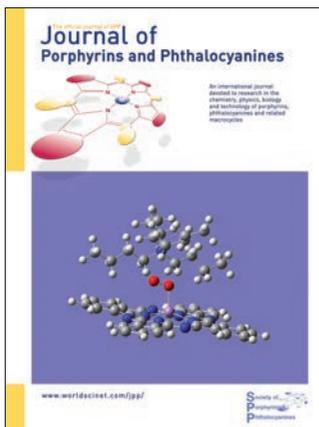


## About the Cover



The cover highlights the article :

### Phthalocyanine as catalyst for rechargeable lithium-oxygen batteries.

Padmakar Kichambare\*, Stanley Rodrigues, Kie Hankins, Perla B. Balbuena, William A. Feld and Lawrence Scanlon\*

Density functional theory was used to investigate the catalytic properties of tetrabutylammonium lithium phthalocyanine, that complexing with molecular oxygen is able to keep oxygen and the reaction intermediates in solution. In addition, the oxygen-oxygen bond elongates due to the weak electrostatic interaction between oxygen and the lithium-ion that helps in the oxygen reduction reaction.

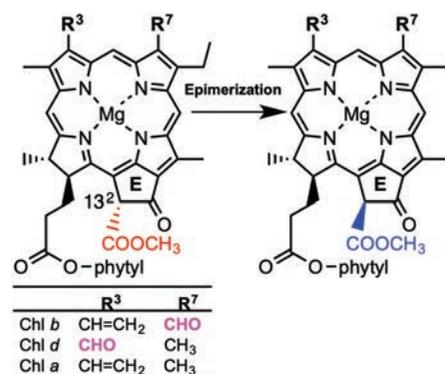
## Articles

### pp. 273–278

#### Effects of peripheral substituents on epimerization kinetics of formylated chlorophylls

Masayuki Tanaka, Aiko Tanaka and Yoshitaka Saga\*

Epimerization kinetics of chlorophyll (Chl) molecules possessing a formyl group, namely Chl *b* and Chl *d*, clearly indicated that the formyl group conjugated to the chlorin macrocycle accelerated the epimerization kinetics. The current analyses also indicated the importance of the combination effect of the substituents directly linked to the chlorin macrocycle for the epimerization of Chl molecules.

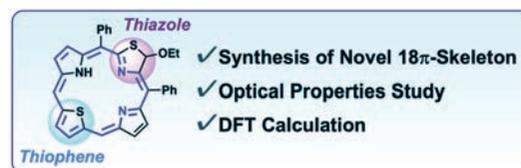


### pp. 279–285

#### First synthesis of a chlorin skeleton containing thiazole and thiophene rings and its optical properties

Takeo Nakano\* and Shigenori Fujikawa

A novel macrocyclic  $\pi$ -skeleton containing thiazole and thiophene rings was synthesized *via* MacDonald [3+1]-type condensation, and its optical properties were investigated. Two sulfur atoms at peripheral and internal positions were effective for the bathochromic shift of the ultraviolet–visible absorption bands in comparison with the traditional porphyrin and chlorin compounds. The characteristics of the absorption spectrum and the nucleus-independent chemical shift calculations show that the  $\pi$ -skeleton is of the chlorin-type compound.

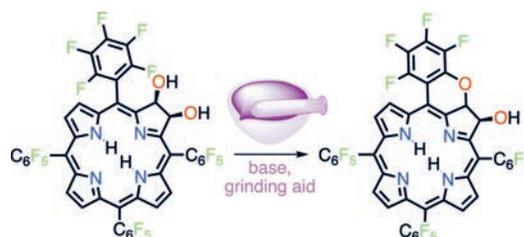


pp. 286–294

**Studies on the mechanochemically induced chromene-annulation of *meso*-tetrakis(pentafluorophenyl)-2,3-dihydroxychlorin: Non-innocence of the grinding aids**

Eric C. Mohan, Adewole O. Atoyebi and Christian Brückner\*

The translation of the solution phase, base-induced formation of a chromene-annulated chlorin from the corresponding *meso*-tetrakis(pentafluorophenyl)-2,3-dihydroxychlorin using a mechanochemical approach (ball milling) is possible, but fraught with unexpectedly large difficulties associated with the grinding aids used.

