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#### **About the Cover**



The 11th International Conference on Porphyrins and Phthalocyanines (ICPP-11) 28 June–3 July, 2021 took the form of a virtual meeting arising from the twice postponed physical conference due to COVID-19 originally planned for Buffalo, New York, USA in June 2020.

The cover image is a montage of Zoom<sup>®</sup> video stills of consenting participants in order to create a partial group photo of the ICPP-11 virtual meeting.

A considerable and respectful 441 participants from 45 different countries contributed for a total of 476 abstracts, which warmed the heart, especially during these difficult times.

A very big thank you to you all for your patience and participation from all the editing team at the JPP Office and we look forward to seeing you all in Madrid 2022 for the reprise of the physical meeting.

#### **Review**

#### pp. 773–793

Pyrrole-based photosensitizers for photodynamic therapy — a Thomas Dougherty award paper

Gabriela I. Vargas-Zúñiga, Hyeong Seok Kim, Mingle Li, Jonathan L. Sessler\* and Jong Seung Kim

Photodynamic therapy (PDT) is a therapeutic modality that uses light to treat malignant or benign diseases. A photosensitizer, light, and oxygen are the three main components needed to generate a cytotoxic effect. Herein we review pyrrolebased photosensitizers that have been studied for possible use in PDT.



## **Articles**

#### pp. 794–799

Synthesis, photophysical properties and photodynamic antimicrobial activity of *meso* 5,10,15,20-tetra(pyren-1-yl)porphyrin and its indium(III) complex

Jackline Khisa, Solomon Derese, John Mack, Edith Amuhaya\* and Tebello Nyokong

5,10,15,20-tetra(pyren-1-yl)porphyrin ( $H_2$ TPyP) and its indium(III) complex (InCITPyP) were successfully synthesized and characterized. A Soret band of InCITPyP showed a 12 nm red shift when compared to  $H_2$ TPyP. The fluorescence quantum yield of InCITPyP was lower than that of  $H_2$ TPyP due to the heavy atom effect of In. InCITPyP showed better photoantimicrobial activity compared to the free-base  $H_2$ TPyP when tested against *Staphylococcus aureus*.



## CONTENTS

## pp. 800–817

Discotic liquid crystals of transition metal complexes 58<sup>†</sup>: Novel phthalocyanine-based mesogenic monomers and polymers exhibiting spontaneous homeotropic alignment and helical tetragonal columnar structure

Ayumi Suzuki-Ichihara, Makiko Sugibayashi-Kajita, Masahiro Ariyoshi, Mikio Yasutake and Kazuchika Ohta\*

Two novel series of phthalocyanine-based discotic liquid crystalline monomers (n, 12) PcCu(OCH<sub>3</sub>)(Acryloyl) (7: e (n = 10), f (n = 12), g (n = 14)) and (n, 12)PcCu(OCH<sub>3</sub>) (Norb) (9e, f, g) were synthesized. The monomers (9) were successfully polymerized by using a Grubbs catalysis to obtain poly-(n, 12)PcCu(OCH<sub>3</sub>)(Norb) (10e, f, g). The liquid crystalline properties of these derivitives were established by polarizing microscopic observations, DSC, and temperature-variable X-ray diffraction measurements. RO - S = RO - OR = R



# Synthesis and photolysis of new BODIPY derivatives with chelated boron centre

Sherif S. Ragab\*

Chelation of the boron centre of BODIPY with different catecholate and salicylate ligands was carried out. Compounds 2–7 were synthesized and their photophysical properties as well as the fluorescence quantum yields ( $\phi_r$ ) were determined. Surprisingly, chelators with electron withdrawing groups did not suppress the fluorescence. Ultraviolet illumination of BODIPYs 6, 7 in MeOH did not produce the fluorescent BODIPY 2, but instead, a decomposition of the photolysis product with concomitant decrease of fluorescence intensity was observed.





