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## CHINESE JOURNAL OF CHEMISTRY

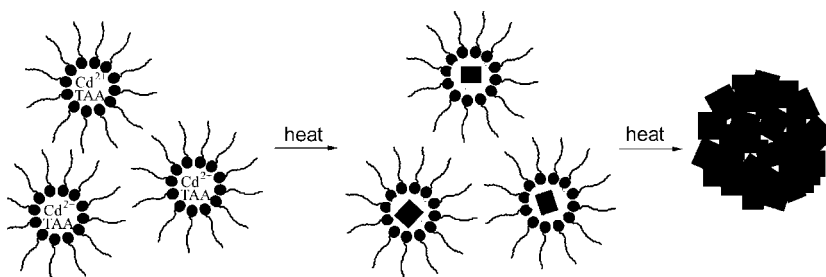
Vol. 23 No. 9 September 2005

Pages 1127—1278

## COMMUNICATIONS

1135

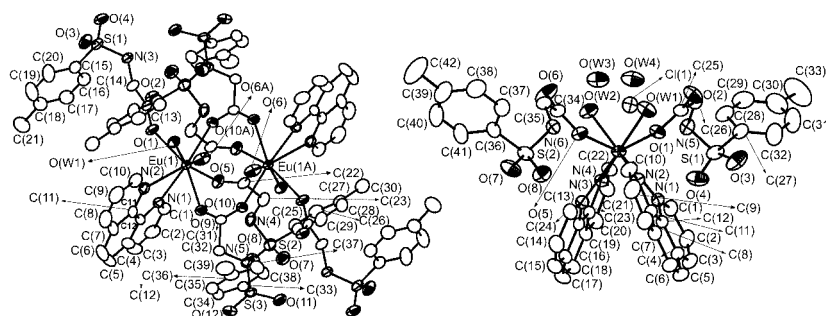
## Synthesis of CdS Microspheres by a Hydrothermal Microemulsion Method



CdS microspheres were prepared by a hydrothermal microemulsion method in cyclohexane/Triton X-100/pentanol/water at 180 °C. The formation process is illustrated in the above figure.

XU, Sheng; PENG, Qing\*

1139

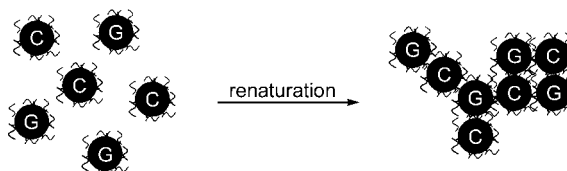
Synthesis and Structures of Lanthanide Complexes of *N-p*-Tolylsulfonylglycinate and 1,10-Phenanthroline

Lanthanide compounds  $[\text{Eu}_2(\text{TsGly})_6(\text{phen})_2(\text{H}_2\text{O})_2]$  (**1**),  $[\text{Ln}(\text{TsGly})_2(\text{phen})_2(\text{H}_2\text{O})_2]\text{Cl} \cdot \text{H}_2\text{O}$  [ $\text{Ln} = \text{Er}$  (**2a**),  $\text{Yb}$  (**2b**)] ( $\text{L} = N$ -*p*-tolylsulfonylglycinate, phen = 1,10-phenanthroline) were synthesized. Structure analyses revealed that compound **1** adopts dinuclear structure with fourfold bridging TsGly ligands between the Eu(III) centers, while compound **2b** features an unusual mononuclear structure.

