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EurJOC is co-owned by 11 societies of ChemPubSoc Europe, a union of European chemical societies for the purpose of publishing high-quality science. All owners merged their national journals to form two leading chemistry journals, the *European Journal of Organic Chemistry* and the *European Journal of Inorganic Chemistry*. Three further members of ChemPubSoc Europe (Austria, Czech Republic and Sweden) are Associates of the two journals.

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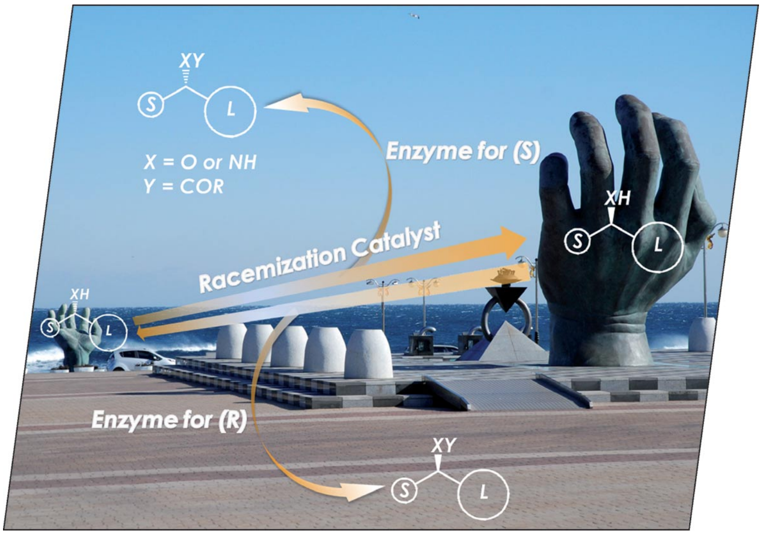
COVER PICTURE

The cover picture shows the synthesis of optically active esters and amides by chemoenzymatic dynamic kinetic resolution (DKR) from racemic alcohols and amines, respectively. Racemic substrates are transformed into single enantiomeric products by the combination of metal-catalyzed racemization and enzymatic acylation. The background is "The Hands of Win-Win" of Homigot, 22 km east of Pohang along the East Sea of Korea. Many people visit Homigot to see the hands and the sun rise. The hands are chiral and racemic. The Microreview by M.-J. Kim, J. Park et al. on p. 999ff. describes the DKR of racemic alcohols and amines by emphasizing the characteristics of the racemization catalysts developed so far.

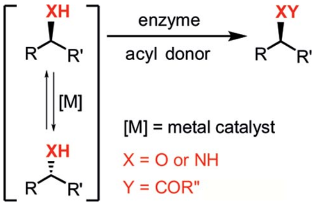


CONTENTS

MICROREVIEW

Dynamic Kinetic Resolution

Keywords: Dynamic kinetic resolution / Transesterification / Enzymes / Alcohols / Amines

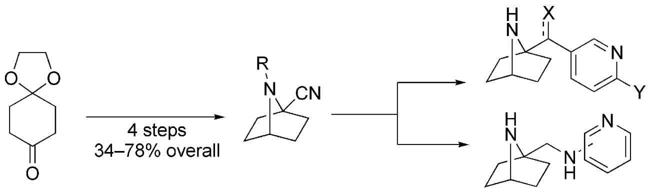


Dynamic kinetic resolution (DKR) is an attractive process for the production of optically active compounds from racemic mixtures. Combinations of the processes of metal-catalyzed racemization and enzymatic acylation in one-pot fashion have shown the potential of DKR of alcohols and amines. This Microreview summarizes developments in and the scope of chemoenzymatic DKR.

SHORT COMMUNICATIONS

Epibatidine Analogues

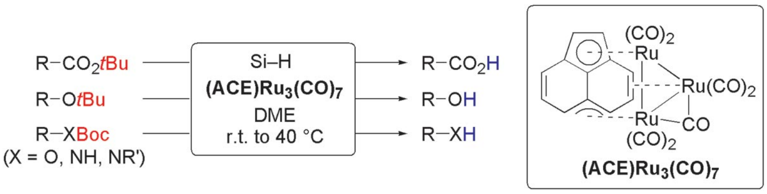
Keywords: Cyanides / Cyclization / Natural products / Neurological agents / Nitrogen heterocycles



Five novel epibatidine analogues were prepared by using a straightforward one-pot method for the synthesis of 7-azabicyclo[2.2.1]heptane-1-carbonitriles, starting from cyclohexanones bearing a leaving group at the 4-position.

