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Papers

1666 Synthesis of novel chiral auxiliaries

A simple and easy route for the preparation of the higher homologue of oxazaborolidine namely dihydrooxazaborin has been reported. Also, the preparations of new bicyclic oxazaborolidines are reported.

S Narasimhan*, S Swarnalakshmi, R Balakumar & S Velmathi

1670 3,3-Disubstituted-1,5-diaryl-1,5-pentanediones as versatile intermediates for spiro heterocycles

The spiro heterocycles 5-8 and 12-15 have been prepared from 3,3-disubstituted-1,5-diaryl-1,5-pentanediones.


1676 Synthesis and characterization of new mesogenic oximes

Synthesis of a homologous series of mesogenic 4-(n-alkoxy)benzaldehyde oximes starting from 4-hydroxybenzaldehyde with n-alkyl bromide under phase transfer condition has been described.

K M Lokanatha Rai*, K Rajashekar Prasad, Nagappa & J Mahadeva

INDIAN J CHEM, 41B (8)2002
Unexpected isomerisation of double bond with DBU: A convenient synthesis of tetrasubstituted α-alkylidene tetrahydrofuranoses

DBU catalysed addition of heterocyclic bases to α,β-unsaturated esters 1 results in the formation of addition products 2 and an unexpected β, γ-unsaturated ester 3.

![Chemical structure](image)

V K Tiwari & R P Tripathi*

NMR and HPLC characterisation of O-alkanoyl lactates prepared by lipase catalysis

Lactic acid esters of organic acids like lauroyl, palmitoyl and stearoyl lactic acids prepared using lipases have been characterised by 1H and 13C NMR spectra and HPLC.

![Chemical structure](image)

K R Kiran & S Divakar*

HMO study on the effect of methyl group perturbations in isoxazoles

The effect of perturbations by methyl groups in isoxazoles have been studied and the results establish that any effects of methyl groups are reflected with the calculated ground state properties. The π-electron densities, π-bond energies, delocalization energies and ionization potentials have been calculated and correlated with the reactivity of isoxazole systems (R1 = R2 = R3 = H/CH3).

Bojja Rajeshwar Rao

INDIAN J CHEM, 41B (8) 2002
1697 AMI study on the conformations of 6-aminopenicillanic acid

The geometry and electronic structure of 6-aminopenicillanic acid (6-APA) molecule having various reaction centers have been fully optimized and calculated by semi-empirical molecular orbital AM1 method. Furthermore, the effect of conformational changes on the electronic properties has been studied. In this connection, the heats of formation, dipole moments, ionization potentials, full atomic charges, and energies of frontier molecular orbital ($E_{\text{HOMO}}$ and $E_{\text{LUMO}}$) have been calculated and discussed. The mechanism of protonation in 6-APA has been studied by comparison of net charges on nitrogen atoms in the different positions of the molecule. The conformational analyses of mono- and di-protonated species have also been performed by AM1 and their stable conformations determined.

Bojja Rajeshwar Rao

1702 AMI study on the conformations of $\alpha$-methyldopa

The geometry and electronic structure of $\alpha$-methyldopa molecule having various reaction centers have been fully optimized by semi-empirical molecular orbital AM1 calculations. Furthermore, the effect of conformational changes on the electronic properties has been studied. The heats of formation, dipole moments, ionization potentials, full atomic charges, and energies of frontier molecular orbital ($E_{\text{HOMO}}$ and $E_{\text{LUMO}}$) have been calculated and discussed. The mechanism of protonation of $\alpha$-methyldopa has been studied by using the comparison of net charges on nitrogen and oxygen atoms in the different positions of the molecule. The conformational analyses of protonated species and zwitterion have also been performed by AM1 method and their stable conformations determined.

Bojja Rajeshwar Rao

1707 Proximity effect in Bergman cyclization: A semiempirical AM1 investigation

Semiempirical AM1 calculation with limited CI(PECI=8) for a series of monocyclic enediynes reproduce the experimentally observed $\pi$-bond proximity effect on activation barrier in Bergman cyclization reactions.

A Pramanik* & Sandip Kumar Kundu
Sydnone derivatives: Part V—Synthesis and pharmacological properties of some novel triazolothiadiazepines

Balakrishna Kalluraya*, M Abdul Rahiman & David Banji

Synthesis and bioassay of O,O-diaryl 0-2-chloroethyl phosphorothionates against *Rhizoctonia solani* and *Sclerotium rolfsii.*

O,O-Diaryl 0-2-chloroethyl phosphorothionates have been prepared by condensing O-2-chloroethyl phosphorodichloridothioate, with various substituted phenols and their fungitoxicity studied against *R. solani* and *S. rolfsii.* O,O-Di (pentachlorophenyl) O-2-chloroethyl phosphorothionate is the most effective against *R. solani* and O,O-di (2-methylphenyl) O-2-chloroethyl phosphorothionate against *S. rolfsii.*

T K Chattapadhyay & R L Gupta*

A convenient and safe synthesis of 4,5-disubstituted 2-oxo-1,3-dioxolens

Employing bis(trichloromethyl)carbonate (BTC), a safe and crystalline substitute of phosgene, 4,5-disubstituted-2-oxo-1,3-dioxolens 3 have been synthesized by cyclocarbonylation of α-hydroxyketones 1 in 47-67% yield.