ZHANG, Man-Bo; HU, Rui-Xiang; LIANG, Fu-Pei\*; MA, Lu-Fang; ZHOU, Zhong-Yuan

1143

## Assembly of Au Nanoparticles with Anisotropic Optical Property Directed by 2'-Phosphorothioate Oligo-DNA

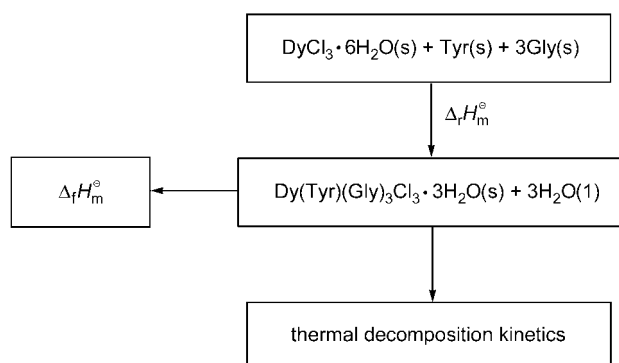


YANG, Bai-Quan; JIANG, Lin; ZHUANG, Jia-Qi\*; LIU, Yi-Chun; XU, Wu; LI Tie-Jin

The assembly of Au nanoparticles with anisotropic optical property was directed by 2'-phosphorothioate oligo-DNA.

## FULL PAPERS

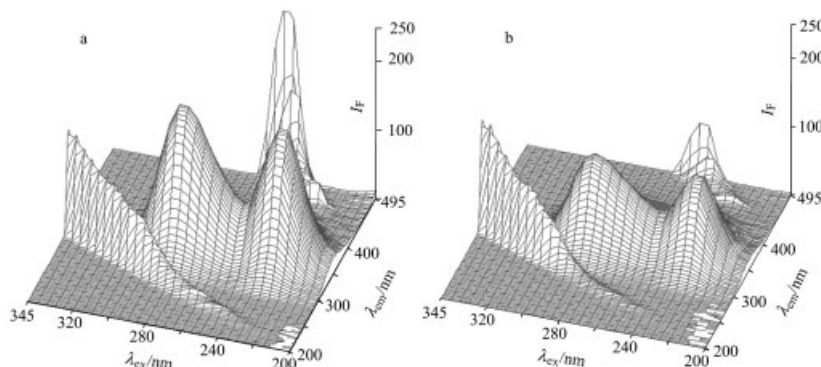
1146

**Study on Thermochemistry and Thermal Decomposition Kinetics of Dy(Tyr)-(Gly)<sub>3</sub>Cl<sub>3</sub>•3H<sub>2</sub>O**


The kinetics of thermal decomposition of the complex was studied by TG-DTG-DTA. The mechanism function of the thermal decomposition reaction for its second step was proposed. The kinetic equation could be expressed as:  $da/dT = 3.14 \times 10^{20} \text{ s}^{-1} / \beta \exp(-209.37 \text{ kJ} \cdot \text{mol}^{-1} / RT)(1-\alpha)^2$ .

ZHANG, Zhong-Hai; KU, Zong-Jun; LIU, Yi\*; QU, Song-Sheng

1151

**Study on Binding Reaction between Flucytosine and Bovine Serum Albumin**


According to three-dimensional fluorescence spectra of BSA (a), and flucytosine-BSA complex (b), two typical fluorescence peaks could be easily found. It is obvious that both fluorescence peaks of BSA have been quenched a lot by flucytosine, but to different extent, indicating that flucytosine has complexed with BSA to change its conformation.

YAN, Cheng-Nong\*; ZHANG, Hua-Xin; MEI, Ping; LIU, Yi

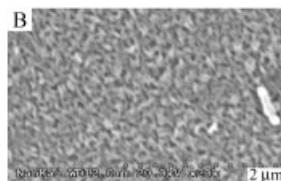
1157

**Effect of Na<sup>+</sup>, K<sup>+</sup> and Ca<sup>2+</sup> Ions on Physico-chemical Properties of Thymine, Cytosine, Thymidine and Cytidine in Aqueous Urea Solution**

Ultrasonic velocity, density and viscosity have been experimentally determined at 298.15 K for two pyrimidine bases thymine and cytosine along with respective nucleosides in aqueous urea solution in the presence of NaCl, KCl and CaCl<sub>2</sub> at different concentrations. UV spectroscopic studies have been carried out for structural studies and a number of thermodynamic parameters have been computed from the experimental measurements to get a broader picture of the interactions involved there of.

PANDEY, Jata Dhari\*; HAROON, Shahla; CHHABRA, Jyotsna; DEY, Ranjan; MISRA, Krishna

1165

**Preparation and Electrochemical Properties of Manganese Hexacyanoferrate Modified Glassy Carbon Electrode**


MnHCF/GC electrode was characterized by scanning electron microscopy (SEM), which further verified the effective deposition of MnHCF film on GC.