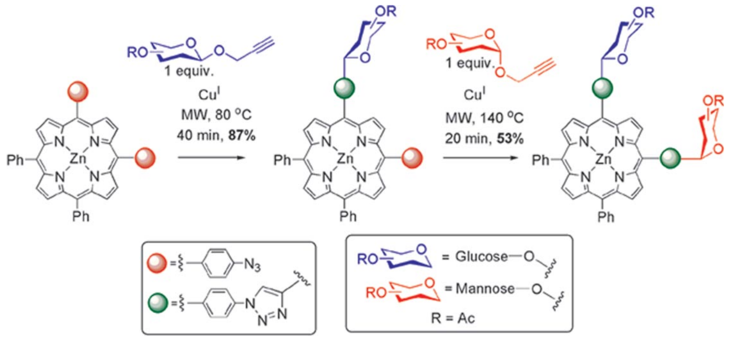
Deprotection

Keywords: Protecting groups / Hydrosilanes / Ruthenium / Cleavage reactions / Si–H activation



Hydrosilanes act as a reagent to cleave the C–O bond of O*t*Bu groups in carbamates, carbonates, esters, and ethers by catalysis of a triruthenium cluster. The reaction offers a novel deprotection method for O*t*Bu groups under neutral conditions. Possible mechanisms for the cleavage of the C–O bond of O*t*Bu groups are discussed on the basis of NMR spectroscopic analysis.

Medicinal Chemistry



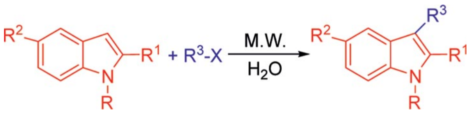
A novel, two-step, sequential "double-click" process allows the preparation of heterogeneous glycoporphyrins in good yields. Microwave heating was used to accelerate reaction times and improve yields for the Cu-catalysed cycloaddition reaction. The latent azide was determined to be stable under these conditions.

O. B. Locos, C. C. Heindl, A. Corral, M. O. Senge, E. M. Scanlan* **1026–1028**

Efficient Synthesis of Glycoporphyrins by Microwave-Mediated "Click" Reactions

Keywords: Porphyrinoids / Glycoporphyrin / Carbohydrates / Click chemistry / Microwave chemistry

Substituted Indoles



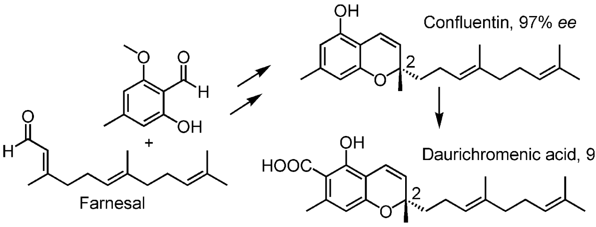
A simple and general protocol for the *C*-alkylation of indoles with benzyl halides in water under microwave irradiation has been developed. The salient features of the methodology are the use of water as green solvent, short reaction times, good adduct yields with high selectivity, easy workup and without the need for any catalyst or additives.

M. De Rosa,* A. Soriente **1029–1032**

Rapid and General Protocol towards Catalyst-Free Friedel–Crafts *C*-Alkylation of Indoles in Water Assisted by Microwave Irradiation

Keywords: Indoles / Friedel–Crafts reaction / Microwave irradiation / Superheated water / Synthetic methods / Nitrogen heterocycles / Microwave chemistry / Alkylation

Natural Products



The synthesis of daurichromenic acid and confluentin, two chromenes from *Rhododendron dauricum*, was achieved using a chiral lactol that was generated from farnesal and 2-methoxy-4-methylsalicylaldehyde by an organocatalytic, highly enantioselective domino aldol/oxa Michael reaction.

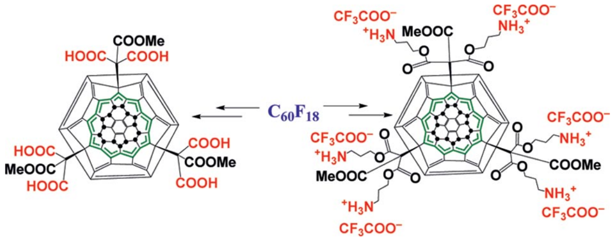
K. Liu, W.-D. Woggon* **1033–1036**

Enantioselective Synthesis of Daurichromenic Acid and Confluentin

Keywords: rganocatalysis / Aldol reactions / Domino reactions / Michael reaction / Chromenes

FULL PAPERS

Chemistry of Fluorofullerenes



The first water-soluble $C_{3}v$-symmetrical trannulene derivatives of fluorofullerene $C_{60}F_{18}$ possessing six carboxylic or ammonium ion groups have been synthesized and spectrally characterized.

