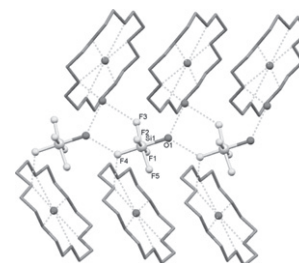




Graphical Abstracts/J. Fluorine Chem. 135 (2012) 1–14

J. Fluorine Chem., 135 (2012) 15

Supramolecular compounds of fluorocomplexes of *p*-elements with crown and azacrown ethers: Synthesis, transformations and crystal structuresVladimir O. Gelmboldt^{a,b}, Eduard V. Ganin^c, Marina S. Fonari^d^aOdessa National Medical University, Valikhovskiy lane 2, 65026 Odessa, Ukraine^bPhysico-Chemical Institute of the Environment and Human Protection, Odessa, Ukraine^cOdessa State Environmental University, Lvovskaya str. 15, 65016 Odessa, Ukraine^dInstitute of Applied Physics, Academy of Sciences of Moldova, Academiei str., 5, MD-2028 Chisinau, Republic of Moldova

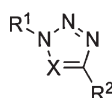
J. Fluorine Chem., 135 (2012) 25

A structure–function study of the surface tension changes of *m*-xylene in the presence of fluorous 1H-1,2,3-triazoles and tetrazoles

Roger W. Read, Xiaobei Wang

School of Chemistry, University of New South Wales, UNSW Sydney, NSW 2052, Australia

Assessment of the surface activity of 28 fluorous 1,2,3-triazoles and 6 fluorous tetrazoles, along with 2 non-fluorous triazoles, through surface tension measurements in *m*-xylene, has provided information on the major factors that contribute to ordered surface activity within these closely related classes of compounds.

 $R^1 = (\text{CH}_2)_n\text{CH}_3; (\text{CH}_2)_n\text{C}_m\text{F}_{2m+1}$ $R^2 = (\text{CH}_2)_n\text{CH}_3; \text{CH}_2\text{O}(\text{CH}_2)_n\text{CH}_3; \text{CH}_2\text{O}(\text{CH}_2)_n\text{C}_m\text{F}_{2m+1}; \text{CH}_2\text{O}(\text{CH}_2\text{CH}_2\text{O})_3\text{CH}_3$ $X = \text{CH}; \text{N}$

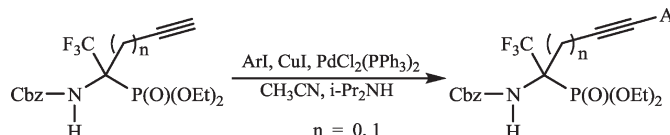
J. Fluorine Chem., 135 (2012) 33

Synthesis of CF_3 -containing α -alkynyl- α -aminophosphonates by Sonogashira cross-coupling reaction

Maria A. Zotova, Tamara P. Vasilyeva, Alexander S. Peregudov, Sergey N. Osipov

A.N. Nesmeyanov Institut of Organoelement Compounds, Russian Academy of Sciences, Vavilov Str. 28, 119991 Moscow, Russian Federation

An efficient route to new α - CF_3 - α -aminophosphonic acid derivatives bearing an arylalkynyl moiety at the α -carbon atom has been developed.



J. Fluorine Chem., 135 (2012) 38

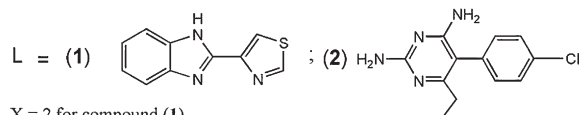
Self-assembly of hydrogen-bonded supramolecular structures based on hexafluorosilicate anion

Velusamy Sethuraman^{ab}, Stanley Nithianantham^a,
Packianathan Thomas Muthiah^a

^aSchool of Chemistry, Bharathidasan University, Tiruchirappalli 620 024, India

^bDepartment of Chemistry, Periyar Maniammai University, Vallam 613 403, Thanjavur, India

Interesting hydrogen-bonded supramolecular patterns have been achieved by hexafluorosilicate anion in the crystal structures of bis(thiabendazole) hexafluorosilicate dihydrate **1** and bis(pyrimethamine) hexafluorosilicate **2**.



