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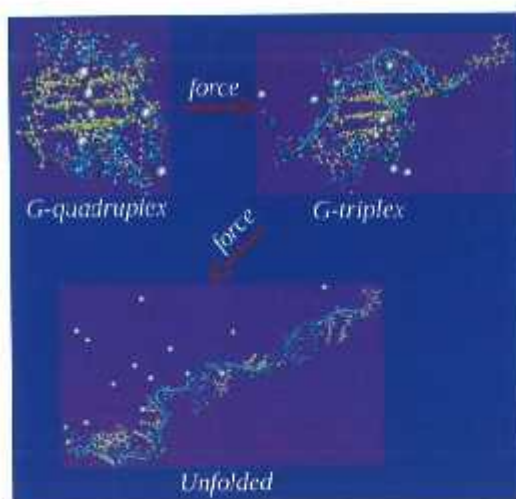
NUMBER 9

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CONTENTS

- 907 **Understanding the unfolding mechanism of human telomeric G-quadruplex using steered molecular dynamics simulation**

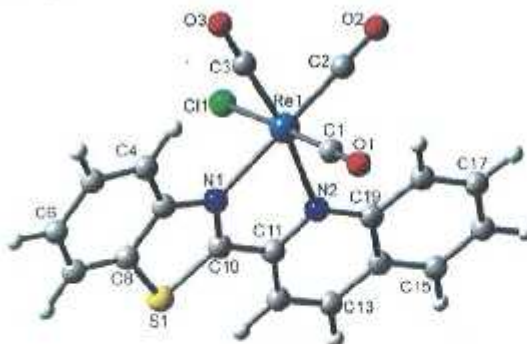
The unfolding pathway of human telomeric G-quadruplex with three G-tetrads in presence of K^+ and Na^+ ions separately, using steered molecular dynamics simulation is reported. The unfolding occurs via G-triplex intermediates, independent of the presence of cations.



Pralok K Samanta & Swapan K Pati*

- 913 **Rhenium(I) complex with 2-(benzothiazol-2-yl)quinoline: Synthesis, characterization, spectral properties and DFT/TDDFT investigations**

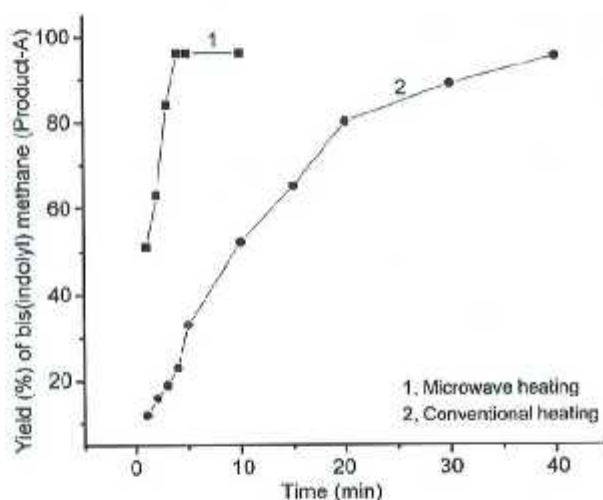
The red colored mononuclear Re(I) complex having *fac*-[Re(CO)₃]⁺ moiety, viz., [Re(CO)₃(N⁺NCl)], is synthesized in excellent yield by reacting [Re(CO)₅Cl] with 2-(benzothiazol-2-yl)quinoline (1:1) in boiling mixture of methanol+chloroform (3:1, v/v) under argon atmosphere. DFT and TDDFT studies reveal the nature of excitations. The lowest lying triplet excited state is associated with the ³MLCT/³ILCT excited state. The emission-like transition is consistent with the strong ³MLCT/³ILCT character.



Rupa Sarkar, Debopam Sinha, Amit Maity & Kajal Krishna Rajak*

925 **Facile synthesis of bis(Indolyl)methanes over cordierite honeycomb coated with modified forms of zirconia under microwave irradiation condition**

Microwave assisted synthesis of bi(indolyl)methane over honeycomb coated with zirconia based solid acid catalysts is reported. Up to 98% yield of bis(indolyl)methane is obtained in a very short reaction time of 4 min. under microwave irradiation. The honeycomb monoliths coated with modified forms of zirconia as catalytic materials are reusable for at least six reaction cycles.

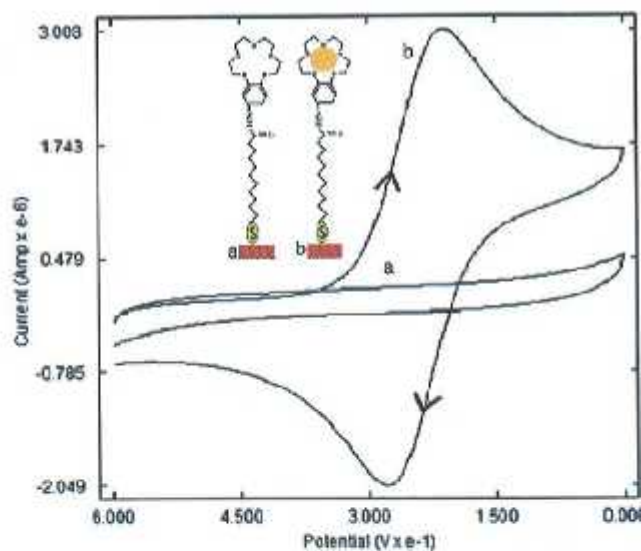


V T Vasantha, S Z Mohamed Shamsuddin*,
Joyce Queeny D'Souza, K Shyamprasad,
S R Pratap & Venkatesh