Devi Prasad Sahu
1724 A facile synthesis of long chain acyclic alkanols via Kolbe coupling: 1-Docosanol and 1-triacontanol

The Kolbe mixed coupling of partially neutralized mono-methyl azelate with appropriate alkanoic acid in methanol, at Pt anode, upon change transfer corresponding to 1.3F mol yields methyl alkanoate, which on LAH reduction affords the desired long chain alcohol.

\[
\text{MeOOC(CH}_2\text{)}_{14}\text{COOH} + \text{CH}_2\text{(CH}_2\text{)}_n\text{COOH} \rightarrow \text{CH}_2\text{(CH}_2\text{)}_n\text{+14COOMe} \rightarrow \text{CH}_2\text{(CH}_2\text{)}_n\text{+14CH}_2\text{OH}
\]

Ashok K Yadav* & Arpita Singh

1727 Synthesis and characterization of 1,3-bis-(2,4,6-trichlorophenyl)-1 H-triazene (BTCPT)

BTCPT has been prepared by diazotisation of 2,4,6-trichloroaniline in the presence of NaNO2/HCl and ethyl alcohol followed by full characterization.

Mehilal, Rajendra B Salunke & J P Agrawal*

1730 Synthesis of dimethyl 2-(N-phenylamido-N-yl)-3-(triphenylphosphoranylidene)butanedioates

A single-step synthesis of highly stabilized ylides 7 is described.

\[
\text{Fmoc-NH-CHR-C-Cl + NaN}_3 \rightarrow \text{Fmoc-NH-CHR-C-N}_3
\]

Ali Ramazani & Leila Karimi-Avargani

1733 Fmoc-amino acid azides in peptide synthesis

Fmoc-amino acid azides can be prepared from their corresponding acid chlorides and NaN3. All the compounds made have been obtained as crystalline solids in good yield and purity. They are found to be stable at room temperature for long periods.

Ganga- Ramu Vasanthakumar, Kuppanna Ananda & Vommina V Suresh Babu*

1736 Synthesis of 1,1,4,4-tetraaryl-1,3-diazabutadienes by oxidation of hydrazones using bis(acetyl-acetonato)-copper (II)

Titled compounds are synthesized by oxidation of hydrazones using Cu(acac)_2.

G S Singh* & K Kopo
Preparation of hydroxybenzophenones using silica-gel supported ferric chloride

Various hydroxybenzophenones have been prepared by using supported heterogeneous catalyst.

Pravin M Bendale & Bhushan M Khadilkar*

Conversion of oximes, phenylhydrazones, 2,4-dinitrophenylhydrazones and semicarbazones to carbonyl compounds with benzyltriphenylphosphonium chlorochromate (BTPPCC) in the presence of aluminium chloride under non-aqueous conditions

Benzyltriphenylphosphonium chlorochromate has been found to be an efficient and novel reagent for the conversion of oximes, phenylhydrazones, 2,4-dinitrophenylhydrazones and semicarbazones to the corresponding carbonyl compounds.

Abdol Reza Hajipour*, Shadpour E Mallakpour*, Iraj Mohammadpoor-Baltork & Hossein Backnejad

Microwave irradiation promoted decomposition of pyrazolines of sesquiterpene lactones

Decomposition of pyrazolines of sesquiterpene lactones has been efficiently achieved under microwave irradiation to yield 13-substituted double bond and alkyl substituted spirocyclopropyl derivatives.

B R Chhabra* & Meenu Jain

Zinc metal assisted hydro-de-halogenation of DDT into DDEthane under sonic conditions

An efficient method for the hydro-de-halogenation of DDT to 1,1-bis (p-chlorophenyl) ethane (DDEthane) exclusively by a simple reaction using commercial zinc dust, is reported. The rate of the reaction is enhanced by irradiating at 35 KHz in a sonic bath at 25°C.

M A Pasha* & D Nagaraja
Substituted benzothiazines 1,1-dioxides as bioactive compounds

An approach towards synthesis of substituted benzothiazine-1,1-dioxides as bioactive compounds and their biological activities have been reported.

V K Pandey* & (Miss) Seema R Pathak

A new triterpenoid from *Ruellia tuberosa* Linn

21-Methyldammar-22-en-3β, 18, 27-triol 1 has been isolated from aerial parts of the plant.

R S Singh*, H S Pandey, R P Pandey & B K Singh

Authors for correspondence are indicated by (*)