

Indian Journal of Chemistry
Sect. A: Inorganic, Bio-inorganic, Physical, Theoretical & Analytical

www.niscair.res.in; http://nopr.niscair.res.in
 CODEN: ICACEC; ISSN: 0376-4710 (Print), 0975-0975 (Online)

VOLUME 54A

NUMBER 11

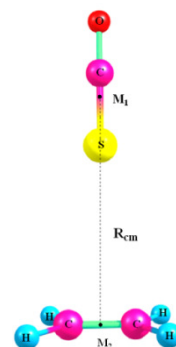
NOVEMBER 2015

CONTENTS

1369 Role of double-hybrid density functionals and correlation consistent basis sets in OCS-hydrocarbon complexes

Five double hybrid density functionals (DHDFs) in conjunction with Dunning's correlation consistent aug-cc-pVDZ, aug-cc-pVTZ and aug-cc-pVQZ basis sets are investigated to describe the weak interaction of the T-shaped isomer of OCS-C₂H₂ and OCS-C₂H₄ weakly bound van der Waals complexes. Amongst these, the mPW2PLYP DHDF with aug-cc-pVQZ basis set gives the best results. Both method and basis set are important for obtaining accurate results for such weakly bound complexes.

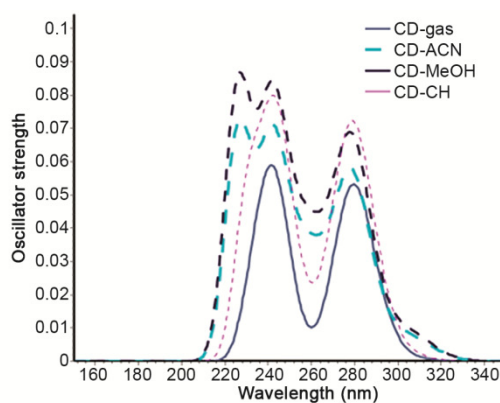
Srimanta Pakhira, Tanay Debnath, Kaushik Sen & Abhijit K Das*



1378 Towards understanding mode of action of L-dopa and carbidopa: DFT/TD-DFT analyses of their electronic and vibration spectra

Electronic absorption and vibrational spectra of L-dopa and carbidopa are recorded experimentally in different solvents and also computed theoretically. Two IR marker bands have been identified for carbidopa. Natural transition orbital analyses clearly indicate that most of the leading transitions in L-dopa and some in carbidopa involve a sizable charge transfer from the aromatic catechol moiety to the aliphatic amino acid side chain. The short wavelength transition, however, shows an opposite trend.

Ghader M Sukker, Nuha Wazzan & Rifaat Hilal*



1387 Mechanistic study of osmium(VIII) promoted oxidation of crotonic acid by aqueous alkaline solution of potassium iodate

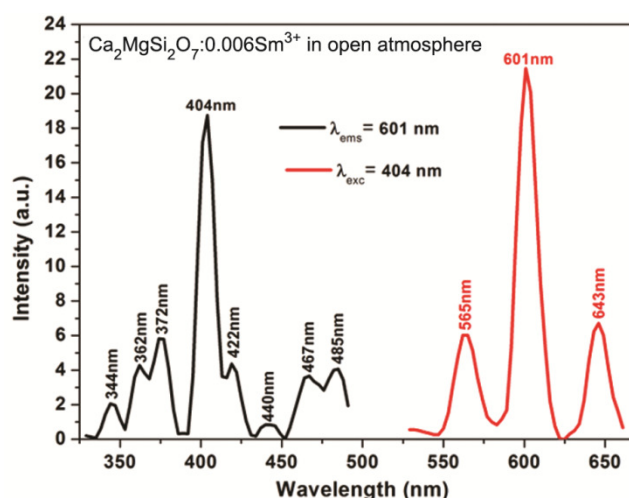
Kinetics and mechanism of osmium(VIII) promoted oxidation of crotonic acid by aqueous alkaline solution of potassium iodate have been investigated in the temperature range of 30–45 °C. A plausible mechanism involving attack of potassium iodate species on the complex formed between the catalytic species of osmium tetroxide and crotonic acid in slow and rate determining step is suggested. The rate law, consistent with observed kinetic results, is presented.

$$\begin{aligned}\text{Rate} &= \frac{-d[\text{KIO}_3]}{dt} \\ &= \frac{kd K_1 K_2 [\text{CA}] [\text{OH}^-] [\text{Os}(\text{VIII})]_T}{1 + K_1 K_2 [\text{CA}] [\text{OH}^-]}\end{aligned}$$