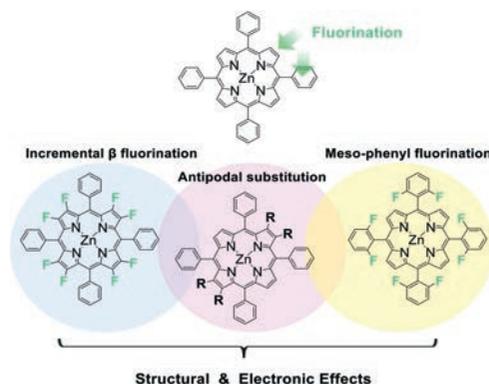


pp. 295–307

**Synthesis and study of fluorine-functionalized ZnTPPs**

Yang Zhang, Jonathan Viereck, Sylvie Rangan, Robert Bartynski and Elena Galoppini\*

Five ZnTPP derivatives, fluorinated either on the *meso* phenyl rings or in  $\beta$ -positions and reference compounds were synthesized and their electronic structure was studied experimentally and computationally to determine the steric and electronic effects of fluorine substitution.

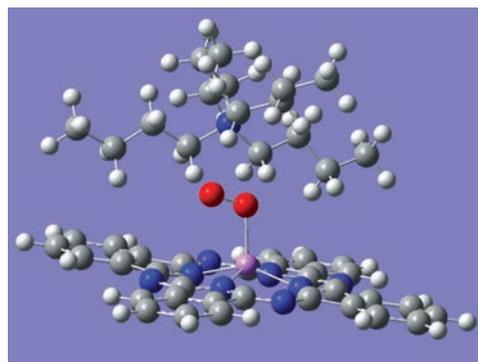


pp. 308–315

**Phthalocyanine as catalyst for rechargeable lithium-oxygen batteries**

Padmakar Kichambare\*, Stanley Rodrigues, Kie Hankins, Perla B. Balbuena, William A. Feld and Lawrence Scanlon\*

Tetrabutylammonium lithium phthalocyanine (TBA-LiPc) can function as a soluble catalyst in low-donor-number (DN) solvents such as tetraethylene glycol dimethyl ether (TEGDME) for rechargeable lithium-oxygen cells. Molecular oxygen forms a complex with the lithium phthalocyanine anion thereby keeping oxygen and the reaction intermediates in solution. Density functional theory (DFT) calculations show the mechanism for complex formation and cyclic voltammetry results show reaction intermediates are soluble in solution during oxygen reduction and oxygen evolution reactions.

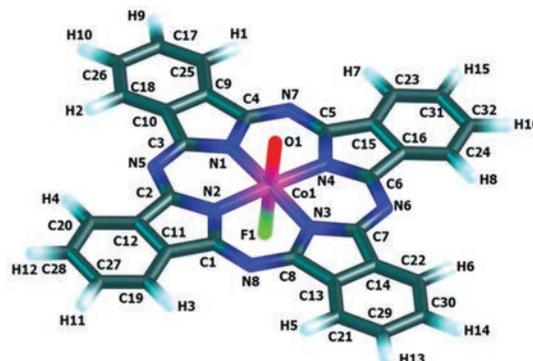


pp. 316–324

**New heteroligand complex of cobalt with phthalocyanine, oxo and fluoro ligands: DFT consideration**

Oleg V. Mikhailov\* and Denis V. Chachkov

The possibility of the existence of a cobalt heteroligand complex contained in the inner coordination sphere of a tetra[benzo]derivative of porphyrazine (phthalocyanine), oxide ( $O^{2-}$ ) and fluoride ( $F^-$ ) ions, with possible oxidation state of Co(V) that is non-characteristic for the given  $3d$ -element, has been shown by means of quantum chemical calculation using the DFT method in the OPBE/TZVP and B3PW91/TZVP levels.