Notes

934 **Functionalized surface for electrochemical sensing of electrochemically inactive alkali metal ion**

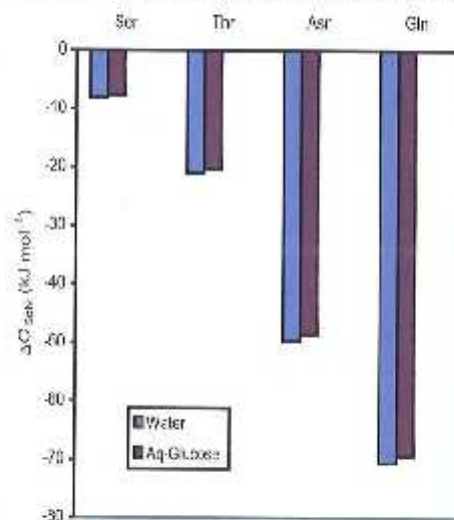
The recognition properties of 4-aminobenzo-15-crown-5 bound to a self-assembled monolayer on the gold surface is found to be selective for Na⁺ ion over Li⁺ and K⁺ ions. The binding of the analyte metal ion to the ionophore has been monitored by cyclic voltammetry using redox couple Fe(CN)₆^{3-/4-} as mediator redox probe.



Urvasini Singh & Sunita Kumbhat*

- 939 **Theoretical study of molecular interactions of amino acids in aqueous carbohydrate solutions by scaled particle theory**

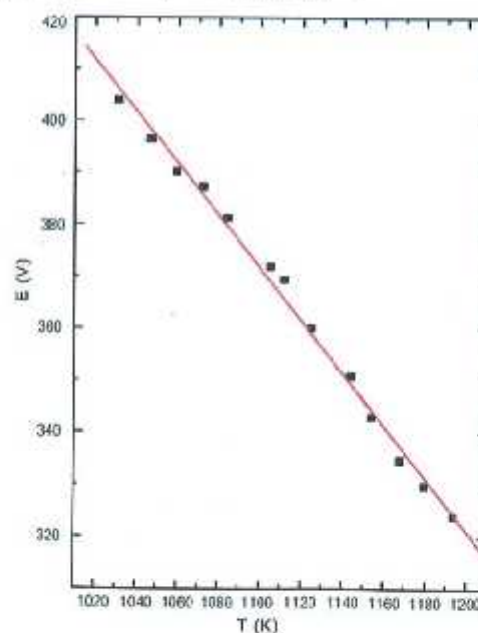
Solvation thermodynamics of some polar and non-polar amino acids in water and in aqueous-glucose at 298.15 K is reported. Results show that while the cavity formation for accommodation of amino acid molecules in aqueous-glucose molecules does not dependent solely on contributions from enthalpy, there is specific contribution from entropy terms. The aqueous glucose-amino acid interactions in the studied systems follow the order: *L*-serine < *L*-threonine < *L*-asparagine < *L*-glutamine in the case of polar amino acids and glycine < *L*-alanine < *L*-valine < *L*-methionine in the case of non-polar amino acids.



A K Nain^a, P Dholiya & J Gupta

- 945 **Thermodynamic properties of the pyrochlore Gd₂Ru₂O₇(s) by solid oxide electrochemical cell**

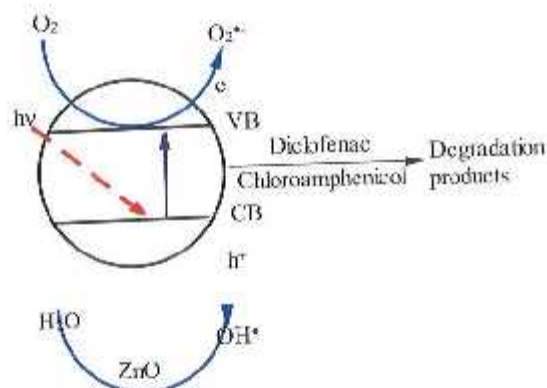
The pyrochlore, Gd₂Ru₂O₇(s), in the Gd-Ru-O system is prepared by the solid state reaction route. From elements in their standard state, the Gibbs energy of formation of Gd₂Ru₂O₇(s) is: $\{\Delta_f G^\circ(\text{Gd}_2\text{Ru}_2\text{O}_7, \text{s}) + 1.7\} = -2549.110.5438 \text{ (J/K)} \times \Delta_f T^\circ(\text{Gd}_2\text{Ru}_2\text{O}_7, \text{s}, 298.15 \text{ K}) = -2584 \text{ kJ mol}^{-1}$.



Aparna Bauerjee

949 Hydrothermal synthesis of zinc oxide nanospheres with sodium alginate as template and its photocatalytic application for degradation of diclofenac and chloramphenicol

ZnO nanospheres of average diameter of 5.0 ± 0.2 nm have been prepared by a simple hydrothermal method using sodium alginate as a template. The photocatalytic activity of the ZnO nanospheres for degradation of the drugs, diclofenac and chloramphenicol, has been studied in presence of UV light of wavelength 365 nm. The total organic content of diclofenac and chloramphenicol is reduced to 12.8% and 6.8% after 180 min under the conditions of the reaction.



Sarika A Shewale, Vilasrao A Kalantre & Gavlisiddappa S Gokavi*

Authors for correspondence are indicated by (*)

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