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Contents

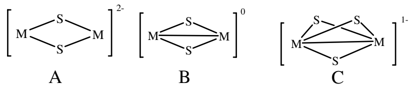
Regular papers

Zhangfeng Zhou, Botao Zhuang, Kechen Wu, Ping Liu, Yongqin Wei, Yuangen Yao

J. Organomet. Chem. 692 (2007) 1411

Synthesis, crystal structures and calculated nonlinear optical properties of seven di-nuclear metal (0, I) carbonyl cyclohexanthiolates, $[M_2(\mu\text{-}SC_6H_{11})_x(CO)_y]^{n-}$ (M = Mo, W; $x = 2, 3; y = 6, 8; n = 0, 1, 2$)

Seven novel di-nuclear molybdenum and tungsten metal cluster complexes with cyclohexanthiolate ligand, $[Et_4N]_2[Mo_2(SC_6H_{11})_2(CO)_8]$ (**1**), $[Et_4N][Mo_2(SC_6H_{11})_3(CO)_6]$ (**2**), $[Ph_4P][Mo_2(SC_6H_{11})_3(CO)_6]$ (**3**), $[(CH_3)_3PhCH_2N][Mo_2(SC_6H_{11})_3(CO)_6]$ (**4**), $[Et_4N]_2[W_2(SC_6H_{11})_2(CO)_8]$ (**5**), $[W_2(SC_6H_{11})_2\ (CO)_8]$ (**6**) and $[Et_4N][W_2(SC_6H_{11})_3(CO)_6]$ (**7**) have been synthesized and characterized. The crystal structures of seven compounds reveal that **1** and **5** contain a planar $M(0)_2S_2$ core (A); **6** contains a planar $M_2(I)S_2$ core(B); **2**, **3**, **4** and **7** contain a $M_2(I)S_3$ core (C) (M = Mo, W). IR of these seven complexes was measured. Compounds **2** and **7** have been predicted to have large first-order hyperpolarizability, 13×10^{-30} esu and 8×10^{-30} esu, respectively, which could be IR second-order nonlinear optical candidate materials.

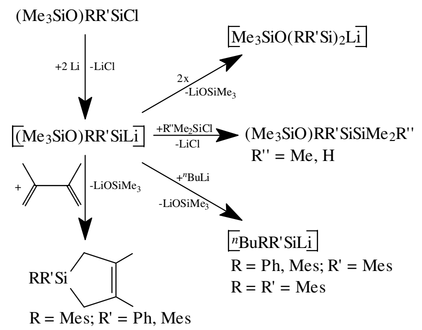


Joerg Harloff, Eckhard Popowski, Helmut Reinke

J. Organomet. Chem. 692 (2007) 1421

Substituted lithiumtrimethylsiloxysilanides $LiSiRR'(OSiMe_3)$ – Investigations of their synthesis, stability and reactivity

Chlorosilanes $(Me_3SiO)RR'SiCl$ (R/R′ = (H, Me, Et, ^{i}Pr, ^{t}Bu, Ph, Mes, Tip)/Ph and Mes/Mes) react with lithium metal to give $Me_3SiO(RR'Si)_nLi$ (n = 1, 2), $Me_3SiRR'SiLi$ and $(LiO)RR'SiLi$. The stability of $(Me_3SiO)RR'SiLi$ depends on substituents and temperature. In the reaction of selected derivatives $(Me_3SiO)RR'SiLi$ with ^{n}BuLi and 2,3-dimethylbuta-1,3-diene n-butylation products and silacyclopentenes are obtained, respectively.



