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CONTENTS

- 143 **Theoretical study of ^{11}B NMR chemical shifts of prototypical boranes: The case of *closo*- $[\text{B}_{12}\text{H}_{12}]^{2-}$, *nest*- $\text{B}_{11}\text{H}_{15}$, and *arachno*- $\text{B}_{10}\text{H}_{16}$**

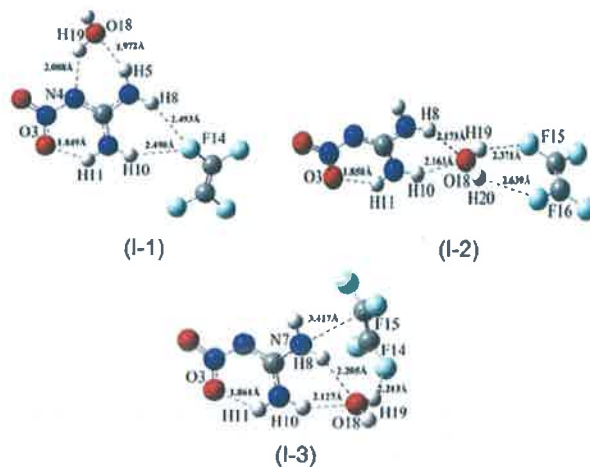
Structural and electronic dependence of ^{11}B chemical shifts are studied by DFT calculations for a series of borane structures, viz., *closo*- $[\text{B}_{12}\text{H}_{12}]^{2-}$, *nest*- $[\text{B}_{11}\text{H}_{15}]$, and *arachno*- $[\text{B}_{10}\text{H}_{16}]$. Three types of environments are identified for the borane systems, in increasing order of chemical shielding as: $\text{B-H} < \text{B-H-B} < \text{B-B-B}$. The obtained chemical shifts are in good agreement with the available experimental results and reflect the extent of heterogeneity of the electronic environments in terms of symmetry and the number of boron cores.



A Morales-Bayuelo, J M Catalán Lavín & R Ramírez-Tagle*

- 150 **Theoretical investigation into the cooperativity effect and thermodynamic property of β -nitroguanidine- $\text{C}_2\text{F}_4\cdots\text{H}_2\text{O}$ ternary complex**

The H-bonding cooperativity effects in $\beta\text{-NQ}\cdots\text{C}_2\text{F}_4\cdots\text{H}_2\text{O}$ ternary complex are investigated by the B3LYP and MP2(full) methods with 6-311++G(2df,2p) basis set. Thermodynamic cooperativity effects are evaluated at 298.15 K. The influence of the $\text{N-H}\cdots\text{O}$ or $\text{O-H}\cdots\text{F}$ H-bonding interaction on the $\text{N-H}\cdots\text{F}$ interaction is more pronounced than that of the latter on the former. Weak cooperativity effect appears in the linear complexes while notable anti-cooperativity effect is seen in the cyclic systems. Enthalpy change is the major factor driving the cooperativity. The complexation energies correlate well with the local minima of surface electrostatic potentials or internal charge separations.

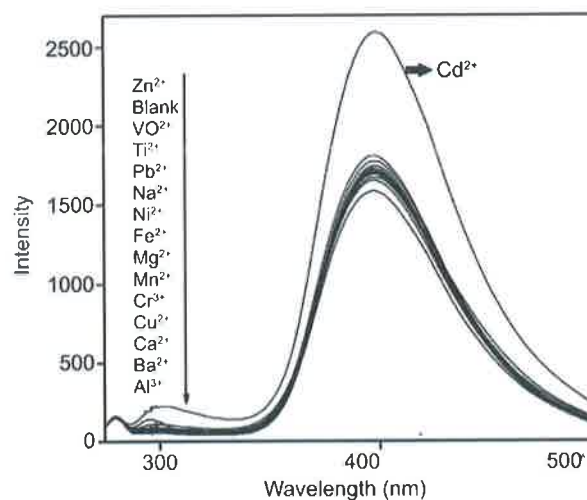


Bin Li*, Guang-ming Zhao & Xiao-juan Guo

Notes

163 Binding interaction of a piperazinylquinoline derivative with β -cyclodextrin and Cd^{2+} ions

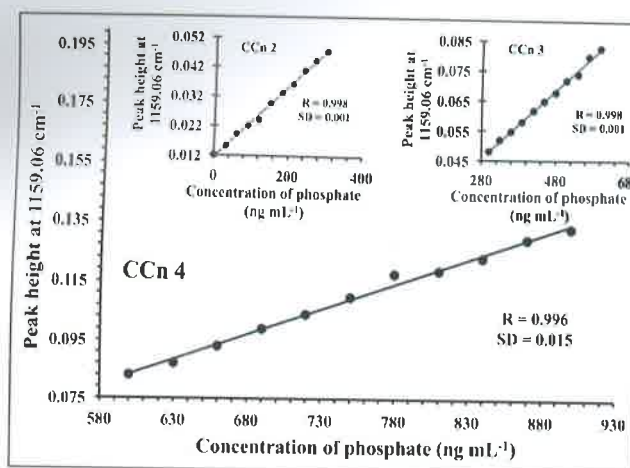
Cd^{2+} ion sensing by 3-methyl-2-(piperazin-1-yl)quinoline using fluorescence spectroscopy is reported. The host-guest complex formation of the quinoline-piperazine conjugate with β -cyclodextrin is studied using UV-visible absorption, fluorescence, and 2-dimensional ROESY spectroscopic methods. The 1:1 Cd^{2+} complexation of the quinoline-piperazine conjugate is achieved on encapsulation by β -cyclodextrin.