P. A. Troshin,* E. A. Khakina, A. V. Zhilenkov, A. S. Peregudov, O. A. Troshina, V. I. Kozlovskii, N. V. Polyakova, R. N. Lyubovskaya **1037–1045**

Synthesis and Spectroscopic Characterization of the First Symmetrically and Non-symmetrically Substituted Fluorinated Emerald-Green Trannulenes $C_{60}F_{15}R_3$ Soluble in Polar Media and Water

Keywords: Fullerenes / Fluorine / Annulenes / Bioorganic chemistry

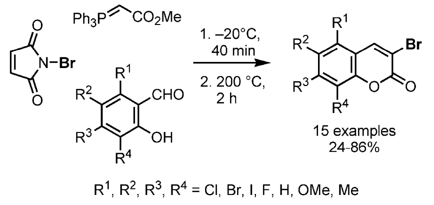
CONTENTS

Three-Component Reactions

D. Audisio, S. Messaoudi,* J.-D. Brion, M. Alami* 1046–1051

A Simple Synthesis of Functionalized 3-Bromocoumarins by a One-Pot Three-Component Reaction

Keywords: Bromine / Multicomponent reactions / Wittig reactions / Oxygen heterocycles / Natural products



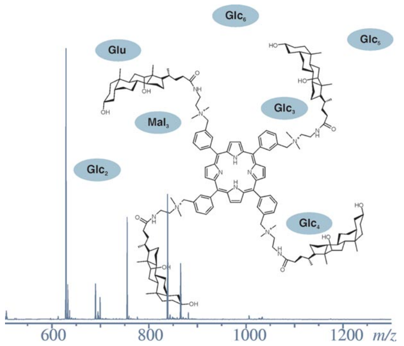
A one-pot three-component reaction between readily available substituted salicylaldehydes, methyl (triphenylphosphoranylidene)acetate and *N*-bromosuccinimide is reported. This simple and straightforward sequence allows the synthesis of a large series of functionalized 3-bromocoumarins.

Molecular Recognition

E. Kalenius,* J. Koivukorpi, E. Kolehmainen, P. Vainiotalo 1052–1058

Noncovalent Saccharide Recognition by Means of a Tetrakis(bile acid)–Porphyrin Conjugate: Selectivity, Cooperation, and Stability

Keywords: Molecular recognition / Saccharide recognition / Porphyrin conjugates / Noncovalent interactions / Mass spectrometry



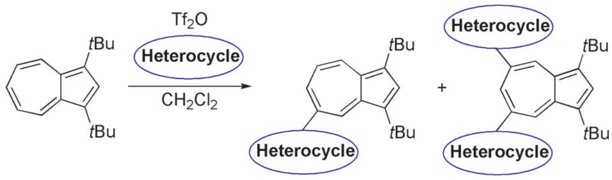
Size-selective complexation of Glu, Glc_2-Glc_6 and Mal_3 with a tetrakis(bile acid)–porphyrin conjugate and properties of the complexes have been studied by mass-spectrometric methods. The bile acid conjugate was observed to form 1:1 noncovalent complexes with size-selectivity towards oligosaccharides with three or more glucose residues.

Azulene Chemistry

T. Shoji,* S. Ito,* K. Toyota, N. Morita 1059–1069

Synthesis of 5-Heteroaryl- and 5,7-Bis(heteroaryl)azulenes by Electrophilic Substitution of 1,3-Di-*tert*-Butylazulene with Triflates of N-Containing Heterocycles

Keywords: Azulene derivatives / Heterocycles / Electrophilic substitution / Electrochemistry / Solvatochromism



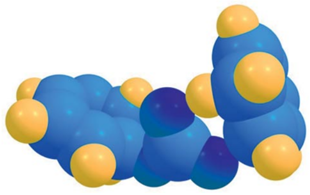
Reaction of 1,3-di-*tert*-butylazulene with triflates of N-containing heterocycles in the presence of excess heterocycles gave 5-heteroaryl- and 5,7-bis(heteroaryl)azulene derivatives. The redox behavior of these new azulene derivatives was examined by cyclic voltammetry and differential pulse voltammetry.

