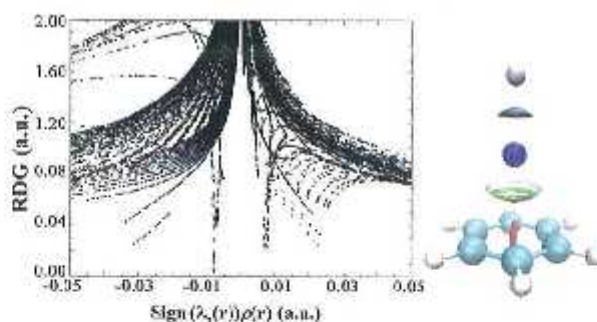


## CONTENTS

709 **Theoretical studies on the H-M $\cdots$  $\pi$  (M=H, Li, Na, K) interactions involving the  $\pi$ -electron donors C<sub>2</sub>H<sub>2</sub>, C<sub>2</sub>H<sub>4</sub> and C<sub>6</sub>H<sub>6</sub>**

There is no clear distinction in the bonding nature between the H-M $\cdots$  $\pi$  and M $\cdots$  $\pi$  interactions (except for the H-Li $\cdots$  $\pi$  and Li $\cdots$  $\pi$  interactions), although the former is stronger than the latter. A noticeable and unusual green RDG isosurface appears above the Li atom in the Li $\cdots$  $\pi$  complexes, like a "cap" on the Li atom.



Jiang-Bo Xie\*, Qiao-Ling Li, Wen-Jing Shi, Fu-de Ren & Hui Song

720 **Does the more notable cooperativity correspond to the higher stability? A comparative theoretical investigation on cooperativity effect upon addition of Na<sup>+</sup> and F<sup>-</sup> into N-(Hydroxymethyl)acetamide dimer**

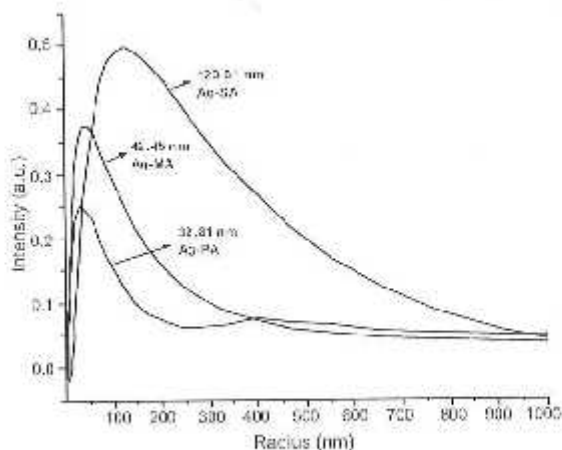
The cooperative structure is more stable than the anti-cooperative structure for the F<sup>-</sup> complex, while it is reverse for the Na<sup>+</sup> system. The thermodynamic cooperativity is not in agreement with the cooperativity effect evaluated by interaction energy.



Wan-li Jia, Wen-jing Shi\*, Fu-de Ren & Xiong Ding

- 734 **Functional modification of agarose: Synthesis of nanosize half-esters of succinic, phthalic and maleic acids**

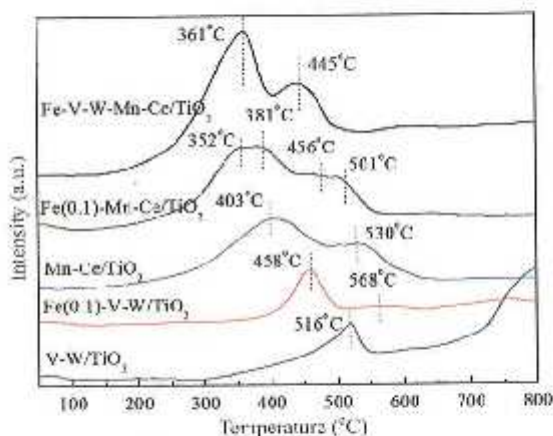
A facile synthetic method for preparing new half-esters of agarose with succinic, phthalic and maleic acids, wherein the acid moieties are attached to the backbone of the agarose, is described. Dynamic light scattering measurements show that nano-sized polymeric vesicles (32–124 nm) are formed in aqueous solution. Ag-SA, Ag-PA and Ag-MA derivatives varying molar ratios of Ag/SA, Ag/PA and Ag/MA (1:1–1:5) show the highest degrees of substitution to be 0.89, 0.69 and 0.39 for Ag-SA (1:4), Ag-PA (1:3) and Ag-MA (1:2) respectively. Aqueous solutions of sodium salts of these esters exhibit enhanced electrical conductivity (ca. 17.5 mS/cm at 40 °C) as compared to those of the parent half-esters (ca. 0.3 mS/cm at 40 °C).