Bharat Singh*, Sandeep Kumar Mishra,
Shipra Tripathi & Deepmala Gupta

1394 Effect of activators and calcination on luminescence properties of åkermanite type phosphors

Novel åkermanite type phosphors, $\text{Eu}^{2+/3+}$, Dy^{3+} , Ce^{3+} , $\text{Pr}^{3+/4+}$, Sm^{3+} separately-doped single-phased $\text{Ca}_2\text{MgSi}_2\text{O}_7$ are synthesized by conventional solid-state reaction method under open (air) atmosphere and/or weak reducing atmosphere comprising nitrogen and hydrogen. The $\text{Ca}_2\text{MgSi}_2\text{O}_7$ host structure exhibits emission of different colors due to the transitions of each doped rare earth ions. The difference in the measured emission spectra is due to either different emission centers or same emission center with different ionic states occupying the same host lattice. The Ce^{3+} -doping generates visible white light emission from the åkermanite type phosphor. The study shows that the rare earth ions change the emission properties of the samples.

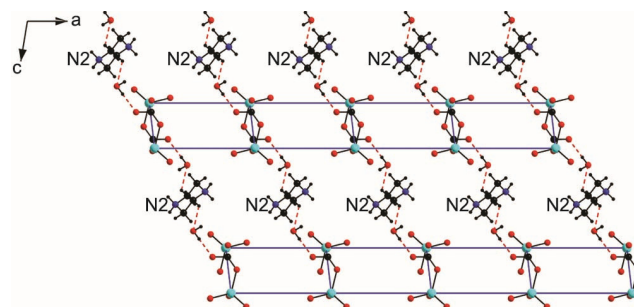


Erkul Karacaoglu* & Bekir Karasu

Notes

1402 Piperazinedium bis(μ_2 -phthalato)zincate(II) monohydrate: A new ladder coordination polymer with a unique supramolecular architecture

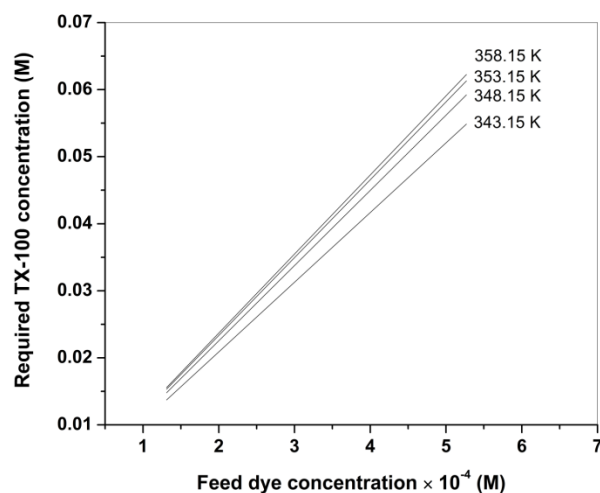
The μ_2 -bridging bidentate coordination modes of the crystallographically unique phthalate ligands in piperazinedium bis(μ_2 -phthalato)zincate(II) monohydrate result in Zn $\cdots$ Zn separations of 5.839(5) and 8.142(3) Å respectively, leading to a one-dimensional Zn(II) ladder. The organic cation, ladder complex anion and lattice water in (pipH₂)[Zn(pt)₂] $\cdot$ H₂O assemble into a unique supramolecular network, resulting in the water $\cdots$ cation $\cdots$ water $\cdots$ ladder $\cdots$ water H-bonded sequence in the crystallographic *ac* plane.



Rita N Jyai & Bikshandarkoil R Srinivasan*

1409 Ionic liquid mediated cloud point extraction of Blue BG dye

Cloud point extraction has been applied successfully for the separation of Blue BG dye using the ionic liquid, tetraethyl ammonium tetrafluoroborate, as an additive with non-ionic surfactant Triton X-100. The extraction of dye is found to increase with increase in temperature, time, surfactant concentration and ionic liquid concentration. A Langmuir type isotherm effectively describes the solubilization isotherms of the dye in TX-100.



Darshak R Bhatt, Kalpana C Maheria & Jigisha K Parikh*



Online Submission for IJCA Articles

From 1 January 2015 onwards, articles submitted for consideration of publication in the Indian J Chem, Sec A, should be uploaded through our Online Submission portal, <http://op.niscair.res.in>.

Authors are requested to register at <http://op.niscair.res.in>. The articles (in MS Word) appended with the certificate of originality, illustrations (jpeg/tiff) and supplementary data, if any, may be uploaded through the User Home page. Further information is available at http://www.niscair.res.in/jinfo/author_guidelines_online_submission.pdf.

It may be noted that from 1 January 2015 onwards, articles submitted by email or postal services shall not be processed.

For technical support and assistance for online submission, Shri Sanjay Burde may be contacted (sanjayburde@niscair.res.in); Tel.: 91-11-25846301.