There exist three clear-cut stages for the deposition of manganese hexacyanoferrate (MnHCF) film on glassy carbon (GC) electrode surface in the whole modification process. The last stage is indispensable to the fabrication of homogenized, stable MnHCF film and must last for an appropriate time. The surface morphology of

LIU, You-Qin\*; YAN, Yun; SHEN, Han-Xi

1173

### Applications of Simple Estimation Scheme of Electron Correlation Energy to Strong Ionic Compounds

ZHUO, Shu-Ping\*; WEI, Ji-Chong; JU, Guan-Zhi

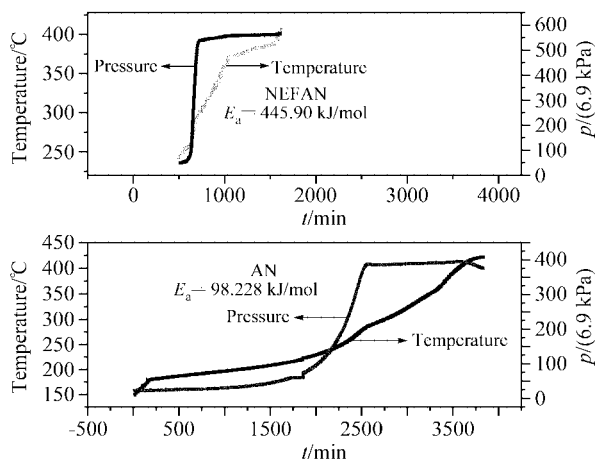
The calculation results of electron correlation energies of KF and (KF)<sub>2</sub> are reported. It is indicated that the estimation of the correlation energies of KF and the (KF)<sub>2</sub> systems can be achieved by applying the simple estimation scheme to the strong ionic compounds.

$$E_{\text{corr}}(\text{KF}) \approx E_{\text{corr}}(\text{K}^+) + E_{\text{corr}}(\text{F}^-)$$

$$E_{\text{corr}}(\text{KF})_2 \approx 2E_{\text{corr}}(\text{KF})$$

1177

### Study on Modification and Test Technology of Nonexplosive and Ir-restorable Fertilizer-grade Ammonium Nitrate

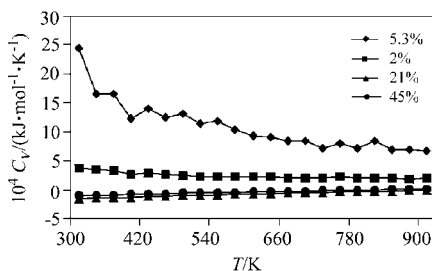


The results of ARC show that the onset thermal decomposition temperature of NEIFAN was 50% higher than that of AN. Furthermore, the activation energy of NEIFAN was about 5 times higher than that of AN. Therefore, NEIFAN has better thermal stability than AN.

SHEN, Li-Jin\*; WANG, Xu-Guang

1182

### Investigation of Microstructures and Anti-corrosion Properties of Aluminium-Zinc Alloys



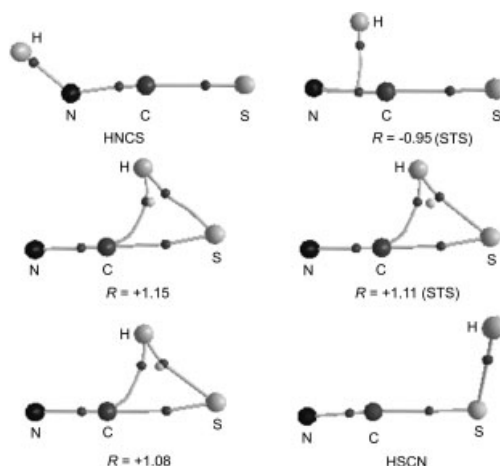
The  $C_V$  values of 21% and 45% aluminium-zinc systems were decreased with the decrease of temperature. The magnitudes of variation in  $C_V$  of these two systems were relatively small compared with other two systems. For the 2% and 5.3% aluminium-zinc systems, the  $C_V$  data were increased with the decrease of temperature. The  $C_V$