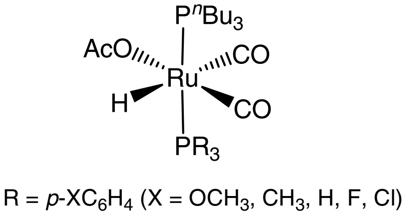
Luca Salvi, Antonella Salvini, Francesca Micoli, Claudio Bianchini, Werner Oberhauser

J. Organomet. Chem. 692 (2007) 1442

Mononuclear ruthenium complexes containing two different phosphines in *trans* position: II. Catalytic hydrogenation of C═C and C═O bonds

Bis(acetate) ruthenium(II) complexes $Ru(CO)_2(OAc)_2(P^nBu_3)[P(p\text{-}XC_6H_4)_3]$, containing different phosphine ligands *trans* to P^nBu_3, have been employed as catalyst precursors for the hydrogenation of alkenes, ketones and α,β-unsaturated ketones.

The heterodiphosphine monohydride catalysts show an excellent selectivity in the hydrogenation of *trans*-4-phenyl-3-buten-2-one to the corresponding allylic alcohol, *trans*-4-phenyl-3-buten-2-ol (>90%).



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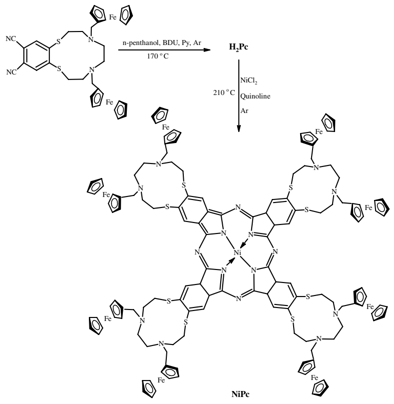
M. Nedim Mısır, Yaşar Gök, Halit Kantekin

J. Organomet. Chem. 692 (2007) 1451

Synthesis and characterization of metal-free and metallophthalocyanines containing N_2S_2-type macrocyclic moieties linked ferrocenyl groups

Metal-free phthalocyanine and metallophthalocyanines containing macrocyclic moieties linked ferrocenyl units have been synthesized by direct cyclotetramerization of the precursor substituted dicyano compound. These compounds were characterized using elemental analysis, UV–Visible, IR, ^{1}H NMR, ^{13}C NMR and MS spectroscopy techniques.

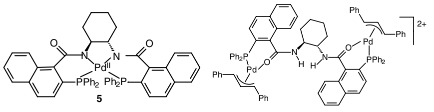


Christian Amatore, Anny Jutand, Laure Mensah, Louis Ricard

J. Organomet. Chem. 692 (2007) 1457

On the formation of Pd(II) complexes of Trost modular ligand involving N–H activation or P,O coordination in Pd-catalyzed allylic alkylations

Side Pd(II) complex **5** formed together with the Pd(0) ligated by the Trost ligand **4**. P,O coordination of the Trost ligand **4** in stable $\{[(\eta^3\text{-allyl})Pd]_2(\mathbf{4})\}^{2+}$.

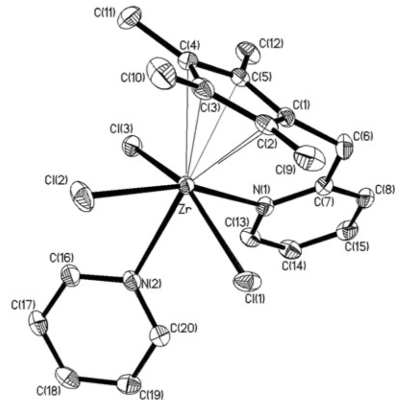


Dmitrii P. Krut'ko, Roman S. Kirsanov, Sergey A. Belov, Maxim V. Borzov, Andrei V. Churakov

J. Organomet. Chem. 692 (2007) 1465

Complexes of titanium and zirconium based on $[C_5Me_4CH_2\text{-}(2\text{-}C_5H_4N)]$ ligand

Half-sandwich $[Cp^{Py}]MCl_3$ (M = Ti, Zr; $Cp^{Py} = C_5Me_4CH_2\text{-}(2\text{-}C_5H_4N)$) and sandwich $[Cp^{Py}][C_5Me_5]ZrCl_2$ complexes were prepared and characterized. Evidence of the intramolecular coordination of the pyridyl group in both half-sandwiches in solutions is provided by NMR data. Crystal structure of $[Cp^{Py}]MCl_3{}^*Py$ was established by X-ray diffraction analysis.

