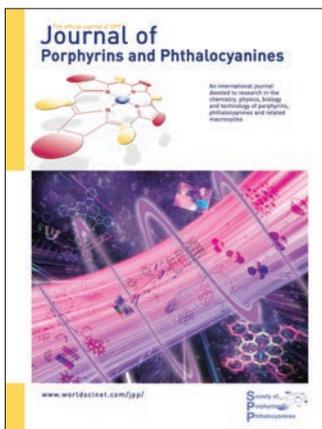


About the Cover



The cover shows a montage of the science presented in the current issue designed by Célia Maisières, on work experience at SPP/JPP Office in conjunction with her 2nd year BTS Support à l'Action Managériale course at Lycée Saint Bénigne in Dijon, France.

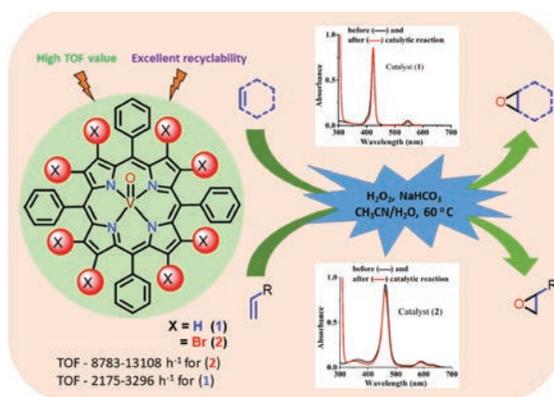
Articles

pp. 187–194

Selective epoxidation of olefins by vanadylporphyrin [V^{IV}O(TPP)] and electron deficient nonplanar β -octabromovanadylporphyrin [V^{IV}O(TPPBr₈)]

Mannar R. Maurya*, Ved Prakash and Muniappan Sankar*

Recyclable vanadyl porphyrins [V^{IV}O(TPP)] (1) and [V^{IV}O(TPPBr₈)] (2) have been utilized as efficient catalysts for the selective epoxidation of olefins. The electron deficient nonplanar porphyrin catalyst 2 exhibited a very high TOF (turnover frequency) as compared to compound 1.

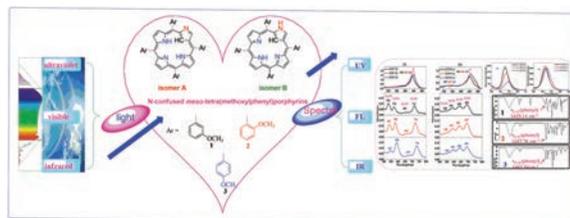


pp. 195–202

UV, FL and IR spectroscopic analysis of N-confused meso-tetra(methoxyphenyl)porphyrins

Su-Hong Peng*, Li-Li Wang, Sha-Sha Cai, Hui-Qing Xiao, Xin-Tong Zhao, Hui Wang and Hai-Yang Liu

UV, FL and IR spectra of isomer A in dichloromethane (DCM) and isomer B in dimethylacetamide (DMAc) of N-confused meso-tetra(*o*-,*m*- or *p*-methoxyphenyl) porphyrins **1**, **2** and **3** were investigated. Significant redshifts in UV-vis absorption and fluorescence spectra were observed from the *o*-isomer **1** to the *p*-isomer **3**. The absorption frequency of the in plane C=C phenyl stretching changed by conjugative and steric effects, respectively, when the methoxy group was in the *ortho* (**1**) or the *meta* (**2**) position in comparison with the *para* (**3**) position.

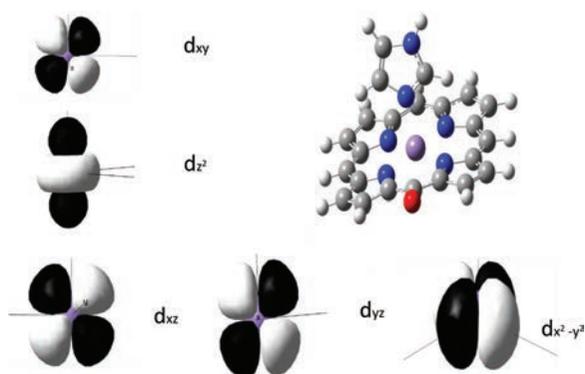


pp. 203–221

Theoretical investigation of five-coordinated manganese(III) oxophlorin with different axial ligands at various spin states using different DFT methods

Pezhman Mirmarghabi and Homayoon Bahrami*

Theoretical investigations of the geometry and electronic configuration of five-coordinated Mn^{III}oxophlorin with different axial ligand at various multiplicity spin states using the MO6-2X method indicate that the oxophlorin complexes with a quintet spin state are more stable than those in other spin states. This finding is due to correspondence between special degeneracy of the manganese d orbitals and what is expected for configuration of atoms in geometries of the aforementioned oxophlorin compounds, namely a pyramid-like structure with a square base.