QI, Zhong-Nan; ZHANG, Chang-Qiao; WANG, Ruo-Xi; LIU, Cheng-Bu\*; CHEN, Zheng-Long

data of 5.3% aluminium-zinc system showed two distinct regions. Below 400 K,  $C_V$  was increased rapidly with the decrease of temperature, but above 400 K,  $C_V$  varied much slowly, indicating that the system exhibited two phases below and above 400 K. At different temperature reduction rate similar trend was found out about  $C_V$  in all systems.

1187

### AIM Study on Reaction $\text{HNCX} \rightarrow \text{HXCN}$ ( $\text{X}=\text{O}, \text{S}$ and $\text{Se}$ )



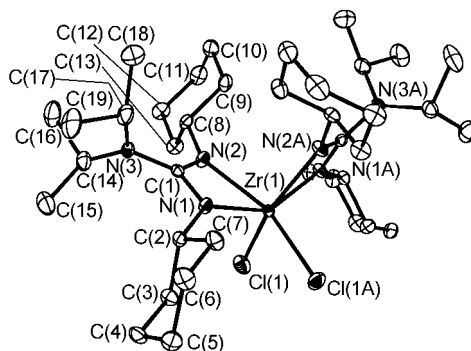
The reactions of HNCX to HOCN, HNCS to HSCN and HNCSe to HSeCN have been studied at MP2/6-311++G(2df,pd)//B3LYP/6-311++G(2df,pd) level. The breakage and formation of the chemical bonds in the reactions have been discussed by the topological analysis method of electronic density. The calculated results show that there are two kinds of structure transition states (STS) in reactions studied.

ZENG, Yan-Li; MENG, Ling-Peng; ZHENG, Shi-Jun\*

1193

### Synthesis and Characterization of Bis(guanidinate) Zirconium Complexes

PANG, Xing-An; YAO, Ying-Ming; WANG, Jun-Feng; SHENG, Hong-Ting; ZHANG, Yong; SHEN, Qi\*

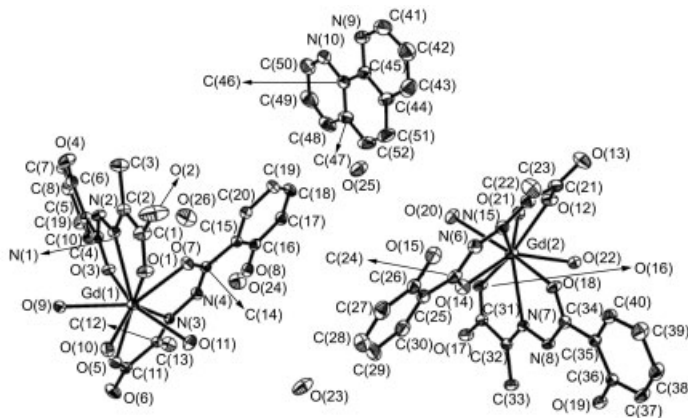


Treatment of  $\text{ZrCl}_4$  with freshly prepared solutions of lithium guanidinate provided a series of bis(guanidinate) complexes of Zr with the general formula of  $\text{Zr}[\text{RNC}(\text{NR}_2)\text{NR}]_2\text{Cl}_2$ .

1198

### Crystal Structure and Bioactivity of Complex $[\text{Gd}(\text{C}_{10}\text{H}_9\text{N}_2\text{O}_4)(\text{C}_{10}\text{H}_8\text{N}_2\text{O}_4)(\text{H}_2\text{O})_3]_2 \cdot \text{phen} \cdot 4\text{H}_2\text{O}$

HE, Shui-Yang\*; YANG, Rui; WU, Wang-Ting; SHI, Qi-Zhen; WANG, Da-Qi; AN, De-Rong



There are two 9-coordinated structure units in every molecule, in which Gd(III) is coordinated by two tridentate  $\text{C}_{10}\text{H}_9\text{N}_2\text{O}_4$  ligands and three water molecules, and the two structural fragments take a distorted monocapped square antiprism. There is a free 1,10-phenanthroline connected with coordinated water by hydrogen bonds in the crystal cell.