Carbonic Acid by Ester Pyrolysis

G. Bucher* 1070–1075

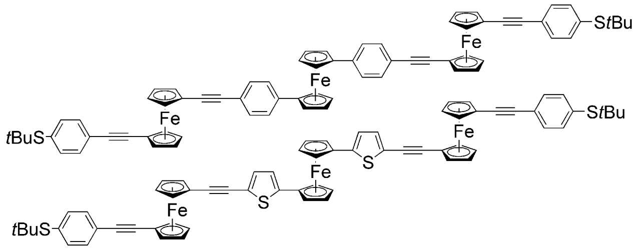
Ester Pyrolysis of Carbonates: Bis(benzene hydrate) Carbonate as Potential Precursor for Monomeric Carbonic Acid

Keywords: Computer chemistry / Thermochemistry / Carbonic acid / Carbonates / Peroxides / Pseudopericyclic reactions



Can monomeric carbonic acid be prepared by twofold ester pyrolysis reaction of carbonates? According to DFT and high level CCSD(T) calculations, the answer is "yes". The carbonate derived from benzene hydrate is predicted to be an excellent precursor. Diethyl carbonate or aldoxime carbonates are predicted to be unsuitable for the generation of carbonic acid, as competing reactions are predicted to be faster than the second ester pyrolysis reaction, and peroxy carbonates suffer from competing O–O bond homolysis.

Ferrocene-Based Extended π Systems



The first ferrocene-based molecular wires with three ferrocene hinges have been prepared by Negishi coupling reactions. A crystal structure analysis of a 1,1′-dithienylferrocene indicates only a slight deviation from planarity of the thiophene and the cyclopentadienyl rings.

I. Baumgardt,
H. Butenschön* **1076–1087**

1,1′-Diaryl-Substituted Ferrocenes: Up to Three Hinges in Oligophenyleneethynylene-Type Molecular Wires

Keywords: Molecular wires / Molecular electronics / Cross-coupling / Cyclic voltammetry / Sandwich complexes / Ferrocene

Sequential Cyclization

Iminophosphoranes obtained through a sequential Ugi four component condensation (4CC)/Staudinger reaction reacted at room temperature with isocyanates to give carbodiimides, which were heated in toluene to give, unexpectedly, 2,3,4-trisubstituted 3,4-dihydroquinazolines, with R^2CO group migration from NR^3 to NR^4.

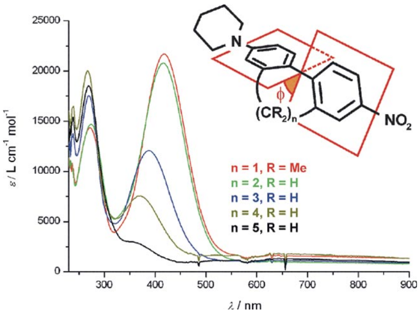
P. He, J. Wu, Y.-B. Nie,
M.-W. Ding* **1088–1095**

Unexpected Synthesis of Rearranged 3,4-Dihydroquinazolines by a Sequential Ugi 4CC/Aza-Wittig/Carbodiimide-Mediated Cyclization

Keywords: 3,4-Dihydroquinazolines / Multicomponent reactions / Ugi reaction / Aza-Wittig reaction / Azides / Cyclization

NLO Model Compounds

Get a Grip on Conjugation: The synthesis of a series of biphenyl push-pull model compounds with restricted torsion angles due to a bridging alkyl chain of varying length is described. The interdependence of the chromophore's π-conjugation and the resulting optical features are reported.



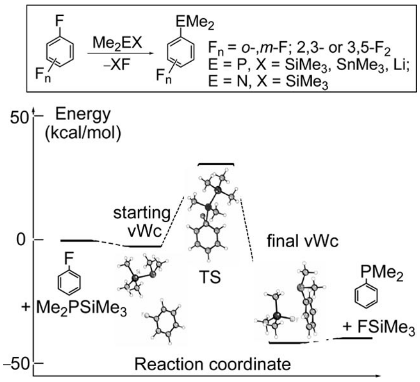
J. Rotzler, D. Vonlanthen,
A. Barsella, A. Boeglin,* A. Fort,
M. Mayor* **1096–1110**