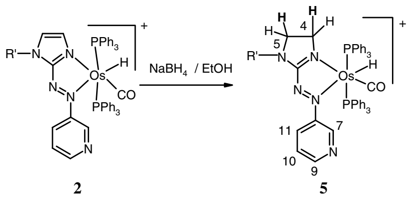


T.K. Mondal, T. Mathur, A.M.Z. Slawin, J.D. Woollins, C. Sinha

J. Organomet. Chem. 692 (2007) 1472

Imidazole → imidazolidine. Preparation by reduction of $[Os(H)(CO)(PPh3)2(PyaiR)]^{+/0}$ with $NaBH_4$ and characterisation of the products (PyaiR = 1-alkyl-2-{3′-(pyridylazo)}-imidazole)

Reduction of $[Os(H)(CO)(PPh_3)_2\ (PyaiR)](PF_6)$ (**2**) with $NaBH_4$ has separated $[Os(H)(CO)(PPh3)2(PyaiR'H2)]^{+/0}$ (**5**), an imidazole (C(4)–C(5)) reduced product. While the reaction of PyaiR and $[Os(H)(Cl)\ (CO)(PPh_3)_3]$ in dry *n*-heptane has separated shining green compound and has been identified azo-anion radical, $[Os(Cl)(CO)(PPh_3)_2(PyaiR^{-\cdot})]$ (**4b–4d**).

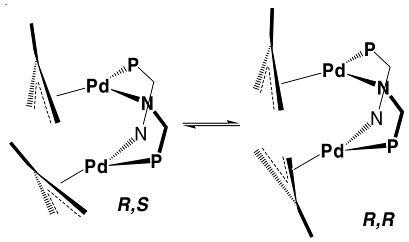


Virginia Díez, Gustavo Espino, Félix A. Jalón, Blanca R. Manzano, Mercedes Pérez-Manrique

J. Organomet. Chem. 692 (2007) 1482

Synthesis and structure of new palladium complexes with the ligand 2-(diphenylphosphino)-1-methylimidazole: Evidence of hemilability

New Palladium(II) derivatives containing the bidentate 2-(diphenylphosphino)-1-methylimidazole, dpim, ligand have been prepared. A water adduct with a hydrogen bond to the coordinated dpim has been obtained and the hemilability of the ligand has been demonstrated. A fluxional process that involves Pd–N bond rupture has been found for the allyl derivative.

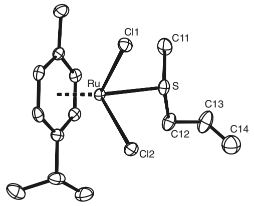


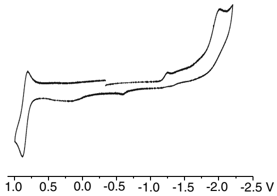
Jadranka Čubrilo, Ingo Hartenbach, Falk Lissner, Thomas Schleid, Mark Niemeyer, Rainer F. Winter

J. Organomet. Chem. 692 (2007) 1496

p-Cymene ruthenium thioether complexes

Simple thioether complexes [(*p*-cymene)$RuCl_2(SRR')$] with methyl, allyl, and alkylaryl substituents have been prepared and studied by X-ray crystallography. Voltammetry suggests thioether dissociation as the primary degradation pathway of the associated radical cations and anions.



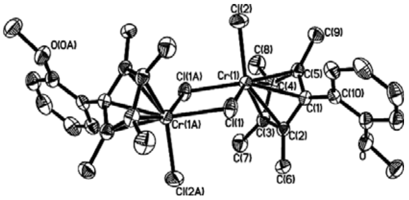


Jiansheng Xu, Wei Gao, Yuetao Zhang, Jincai Li, Ying Mu

J. Organomet. Chem. 692 (2007) 1505

New *o*-methoxyphenylcyclopentadienylchromium (III) complexes: Synthesis, structures and catalytic properties for ethylene polymerization

Two new chromium complexes η^5-1-(2-methoxyphenyl)-3,4-diphenylcyclopentadienyl chromium dichloride and η^5-1-(2-methoxyphenyl)-2,3,4,5-tetramethylcyclopentadienyl chromium dichloride were synthesized and characterized. Both complexes exhibited high catalytic activities for ethylene polymerization in the presence of $Al(^iBu)_3$ and $Ph_3C^+B(C_6F_5)_4^-$.