1203

### Studies of Iron-Sulfur Covalency in the Model System and Proteins

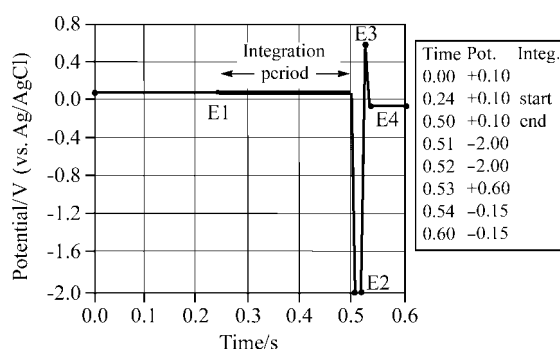
QIN, Xiu-Juan; CHEN, Yan; GAO, Fa-Ming\*

It was found that the highly covalent nature of the metal-ligand interactions in the Fe-S cluster clearly played an important role in determining the reactivity of the sites. A semi-empirical model, based on the Phillips theory of bonding was developed for quantitative explanation of covalency in Fe-S cluster, showing that Mossbauer spectroscopy and electronic absorption spectroscopy provided the direct experimental probe of covalency of  $\text{Fe-S}_4$  clusters.

1207

### Optimizing the Quadruple-potential Waveform for the Determination of Gentamicin Sulfate by High Performance Liquid Chromatography with Pulsed Electrochemical Detection

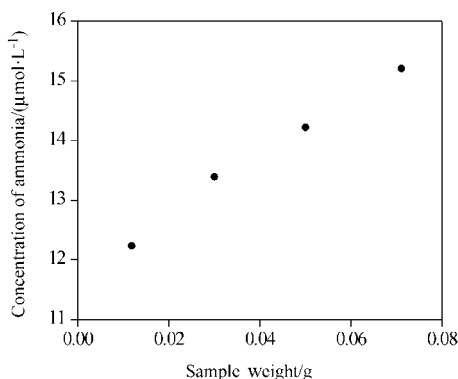
CAI, Ya-Qi; MOU, Shi-Fen\*



way, the formation of gold oxide resulting from the application of high positive potential during the analyte detection and electrode cleaning were greatly reduced, and therefore, the dissolution and recession of gold working electrode was also reduced. The good condition of gold working electrode achieved by this quadruple-potential waveform can help us to obtain a good reproducibility.

A quadruple-potential waveform was investigated and optimized for the determination of gentamicin by reversed phase ion-pair chromatography. Instead of a relatively high positive potential, a negative potential was adopted as a potential for the cleaning of gold working electrode. By this

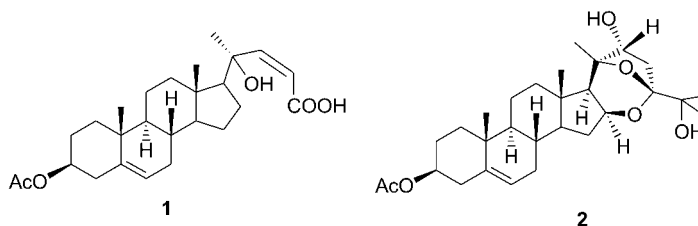
1213

**Reduction of Nitrogen on Gallium Phosphide Nanoparticles**

Under ambient conditions gallium phosphide (GaP) nanoparticles were employed to carry out the reduction of nitrogen. By using Nessler's reagent ammonia was detected.