Variation of the Backbone Conjugation in NLO Model Compounds: Torsion-Angle-Restricted, Biphenyl-Based Push-Pull-Systems

Keywords: Nonlinear optics / Conjugation / Chromophores / Push-pull systems / Torsion angle / Oxidation / Biphenyl

Aromatic Nucleophilic Substitution

Experimental observations (substrate selectivities and regioselectivities) and high-level quantum-chemical DFT and MP2 calculations reveal that the synthetically significant reactions between di- or trifluorobenzene and Me_2EX ($E = P$, $X = SiMe_3$, $SnMe_3$, Li; $E = N$, $X = SiMe_3$) in the gas phase or in nonpolar media each proceed by a concerted mechanism with a single transition state.



L. I. Goryunov, J. Grobe,* D. Le Van,
V. D. Shteingarts,* R. Mews, E. Lork,
E.-U. Würthwein* **1111–1123**

Di- and Trifluorobenzenes in Reactions with Me_2EM ($E = P$, N; $M = SiMe_3$, $SnMe_3$, Li) Reagents: Evidence for a Concerted Mechanism of Aromatic Nucleophilic Substitution

Keywords: Phosphanes / Polyfluoroarenes / Aromatic substitution / Nucleophilic substitution / Ab initio calculations / Bis(phosphane)palladium dichloride complexes

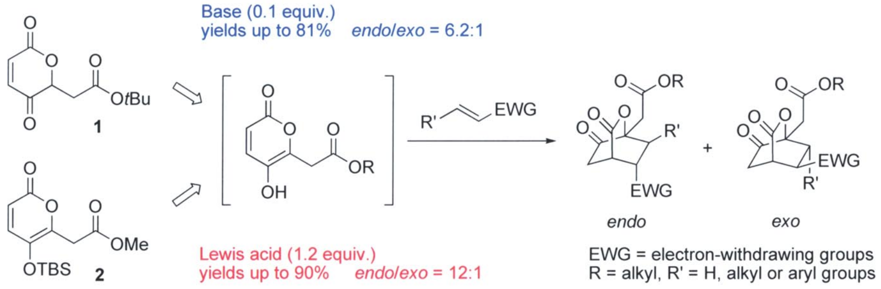
CONTENTS

2-Pyrone Diels–Alder Cycloaddition

W. Wu, S. He, X. Zhou, C.-S. Lee* 1124–1133

Diels–Alder Cycloadditions of 5-Hydroxy-2-pyrones: 2*H*-Pyran-2,5-diones and 5-(*tert*-Butyldimethylsilyloxy)-2-pyrones as Synthons

Keywords: Cycloaddition / Lactones / 2-Pyrones



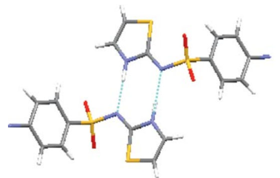
Both 2*H*-pyran-2,5-diones and 5-(*tert*-butyldimethylsilyloxy)-2-pyrones have been successfully utilized as synthons for 5-hydroxy-2-pyrones in Diels–Alder (DA) cycloadditions at RT. The equilibration/DA cycloaddition of **1** was optimized with *c*Hex$_2$NMe in *t*BuOH and the Lewis-acid-promoted DA cycloaddition of **2** was optimized with BF$_3$·OEt$_2$ in CH$_2$Cl$_2$.

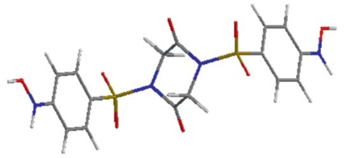
Crystal Polymorphism

S. E. Lawrence, M. T. McAuliffe, H. A. Moynihan* 1134–1141

Mimics of a $R_2^2(8)$ Hydrogen-Bond Dimer Motif: Synthesis and Influence on the Crystallisation of Sulfathiazole and Sulfapyridine

Keywords: Crystal polymorphism / Hydrogen bonds / Sulfathiazole / Sulfapyridine / Polymorphism / Sulfur heterocycles





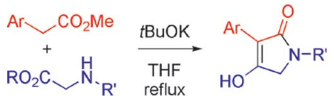
The syntheses and effects of three compounds, which mimic a specific hydrogen-bonding motif, on crystallisations of sulfathiazole and sulfapyridine are reported.