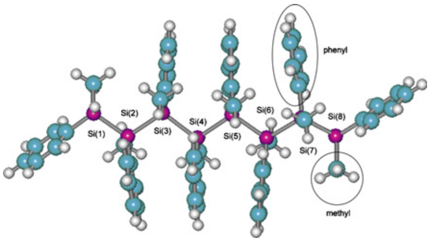


Hiroto Tachikawa, Hiroshi Kawabata

J. Organomet. Chem. 692 (2007) 1511

Electronic states of radical cations of all-*trans* oligo[methyl(phenyl)silane]

The electronic states of radical cations of oligo[methyl(phenyl)silane] ($OMPSi^+$) with all *trans* form (n = 2–8, where n is number of monomer unit of OMPSi) have been investigated by means of density functional theory (DFT) calculation to shed light on the mechanism of hole-transport in oligosilanes with phenyl group in the side chain.

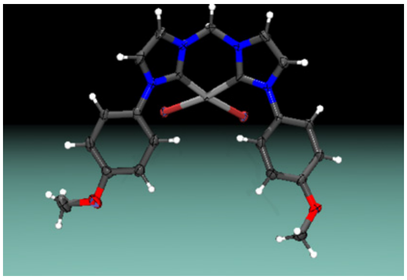


**Maria A. Taige, Alexander Zeller,
Sebastian Ahrens, Sigrid Goutal,
Eberhardt Herdtweck, Thomas Strassner**

J. Organomet. Chem. 692 (2007) 1519

New Pd–NHC-complexes for the Mizoroki–Heck reaction

The synthesis, structural characterization and catalytic application of novel bridged *N*-aryl substituted palladium(II)–biscarbenecomplexes in the Mizoroki–Heck reaction are reported. The activity of the investigated aryl substituted catalysts is significantly higher compared to the corresponding methyl substituted NHC complexes.

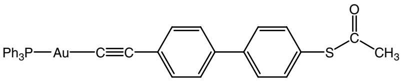


**Katrin Rößler, Tobias Rüffer,
Bernhard Walfort, Rico Packheiser,
Rudolf Holze, Michael Zharnikov,
Heinrich Lang**

J. Organomet. Chem. 692 (2007) 1530

Synthesis, characterization and electrochemical behavior of unsymmetric transition metal-terminated biphenyl ethynyl thiols

The synthesis, characterization and electrochemical behavior of R'–C≡C–C_6H_4–C_6H_4–SR (R' = $SiMe_3$, R = C(O)Me; R' = $SiMe_3$, R = H; R' = H, R = C(O)Me) and L_nM'–C≡C–C_6H_4–C_6H_4–SR (L_nM = Fc, R = C(O)Me; L_nM = Fc, R = H; L_nM = $(Ph_3P)Au$, R = C(O)Me; L_nM = $FcPPh_2$-Au, R = C(O)Me; Fc = $(\eta^5\text{-}C_5H_5)(\eta^5\text{-}C_5H_4)Fe$; $FcPPh_2$ = $(\eta^5\text{-}C_5H_5)(\eta^5\text{-}C_5H_4PPh_2)Fe$) is discussed. The solid state structures of six compounds are reported as well.