ZHANG, Zhao-Chun\*; CUI, De-Liang

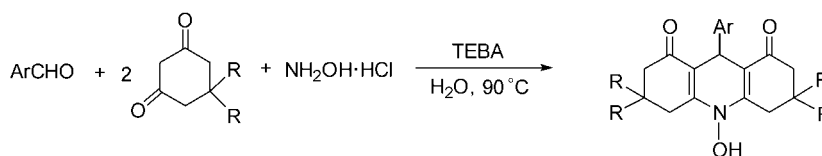
1218

**Three Polyoxygenated Steroids from the South China Sea Gorgonian Coral *Subergorgia reticulata***

Two new polyoxygenated steroids (**1** and **2**) were isolated from the South China Sea gorgonian coral *Subergorgia reticulata*. Their structures were established on the basis of 1D, 2D NMR spectroscopic analysis and the X-ray crystallographic analysis.

YANG, Jin; QI, Shu-Hua; ZHANG, Si\*; WU, Jun; XIAO, Zhi-Hui

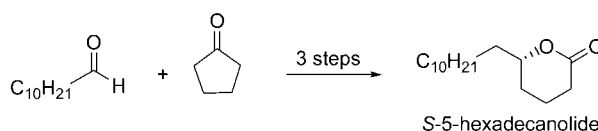
1223

**One-pot Synthesis of *N*-Hydroxylacridine Derivatives in Water**

*N*-Hydroxylacridinedione derivatives were synthesized by three-component reaction of aromatic aldehydes, 1,3-dicarbonyl compounds and hydroxylamine hydrochloride using triethylbenzylammonium chloride (TEBA) as the catalysis in water. The reaction has many advantages including good yields, easy to be separated and environmental friendliness.

SHI, Da-Qing\*; MOU, Jie; ZHUANG, Qi-Ya; WANG, Xiang-Shan

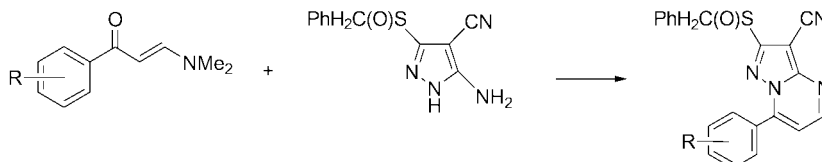
1228

**Asymmetric Synthesis of *S*-Hexadecanolide**

Optically pure *S*-5-hexadecanolide has been easily prepared from aldehyde and cyclopentanone.

SUN, Bin; ZHANG, Chao-Xin; ZHANG, Gui-Min; LI, Ying\*; LI, Yu-Lin; PENG, Li-Zeng\*

1231

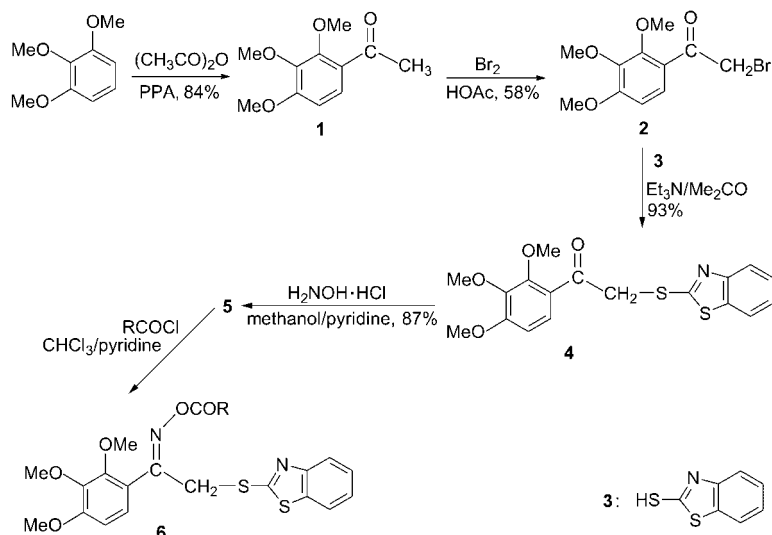
**Reaction of Enaminones with Amino-pyrazoles: Synthesis, Structures and Bioactivities of 7-Aryl-3-cyano-2-substituted Pyrazolo[1,5-*a*]pyrimidines**

The condensation reactions of 5-amino-4-cyano-3-substituted-1*H*-pyrazole **2** or **3** with enaminones **1** in the presence of glacial acetic acid gave twelve new 7-aryl-3-cyano-2-substituted pyrazolo[1,5-*a*]pyrimidines **4** and **5** at room temperature. Their structures were characterized by elemental analysis, IR and <sup>1</sup>H NMR spectra. The structure of **4a** was further confirmed by X-ray crystallography analysis. A plausible reaction mechanism for the formation of the title compounds was also proposed. The bioassay tests showed that compounds **4a**, **4c**, **4e**, **4f**, **5a** and **5d** possessed moderate herbicidal activity.