#### pp. 825–834

# Reaction, structure and spectroscopic properties of bis(cyano)cobalt(III) porphyrin complexes

Jianping Zhao, Mingrui He, Zhen Yao, Hongli Cao, Yiwen Yuan, Yongzhong Bian\* and Jianfeng Li\*

Two different mechanisms with(out) the addition of crown ether/cryptand are reported for the isolation of two six-coordinate low spin bis(cyano) [K(222)] [Co<sup>III</sup>(TPP)(CN)<sub>2</sub>] and [K(222)][Co<sup>III</sup>(TMP)(CN)<sub>2</sub>]. In the reaction without addition of crown ether/cryptand, a trace amount of (unstable) radical is generated, in contrast to the stable radical in the pathway mediated by crown ether/cryptand. Both radicals are produced by attack of cyanide to the Co<sup>II</sup> metal center, consistent with the strong  $\sigma$  donation of the cyanide ligand.

#### pp. 835–842

# Bioinformatic and chemoneurocytological analysis of the pharmacological properties of vitamin $B_{12}$ and some of its derivatives

Olga A. Gromova\*, Ivan Yu. Torshin, Larissa A. Maiorova\*, Oscar I. Koifman and Denis S. Salnikov

Chemoneurocytological analysis of compounds showed that cyanocobalamin (B12-1) and aquacobalamin (B12-2) may have the greatest neuroprotective effects. Increase in the concentration of the substances by 1 mmol/L causes the estimate of neuronal survival to increase by 25%. The neuroprotective effects for other substances were nearer 50%, and the survival rate of neurons did not significantly change with an increase in the concentrations of compounds.





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### pp. 843–857

Discotic liquid crystals of transition metal complexes  $59^{\dagger}$ : Parity effect of the number of *d*-electrons on the columnar mesomorphism and homeotropic alignment of 1,4-diazatriphenylenocyaninato metal(II) complexes

Masahiro Shichi, Mikio Yasutake and Kazuchika Ohta\*

20 super-discotic metallomesogens were synthesized based on a largely expanded  $\pi$ -conjugated macrocycle of 1,4-diazatriphenylenocyaninato metal(II) complex,  $(C_n O)_{16}$ TzM (M = Co, Ni, Cu, Zn;  $n = 8 \sim 16$ ). The Co(II)[ $d^7$ ] and Cu(II)[ $d^9$ ] complexes exhibit a Col<sub>tet</sub> mesophase accompanied by homeotropic alignment for  $n = 8 \sim 14$ , whereas the Ni(II)[ $d^8$ ] and Zn(II)[ $d^{10}$ ] derivatives do not. The parity effect originates from the number of d-electrons in the central metal ion.

#### pp. 858-865

#### (*H,H*)-Isomerism of *cis*- and *trans*-di[benzo]porphyrazines: Quantum chemical modeling within the framework of the DFT method

#### Oleg V. Mikhailov\* and Denis V. Chachkov

A quantum-chemical calculation of key structural parameters for molecular structures of (*H*,*H*)-isomeric (*NNNN*)-donoratomic macrocyclic tetradentate ligands, namely *cis*-di[benzo]porphyrazines (4 isomeric forms) and *trans*-di[benzo] porphyrazines (2 isomeric forms), was carried out using density functional theory (DFT) B3PW91/TZVP.

#### pp. 866-877

# A temperature switchable pyridyl-zinc(II) side arm porphyrin with functionality for surface immobilisation

Rhys B. Murphy and Martin R. Johnston\*

A side arm porphyrin appended with decyl chains undergoes reversible switching in solution, laying the foundation for surface mounted switchability.

#### pp. 878–884

#### Controlled synthesis of metal-organic frameworks with skeletal and pore-filling iron(III) porphyrins for electrochemical oxygen reduction

Yunlong Zhang, Hongsa Han, Jiaqi Qin, Na Zhang, Guanghui Zhang and Yujiang Song\*

Fe porphyrins have been employed to modify both the pores and the skeleton of metal-organic frameworks, which were further pyrolyzed to synthesize atomically dispersed Fe–N–C electrocatalysts with effective activity and durability toward oxygen reduction reaction. Furthermore, the Fe–N–C sites may exist in the configuration of distorted octahedral  $(O/N)_2$ –Fe<sup>III</sup>–N<sub>4</sub>.