M Sumithra, G Tamil Selvan, S Suganthi,
P Mosae Selvakumar & Israel V M V Enoch*

168 Ion-pair single-drop microextraction with ATR-FTIR determination of phosphate in water samples

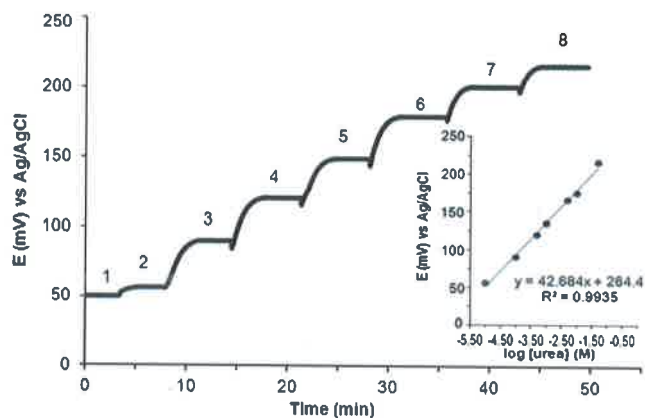
An ion-pair single-drop microextraction procedure followed by ATR-FTIR has been developed for analysis of phosphate in water samples. This method is based on the extraction of the phosphate-cetyltrimethylammonium bromide ion-pair by single-drop extraction procedure. The calibration plot for phosphate is linear over the range of 1–900 ng mL^{-1} ($r^2 = 0.998$). The limit of detection, limit of quantification, standard deviation and relative standard deviation of six replicate measurements are respectively 0.34 ng mL^{-1} , 1.12 ng mL^{-1} , 0.001 and 0.94–3.36%.



Swati Chandrawanshi, Santosh Kumar Verma &
Manas Kanti Deb*

175 Urease immobilized potentiometric biosensor for determination of urea

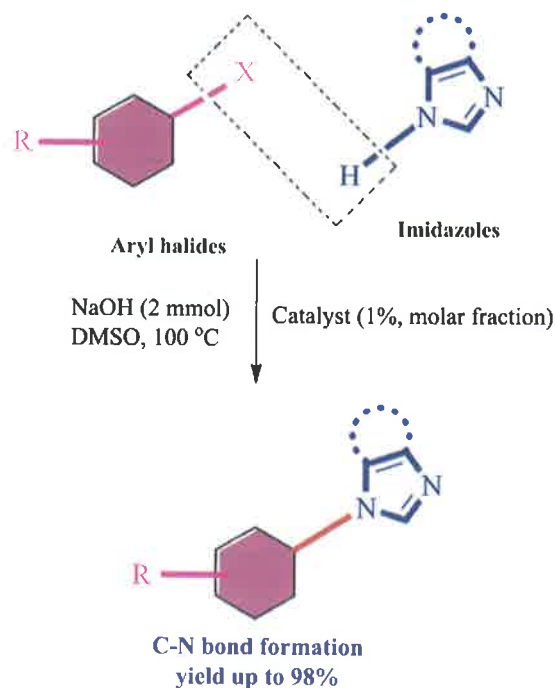
Potentiometric urea biosensor is constructed by immobilizing urease at tungsten electrode using polyvinyl alcohol matrix followed by sealing with plasticised polyvinyl chloride. The sensing device gives fast, linear and sensitive response to urea over 0.01–50 mM (slope 42.7 mV per decade urea, $r^2 = 0.993$), with detection limit of 0.01 mM urea.



Kawan Sihombing, Monica Chrisdayanti Tamba, Winry Sulistiani Marbun & Manihar Situmorang*

181 Functional 1,8-naphthyridine copper(I) complex as efficient catalyst for *n*-arylation of imidazoles coupling reactions

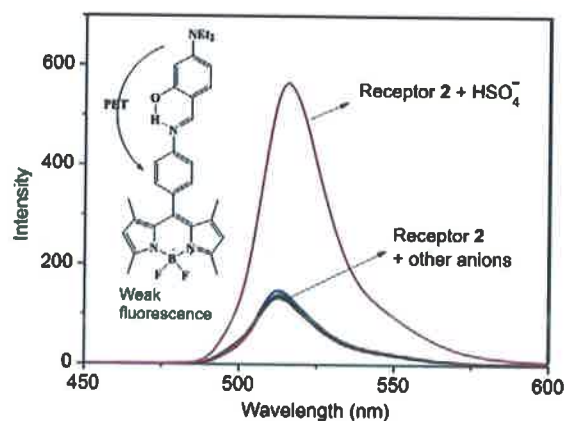
The functional 1,8-naphthyridine copper(I) complex catalyzes the cross-coupling reaction of aryl halides with imidazoles by C–N bond formation with a low catalyst loading (1%, molar fraction) and cheap base even under aerobic conditions. The procedure tolerates aryl halides with various functional groups (such as methyl, methoxy, acetyl, fluoro, nitrile and nitro groups) and gives the corresponding coupling products in moderate to high yields.



Gao-Zhang Gou*, Na Wu, Ju-Cheng Zhang, Ling Shi, Gui-Yang Liu, Wei Liu, Chao-Yong Mang & Shao-Ming Chi*

186 **BODIPY-based fluorescent sensors with tunable binding ability to fluoride and hydrogen sulfate anions**

The binding and sensing abilities of BODIPY based fluorescent sensors **1** and **2** towards various anions are studied by absorption, emission and ^1H NMR titrations spectroscopy. Sensor **1** shows selective response toward fluoride anions through hydrogen bonding interaction, while sensor **2** acts as a highly selective "Off-On" fluorescent sensor for hydrogen sulfate anion in DMSO solvent.



Qian Li*, Yehong Guo & Yuan Chen

193 **Guide to Authors**

Authors for correspondence are indicated by (*)

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