WEN, Li-Rong; WANG, Shu-Wen; LI, Ming\*; YANG, Hua-Zheng

1236

### Synthesis and Anticancer Activity of 2,3,4-Trimethoxyacetophenoxime Ester Containing Benzothiazole Moiety



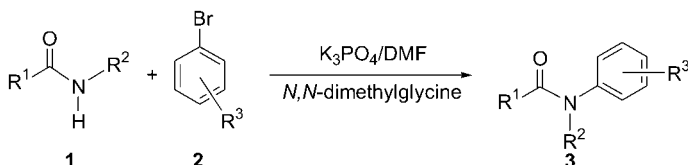
SONG, Bao-An\*; LIU, Xin-Hua; YANG, Song; HU, De-Yu; JIN, Lin-Hong; ZHANG, Hua

Starting from trimethoxybenzene, nine 2,3,4-trimethoxyacetophenoxime esters containing benzothiazole moiety were synthesized through five reaction steps. Their inhibitive bioactivity to cancer cell proliferation and ERK phosphorylation induced by PDGF were tested.

1241

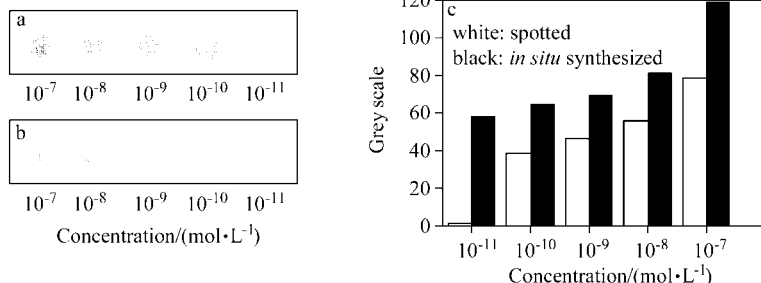
### Mild and Efficient CuI Catalyzed Coupling Reactions of Amides with Bromides

DENG, Wei; ZHANG, Chen; LIU, Min; ZOU, Yan; LIU, Lei; GUO, Qing-Xiang\*



1247

### In situ Synthesis of Oligonucleotide and Detection of Gold-label-silver-stain on PTFE Slices



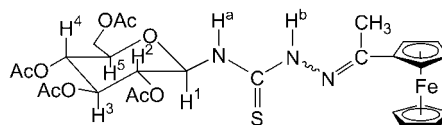
TAN, Mei-Jun; TANG, Jian-Xin\*; CHEN, Hong\*

Poly(tetrafluoroethylene) (PTFE) was treated with plasma in a mixture of nitrogen and hydrogen (1 : 2 in volume), and then successively applied to the *in situ* synthesis of oligonucleotides. With the detection of gold-label-silver-stain, the hybridization signals were recorded with a gel document and analysis system. A target DNA concentration as low as 10 pmol/L was detected. The sensitivity of *in situ* synthesis system was 1 order of magnitude higher than that of spotting system, and the signals of the former was about 1.8 times stronger than that of the latter under the same target DNA concentration.

1253

### Facile Synthesis and Characterization of Bioactive N-[(1-Ferrocenylethylidene)amino]-N'-β-D-glycopyranosylthiourea

ZHANG, Shu-Sheng\*; YANG, Bo; LI, Hui-Xiang; JIAO, Kui

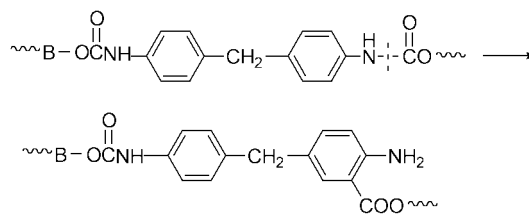


Several novel *N*-[(1-ferrocenylethylidene)amino]-*N'*-β-*D*-glycopyranosylthiourea have been efficiently synthesized and characterized. An initially alternative synthetic route, which was seemingly reasonable, has been excluded due to its inefficiency.