S Kondaveeti, N A Chudasama, J P Chaudhary, R Meena & A K Siddhanta\*

- 744 **FeOx-VOx-WOx-MnOx-CeOx/TiO<sub>2</sub> as a catalyst for selective catalytic reduction of NO<sub>x</sub> with NH<sub>3</sub> and the role of iron**

FeOx-VOx-WOx-MnOx-CeOx/TiO<sub>2</sub> catalyst prepared by ultrasound-substep-wet impregnation method for removing NO<sub>x</sub> from diesel engine exhausts demonstrates excellent low-temperature selective catalytic reduction activity over a broad temperature window of 150–300 °C. Results show that the excellent activity is due to the well-dispersed active components, the moderate ratio of V<sup>4+</sup>/V<sup>5+</sup> and (Mn<sup>3+</sup>+Mn<sup>2+</sup>)/Mn<sup>2+</sup>, the excellent redox property and the abundant acid sites. Iron plays the important role of inhibiting the agglomeration of metal oxide during the catalyst sintering and converting V and Mn to their higher oxidation states.

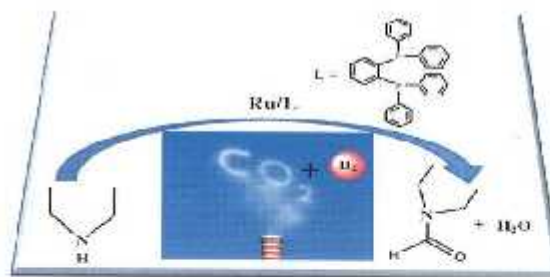


Su Yu\*, Dong Guojun\*, Zhao Yuan, Zhang Yufeng & Wang Yajie

## Notes

752. Ru catalyzed formylation of diethylamine with CO<sub>2</sub> and H<sub>2</sub> under moderate pressure condition

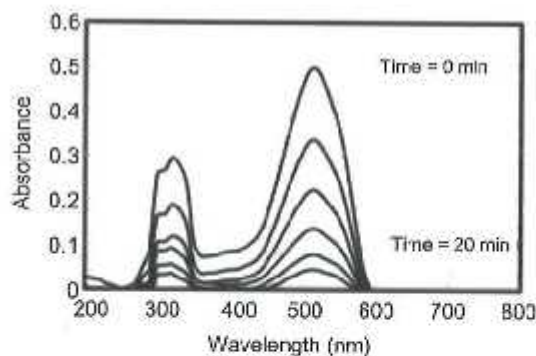
Ru catalyzed formylation of diethylamine (bulky secondary amine) with CO<sub>2</sub> and H<sub>2</sub> is investigated using a series of phosphine ligands. The Ru catalyst with the ligand, 1,2-bis(diphenylphosphino)benzene exhibits the highest catalyst performance (TON up to 2475). The high conversion (99%) and high selectivity to the corresponding formamide (up to 90-98%) is achieved at 150 °C and moderate pressure conditions.



Aasif A Dabbawala, Sudheesh N & Hari C Bajaj\*

757. Degradation of Acid Red 14 in contaminated water by Ag-SiO<sub>2</sub> nanocomposite

Silica aerogel doped with 12 wt% Ag, prepared by the alkoxide sol-gel method with tetraethyl orthosilicate as precursor, has been tested for degradation of Acid Red 14. Complete oxidation of the dye is achieved within 30 min under the optimum conditions.



Shahla Masoudian\*, Mohammad Hossein Rasoulifard  
& Parvaneh Pakravan

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