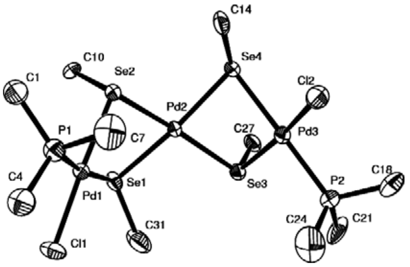


**Liladhar B. Kumbhare, Vimal K. Jain,
Prasad P. Phadnis, Munirathinam Nethaji**

J. Organomet. Chem. 692 (2007) 1546

Palladium(II) and platinum(II) 2-(methoxycarbonyl)ethylselenolates: Synthesis, spectroscopy, structures and their conversion into metal selenide

Reactions of $MeOOCCH_2CH_2SeNa$ with $[M_2Cl_2(\mu\text{-}Cl)_2(PR_3)_2]$ yield a variety of products of compositions $[M_2Cl_2(\mu\text{-}SeCH_2CH_2COOMe)_2(PR_3)_2]$(**2**), $[M_2Cl_2(\mu\text{-}Cl)(\mu\text{-}SeCH_2CH_2COOMe)(PR_3)_2]$(**3**), $[Pd_2(SeCH_2CH_2COOMe)_2(\mu\text{-}SeCH_2CH_2COOMe)_2(PR_3)_2]$(**4**) and $[Pd_3Cl_2(\mu\text{-}SeCH_2CH_2COOMe)_4(PR_3)_2]$ (**5**). A homoleptic palladium complex, $[Pd(SeCH_2CH_2COOMe)_2]_6$ (**6**) is formed by a reaction between Na_2PdCl_4 and $MeOOCCH_2CH_2SeNa$. These complexes have been characterized by elemental analysis, IR, UV–Vis and NMR (^1H, ^{13}C, ^{31}P, ^{77}Se, ^{195}Pt) spectroscopy and X-ray crystallography for representative complexes. Pyrolysis of $[Pd_2Cl_2(\mu\text{-}SeCH_2CH_2COOMe)_2(P''Pr_3)_2]$ in tributylphosphate at 195 °C gave $Pd_{17}Se_{15}$ nanoparticles which were characterized by XRD and EDAX.

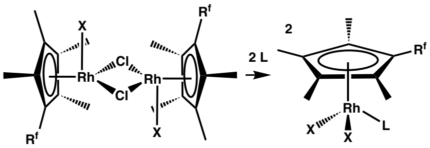


**Jan Čermák, Jaroslav Žádný, Alena Krupková,
Kateřina Lopatová, Alena Vlachová,
Thu Huong Nguyen Thi, Jana Šauliová,
Jan Sýkora, Ivana Císařová**

J. Organomet. Chem. 692 (2007) 1557

Tetramethyl(perfluoroalkyl) cyclopentadienyl rhodium(III) complexes containing phosphorus and nitrogen monodentate donors. Crystal structure of $[(\eta_5\text{-}C_5Me_4C_4F_9)Rh(PPr_3^{\,i})Cl_2]$

Rh(III) piano-stool type complexes $[(C_5Me_4C_nF_{2n+1})RhX_2L]$ (n = 4, 6; X = Cl, Br; L = two-electron donor) were prepared, crystal structure of $[(\eta^5\text{-}C_5Me_4C_4F_9)Rh(PPr_3^{\,i})Cl_2]$ was determined by X-ray. Hindered rotation of triarylphosphine and 2-substituted pyridine ligands around Rh–L bond was observed and analyzed with the help of variable temperature NMR.



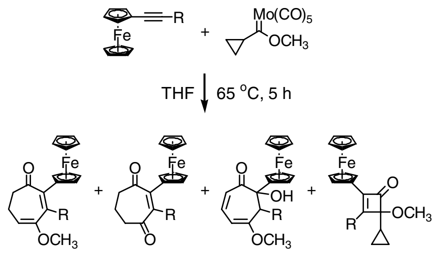
X = Cl, Br; R^f = C_4F_9, C_6F_{13}; L: alkylphosphines, arylphosphines, phosphites, pyridine-derived heterocyclic amines

Metin Zora, Canet Açıkgöz, Mustafa Odabaşoğlu, Orhan Büyükgüngör

J. Organomet. Chem. 692 (2007) 1571

Coupling of pentacarbonyl[(cyclopropyl) methoxymethylene]molybdenum complex with ferrocenyl alkynes: Synthesis of ferrocenyl-substituted cycloheptadienones and cycloheptenediones

The coupling of pentacarbonyl[(cyclopropyl)methoxymethylene]molybdenum complex with ferrocenyl alkynes produces ferrocenyl-substituted cycloheptadienones as the major products, accompanied by varying amounts of cycloheptenediones and/or cyclobutenones.