X = 2 for compound (1)

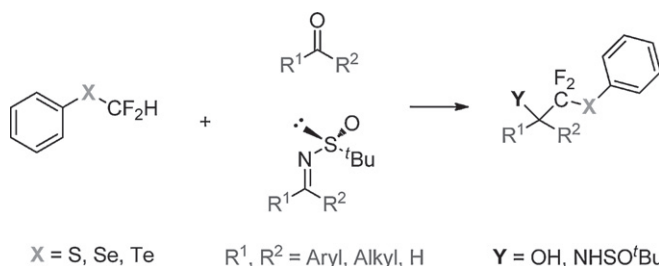
X = 0 for compound (2)

J. Fluorine Chem., 135 (2012) 45

Difluoro(phenylchalcogen)methylation of aldehydes, ketones, and imines with S-, Se-, and Te-containing reagents PhXCF₂H (X = S, Se, Te)

Mingyou Hu, Fei Wang, Yanchuan Zhao, Zhengbiao He,
Wei Zhang, Jinbo Hu

Key Laboratory of Organofluorine Chemistry, Shanghai Institute
of Organic Chemistry, Chinese Academy of Sciences, 345 Ling-Ling Road,
Shanghai 200032, China



J. Fluorine Chem., 135 (2012) 59

An in-depth *in situ* IR study of the thermal decomposition of copper trifluoroacetate hydrate

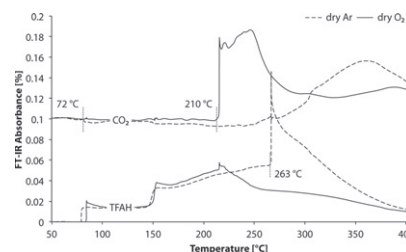
M. Mosiadz^a, K.L. Juda^{ab}, S.C. Hopkins^a, J. Soloduch^b, B.A. Glowacki^{ac}

^aDepartment of Materials Science and Metallurgy, University of Cambridge, Pembroke Street,
Cambridge, CB2 3QZ, United Kingdom

^bDepartment of Chemistry, Wrocław University of Technology, Wybrzeże Wyspiańskiego 27, 50-370
Wrocław, Poland

^cInstitute of Power Engineering, ul. Augustowska 6, 02-981 Warsaw, Poland

The different decomposition reaction paths of copper trifluoroacetate hydrate under flowing Ar and O₂ atmospheres have been identified. The violent exothermic nature of pyrolysis in an O₂ atmosphere has implications for sol-gel processing.



J. Fluorine Chem., 135 (2012) 68

Synthesis of pentafluoro-λ⁶-sulfanyl substituted acetylenes for novel liquid crystals

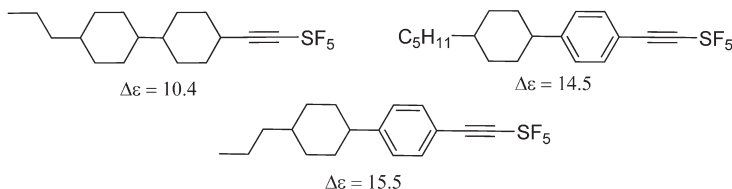
Maxim V. Ponomarenko^{ab}, Nataliya Kalinovich^a,
Yurii A. Serguchev^b, Matthias Bremer^c,
Gerd-Volker Rösenthaller^a

^aSchool of Engineering and Science, Jacobs University Bremen gGmbH,
Campus Ring 1, 28759 Bremen, Germany

^bInstitute of Organic Chemistry, National Academy of Sciences of Ukraine, 5 Murmanskaya, 02094 Kiev, Ukraine

^cMerck KGaA, 250 Frankfurterstr., 64271 Darmstadt, Germany

New, acetylenic liquid crystals with a pentafluoro-λ⁶-sulfanyl function as a terminal group were prepared and their physical properties were examined.