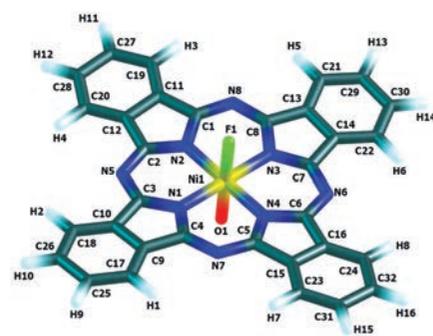


pp. 222–231

Nickel macrocyclic complexes with porphyrzine and some [benzo]substituted, oxo and fluoro ligands: DFT analysis

Denis V. Chachkov and Oleg V. Mikhailov*

By using DFT OPBE/TZVP and DFT B3PW91/TZVP methods, the principal possibility of the existence of three heteroligand Ni(V) complexes was shown, each of which contained in the inner coordination sphere porphyrzine or di[benzo]- and tetra[benzo]porphyrzine, oxygen (O²⁻) and fluorine (F⁻) ions.

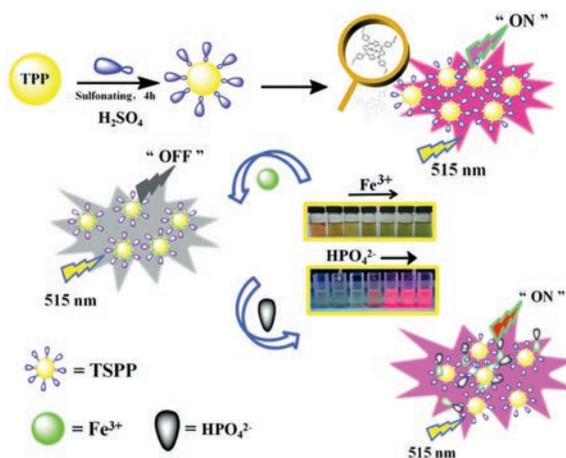


pp. 232–241

A novel fluorescent “on-off-on” sensor for monohydrogen phosphate based on the 5, 10, 15, 20-(4-sulphonatophenyl)porphyrin (TSPP) in nutrient solution and DFT calculation

Qin Ma, Baocheng Ran, Jiang Wu, Rong Zhang, Zechen Wei and Huan Wang*

A novel fluorescent “on-off-on” sensor for HPO₄²⁻ in the nutrient solution using the appealing fluorescence of TSPP with high efficiency and sensitivity is proposed. A switchable sensor based on TSPP was developed to determine HPO₄²⁻ via fluorescence quenching of TSPP solution by Fe³⁺ (off) and recovery by HPO₄²⁻ (on). With the addition of Fe³⁺, a very fast color change can be observed from light pink to green under daylight by the naked eye with a great decrease in the fluorescence intensity of TSPP. However, the fluorescence and the color is rapidly recovered by adding a certain amount of HPO₄²⁻ into the complex of TSPP-Fe³⁺. Based on the above phenomenon, a novel switch sensor for detection of HPO₄²⁻ has been developed.

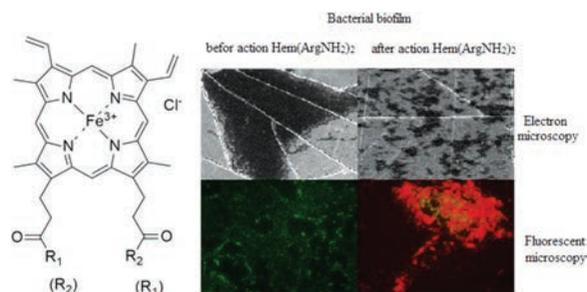


pp. 242–252

Improving the synthesis of hemin derivatives and their effect on bacterial biofilms

Sergey V. Blagodarov*, Galina A. Zheltukhina, Yuliya M. Romanova, Natalia V. Alekseeva, Lyudmila D. Iskhakova, Maria I. Semashko, Eteri R. Tolordava and Vladimir E. Nebolsin

This research was aimed at improving the synthesis of HDs (4) and (5) to increase their yield, simplify the process and minimize the side reactions, as well as to establish their antimicrobial and destructive effect on biofilms, including those consisting of antibiotic-resistant bacteria.

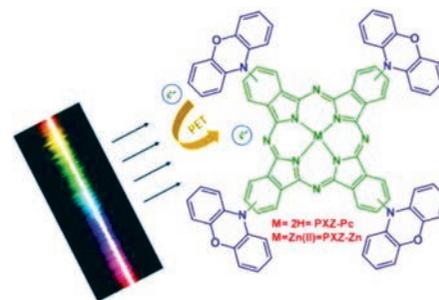


pp. 253–262

Photo-induced intramolecular electron transfer in phenoxazine-phthalocyanine donor-acceptor systems

K.S. Srivishnu, Madarapu Naresh, J. Laxmikanth Rao and Lingamallu Giribabu*

Donor-acceptor systems based on phenoxazine and phthalocyanine were designed and their excited state properties indicated photo-induced intramolecular electron transfer from the ground state of phenoxazine to the excited state of phthalocyanine.



pp. 263–272

Synthesis, redox properties, and catalytic hydrogen gas generation of porphycene cobalt complexes

Zihan Zhou, Taro Koide*, Yoshihito Shiota, Yoshio Yano, Ning Xu, Toshikazu Ono, Hisashi Shimakoshi, Kazunari Yoshizawa and Yoshio Hisaeda*

A new porphycene having four 3,5-di-*tert*-butylphenyl groups at the *meso*-positions and its cobalt complex were synthesized and characterized. The electrocatalytic hydrogen evolution reaction *via* the ligand-centered reduction of porphycene cobalt complexes was investigated. The reaction process was revealed by experimental results and theoretical calculations and was clearly different from the system *via* metal-centered reduction using porphyrin cobalt complex.