## pp. 325–333

**Experimental analysis of excited state dynamics in Anderson-type POM@porphyrin hybrids in relevance to third-order nonlinear optical properties**

Sonia Rani, Rabbia Khan, Muhammad Tariq, Zahoor Ahmad, Hafiz M. Asif\* and Muhammad A. Khan\*

Di-Tris-NPor@Di-AndPOM-1 showed better nonlinear optics ( $\chi^3$ ,  $\chi$  and  $\beta$ ) than Di-TrisPor@Di-AndPOM-2 with excited state dynamics ( $\tau_1 = 3.86$  ns). Moreover, easy electron transfer was also observed in Di-Tris-NPor@Di-AndPOM-1 with a charge separated state of 0.88 eV.

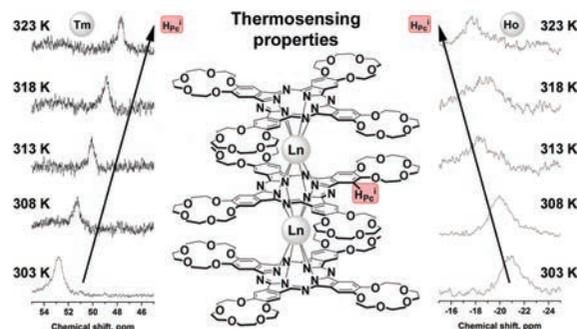


## pp. 334–339

**Nuclear magnetic resonance thermosensing properties of holmium(III) and thulium(III) tris(tetra-15-crown-5-phthalocyaninato) complexes**

Sergey P. Babailov, Marina A. Polovkova, Evgeny N. Zapolotsky, Gayane A. Kirakosyan, Alexander G. Martynov and Yulia G. Gorbunova\*

Temperature dependences of paramagnetic chemical shifts in NMR spectra of holmium(III) and thulium(III) trisphthalocyaninates were studied, revealing that these kinetically and thermodynamically stable complexes can be considered as promising designs of thermosensitive NMR probes for determination of the local temperature in nonpolar solutions.

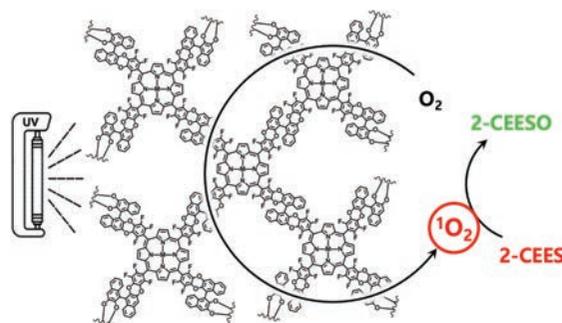


## pp. 340–347

**Use of porphyrin-containing polymers of intrinsic microporosity as selective photocatalysts for oxidative detoxification of chemical warfare agent simulant**

Hye Min Choi, Ye Ji Kim, E Tae Choi, Tai Yong Lee and Suk Joong Lee\*

Porphyrin-based polymers of intrinsic microporosity (PIMs) in photocatalytic degradation of a mustard-gas simulant (2-chloroethyl ethyl sulfide (2-CEES)) was demonstrated. Under blue-ultraviolet (UV) light-emitting diode (LED) irradiation, porphyrin-based PIMs **PP-H2** and **PP-Zn(II)** worked as effective heterogeneous photocatalysts for oxidation of 2-CEES.



## pp. 348–354

**Porphyrin-BODIPY light harvesting [3]rotaxane**

Maher Fathalla\*

A light harvesting [3]rotaxane comprising of a central Zn porphyrin and four boron dipyrin (BODIPY) moieties was constructed *via* the threading of alkyne substituted dibenzyl ammonium axle into dibenzo-24-crown-8 macrocycles of Zn-porphyrin followed by stoppering the resulting [3]pseudorotaxane with four azide functionalized BODIPY molecules *via* “click” reaction. Steady-state fluorescence studies demonstrated an efficient photoinduced energy transfer from BODIPY moieties to the central Zn porphyrin within [3]rotaxane.