Heterocycle Synthesis

A. Mallinger, B. Nadal, N. Chopin, T. Le Gall* 1142–1148

One-Pot Synthesis of 3-Aryltetramic Acids

Keywords: Tetramic acid / Nitrogen heterocycles / Amides / Ring closure / Dieckmann condensation / Synthetic methods



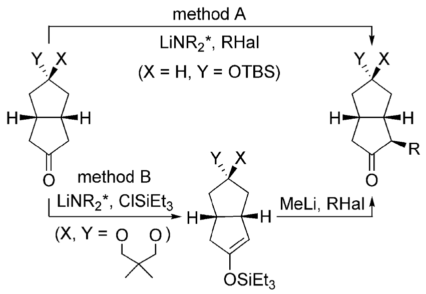
A tandem process that combines an amide formation and a condensation reaction allowed the straightforward, one-pot preparation of several 3-aryltetramic acids from amino esters and methyl arylacetates.

Enantioselective Deprotonation

V. Lutz, A. Baro, P. Fischer, S. Laschat* 1149–1157

Synthesis of Functionalized Hydropentalenes by an Asymmetric Deprotonation/Alkylation Strategy

Keywords: Alkylation / Asymmetric synthesis / Bicyclic compounds / Chiral bases / Weiss diketone / Chiral auxiliaries

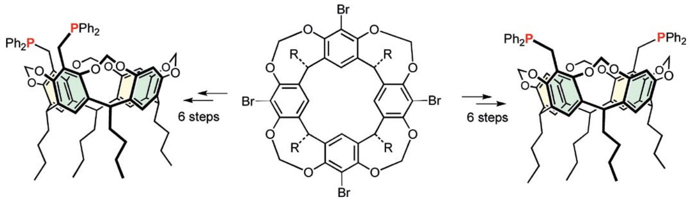


α-Alkylated hydropentalenones are accessible with good diastereoselectivities from differently substituted ketones either by a direct enantioselective deprotonation/alkylation route (Method A) or by an enantioselective deprotonation/trapping/alkylation sequence via the corresponding silyl enol ethers (Method B), depending on the substituents X and Y.

Cavity-Shaped Diphosphanes

Regioselective Grafting of Two $-CH_2P(X)Ph_2$ Units (X = O, Lone Pair) onto a Resorcin[4]arene-Derived Cavitand

Keywords: Resorcinarene / Cavitands / Phosphanes / Phosphane oxides / Ruthenium

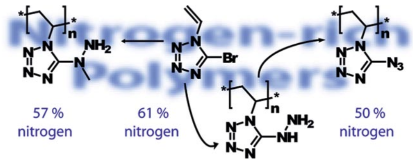


The first diphosphanes based on a resorcinarene cavitand were conveniently prepared in six steps from a tetrabrominated precursor. The new ligands were shown to be suitable for the preparation of bimetallic complexes without alteration of the shape of the generic cavitand core.

Nitrogen-Rich Polymer

Nitrogen-Rich Polymers Based on 5-Bromo-1-vinyl-1*H*-tetrazole

Keywords: Nitrogen heterocycles / Nitrogen-rich compounds / Tetrazole / Polymers / Polymerization

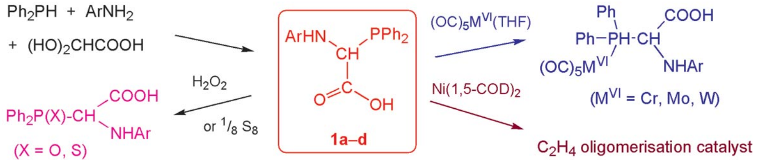


Starting from 5-bromo-1-vinyl-1*H*-tetrazole several nitrogen-rich polymers were synthesized by radical polymerization. The polymers possess nitrogen contents ranging from 50−60 %. They have moderate energetic properties, along with thermal stabilities up to 270 °C.

α-Phosphanylglycines

α-Phosphanyl Amino Acids: Synthesis, Structure and Reactivity of *N*-Aryl-α-phosphanylglycines 💻

Keywords: P ligands / Amino acids / Hydrolysis / Solvent effects / Oligomerization



N-Aryl-α-phosphanylglycines have been prepared by one-pot three-component reactions of diphenylphosphane, primary arylamines, and glyoxylic acid hydrate at ambient temperature. The properties, structural aspects and selected reactions characterize the new α-phosphanyl amino acids, their reactivity and potential use.

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* Author to whom correspondence should be addressed.

💻 Supporting information on the WWW (see article for access details).