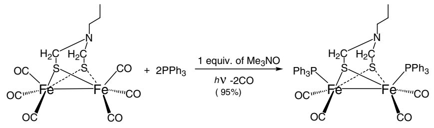


Weiming Gao, Jianhui Liu, Björn Åkermark, Licheng Sun

J. Organomet. Chem. 692 (2007) 1579

Facile and highly efficient light-induced PR_3/CO ligand exchange: A novel approach to the synthesis of $[(\mu\text{-}SCH_2N^nPrCH_2S)Fe_2(CO)_4(PR_3)_2]$

An efficient and improved approach towards the transformation of the Fe–S complex $[(\mu\text{-}SCH_2N^nPrCH_2S)Fe_2(CO)_6]$ to its double phosphine coordinated analogue $[(\mu\text{-}SCH_2N^nPrCH_2S)Fe_2(CO)_4(PR_3)_2]$ (R = Ph, Me) was disclosed.

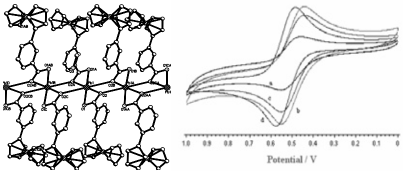


Jinpeng Li, Yinglin Song, Hongwei Hou, Mingsheng Tang, Yaoting Fan, Yu Zhu

J. Organomet. Chem. 692 (2007) 1584

1-D Polymeric divalent metal *m*-ferrocenylbenzoates: Structures, NLO and electrochemical properties

Three 1-D *m*-ferrocenylbenzoate metal polymers: $\{[Pb(\mu_2\text{-}\eta^2\text{-}OOCH_4C_6Fc)_2]\cdot(CH_3OH)_2\}_n$(**1**), $[Zn(OOCH_4C_6Fc)_2(bpe)]_n$ (**2**) and $[Mn(\eta^2\text{-}OCH_4C_6Fc)_2(4,4'\text{-}bpy)]_n$ (**3**) were synthesized and structurally characterized. By quantum chemistry calculation we elucidate the possible reason for their electrochemical behaviors and confirm the nonlinear refractive behaviors of the three polymers mainly come of the ferrocenyl ligands and organic adjuvant ligands; Mn(II) ions and Pb(II) ions have also some influence on NLO properties.

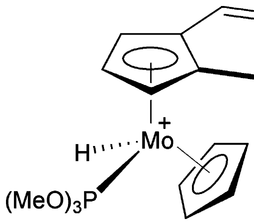


Isabel S. Gonçalves, Cláudia C.L. Pereira, Carla A. Gamelas, Alan Hazell, Carlos C. Romão

J. Organomet. Chem. 692 (2007) 1593

Synthesis and structural characterization of new mixed-ring indenyl derivatives of molybdenum containing phosphorus ligands

A group of novel mixed ring molybdenum cations containing phosphorus ligands is reported, starting from the dicationic compounds $[IndCpMoL_2][BF_4]_2$ with L = dppe or $P(OMe)_3$. The diene complexes of the type $[IndMo\{\eta^4\text{-}C_5H_5(R)\}L_2]^+$ (L = dppe or $P(OMe)_3$; R = H, CH_2Cl) and also the asymmetric hydride complex $[IndCpMoH\{P(OMe)_3\}]PF_6$ were characterized by experimental techniques, including X-ray crystallographic studies and cyclic voltammetry.