1257

**Photochemical Degradation Study of Polyurethanes as Relic Protection Materials by FTIR-ATR**

WANG, Li-Qin; LIANG, Guo-Zheng; DANG, Gao-Chao\*; WANG, Fang; FAN, Xiao-Pan; FU, Wen-Bin



1264

**Penta-Coordinate Phosphorus Intermediates Analysis on Phospho-related Proteins**

LI, Wu; MA, Yuan; ZHAO, Yu-Fen

In this paper, based on known crystal structures of square pyramid (SP) and trigonal bipyramid (TBP) penta coordinated phosphorus compounds containing amino acid side chains, such as amino, carboxyl, hydroxyl or thioal, a software for survey the P(5)-structure of phosphorylated proteins was derived. By this software, it was found that 382 of 398 phosphorus related kinases (96%) from current PDB could go through the penta-coordinated phosphorus transition state or intermediate.

1267

**New Aspects in the Chemistry of Three-membered Ring Compounds Containing a Highly Coordinate Main Group Element**

TAKAYUKI, Kawashima

The title compounds were synthesized by taking advantage of the Martin ligand. Their structures were determined by X-ray crystallography. Pentacoordinate thiasiliranides were hydrolyzed to give the corresponding thiol. Pentacoordinate chalcogenaphosphoranes were found to have polar P-chalcogen bonds, which were confirmed by their reactions with  $\text{CF}_3\text{SO}_3\text{Me}$  to give the corresponding 1-(methylchalcogena)alkylphosphonium triflates and by the solvent-dependent NMR studies.

1270

**New Methods and Synthetic Applications of Asymmetric Nitrogen Transfer**

ARMSTRONG, Alan; EDMONDS, Ian; COOKE, Richard S.; SHANAHAN, Stephen E.; KNIGHT, Jamie D.; CUMMING, Graham R.

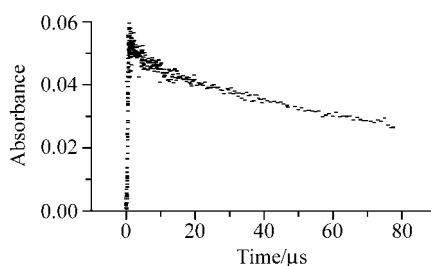
Structure/reactivity relationships of *N*-alkoxycarbonyl- and *N*-carboxamidooxaziridines are explored, and conditions are discovered for the efficient amination of sulfides and primary amines. Reactions of these oxaziridines with alkenes are also examined, and lead to interesting new heteroatom transfer reaction products. Finally, the aminative rearrangement of 2-alkoxydihydropyrans leads to a useful stereocontrolled synthesis of pyrrolidines which can undergo synthetic manipulations to give [2.2.1]- and [3.2.1]-azabicycles.

**NOTES**

1273

**Reactions of Hydroxyl Radical with Salicylic Acid Derivatives: A Pulse Radiolysis Study**

MA, Jian-Hua\*

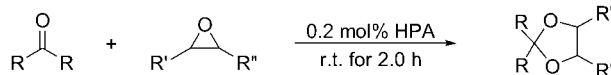


The rate constant for reactions of hydroxyl radical with benzylsalicylate was determined by growth trace of transient absorptions arising from the scavenging of hydroxyl radical by benzylsalicylate.

1275

**Heteropolyacid-catalyzed Reaction of Epoxides with Ketones: Efficient Synthesis of 1,3-Dioxolane Derivatives**

HE, Jun-Yi; GAO, Fei-Xue; HUA, Rui-Mao\*



An efficient method for the preparation of 1,3-dioxolanes via the coupling of epoxides with ketones catalyzed by heteropolyacids at ambient temperature has been described.