, Efe Baturhan Orman, Ümit Salan*, Ali Rıza Özkaya* and Mustafa Bulut

Novel peripheral and non-peripheral tetra substituted 6-hydroxyflavonoxy zinc(II), cobalt(II) and metal free phthalocyanines were synthesized. Electron transfer properties of the compounds were investigated by voltammetric and *in situ* spectroelectrochemical measurements in nonaqueous solution medium.