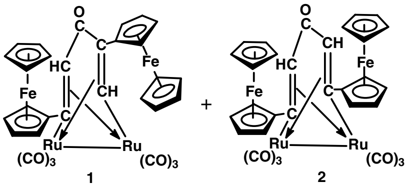


Pradeep Mathur, Saurav Chatterjee,
Atanu Das, Goutam K. Lahiri, Somnath Maji,
Shaikh M. Mobin

J. Organomet. Chem. 692 (2007) 1601

Synthesis, structure and electrochemistry of CO incorporated diruthenium metallacyclic compounds $[Ru_2(CO)_6\{\mu\text{-}\eta^1:\eta^1:\eta^2:\eta^2\text{-}1,4\text{-}Fc_2C_5H_2O\}]$ and $[Ru_2(CO)_6\{\mu\text{-}\eta^1:\eta^1:\eta^2:\eta^2\text{-}1,5\text{-}Fc_2C_5H_2O\}]$

Ferrocenyl substituted ruthenium metallacyclic compounds, $[Ru_2(CO)_6\{\mu\text{-}\eta^1:\eta^1:\eta^2:\eta^2\text{-}1,4\text{-}Fc_2C_5H_2O\}]$ (**1**) and $[Ru_2(CO)_6\{\mu\text{-}\eta^1:\eta^1:\eta^2:\eta^2\text{-}1,5\text{-}Fc_2C_5H_2O\}]$ (**2**) have been synthesized and structurally characterized. Electrochemical studies for **1** and **2** and the respective quinones, **3** and **4** show electrochemical coupling between the two redox active ferrocenyl units via the bridging ligand. The electrochemical coupling has been observed to depend upon the orientation and position of the ferrocenyl units.



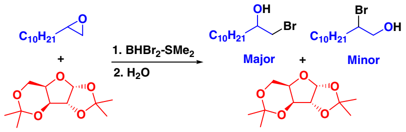
Notes

Chandra D. Roy, Herbert C. Brown

J. Organomet. Chem. 692 (2007) 1608

A highly regio- and chemoselective synthesis of vicinal bromohydrins by ring opening of terminal epoxides with dibromoborane–dimethyl sulfide

Regio- and chemoselective cleavage of epoxides into β-bromohydrins utilizing the commercially available reagent, $BHBr_2–SMe_2$, is described. Several reactive and reducible functional groups, such as, alkene, alkyne, allene, ethers, acetal, ketal, chloride, aldehyde, ketone, azide, ester, nitrile and *tert*-amino ester, have been successfully accommodated during the epoxide opening reactions.

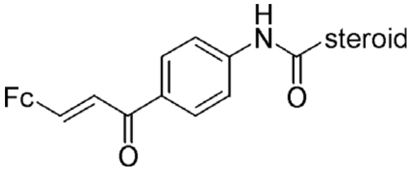


János Balogh, Virág Zsoldos-Mády,
Dávid Frigyes, Attila C. Bényei,
Rita Skoda-Földes, Pál Sohár

J. Organomet. Chem. 692 (2007) 1614

Synthesis of novel ferrocene labelled steroidal derivatives via palladium-catalysed carbonylation. X-ray structure of 17-(*N*-(4′-((2-ferrocenyl-ethenyl)-carbonyl)-phenyl)carbamoyl)-5α-androst-16-ene

Palladium-catalysed aminocarbonylation of steroidal alkenyl iodides has been carried out in the presence of ferrocenyl chalcone **6**. The products were obtained in moderate to good yield and were characterised with various spectroscopic methods. The solid state structure of 17-(*N*-(4′-((2-ferrocenyl-ethenyl)-carbonyl)-phenyl)-carbamoyl)-5α-androst-16-ene (**1a**) has been determined by X-ray crystallography.



Weiying Lin, Lingliang long, Daiwei Peng, Cancheng Guo

J. Organomet. Chem. 692 (2007) 1619

A novel application of tin-based alkoxide anion for deacetylation

A combination of cyclic dialkyltin alkoxide with CsF can deacetylate acetates under very mild condition, and a likely deacetylation mechanism is proposed.