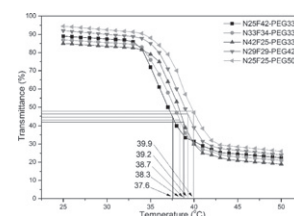


J. Fluorine Chem., 135 (2012) 75

Fluorine-containing thermo-sensitive core/shell microgel particles: Preparation, characterization, and their applications in controlled drug release

Guoqiang Liu^a, Xiaolong Li^a, Shengdong Xiong^a, Ling Li^a, Paul K. Chu^b, Shuilin Wu^{ab}, Zushun Xu^{ab}^aMinistry-of-Education Key Laboratory for the Green Preparation and Application of Functional Materials, Hubei University, Wuhan 430062, China^bDepartment of Physics & Materials Science, City University of Hong Kong, Tat Chee Avenue, Kowloon, Hong Kong, China

A novel series of fluorine-containing thermo-sensitive core/shell microgel particles were prepared via surfactant free emulsion polymerization. The copolymer microgels exhibited a lower critical solution temperature (LCST) above the normal human physiological temperature. The size and morphology of the microgel particles were both sensitive to the change of temperature. Furthermore, the drug-loaded microgels showed a desired thermo-responsive drug release behavior. The study indicated that the fluorine-containing thermo-sensitive copolymer microgels had promising potential applications as a "smart" drug carrier in biomedical field.



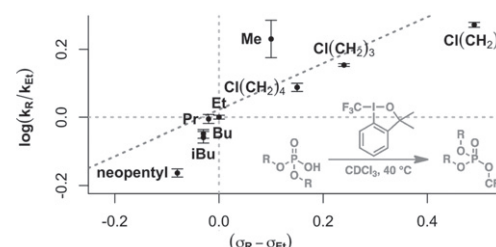
J. Fluorine Chem., 135 (2012) 83

Reactivity of an electrophilic hypervalent iodine trifluoromethylation reagent with hydrogen phosphates—A mechanistic study

Nico Santschi, Patrik Geissbühler, Antonio Togni

Department of Chemistry and Applied Biosciences, Swiss Federal Institute of Technology, Wolfgang-Pauli-Strasse 10, ETH Zürich, CH-8093 Zürich, Switzerland

A mechanistic study of the formation of trifluoromethyl phosphates by electrophilic trifluoromethylation of hydrogen phosphates is presented. The products easily decompose to corresponding fluorophosphates.



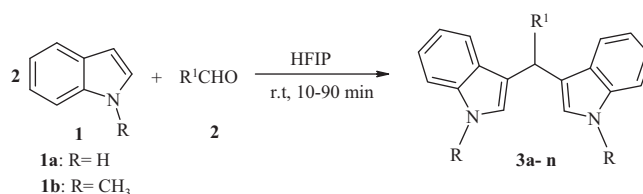
J. Fluorine Chem., 135 (2012) 87

A simple, efficient and green procedure for the synthesis of bis-indolyl methanes in 1,1,1,3,3,3-hexafluoro-2-propanol

Samad Khaksar, Saeed Mohammadzadeh Talesh

Chemistry Department, Ayatollah Amoli Branch, Islamic Azad University, PO Box 678, Amol, Iran

Bis-indolyl methanes derivatives were synthesized in excellent yield in hexafluoroisopropanol.

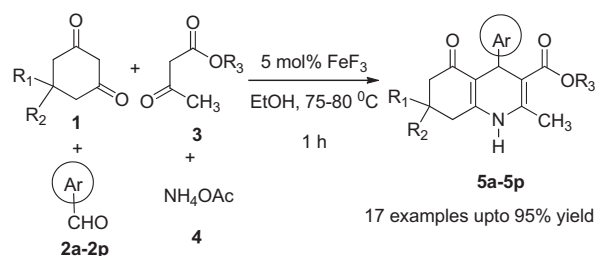


J. Fluorine Chem., 135 (2012) 91

FeF₃ as a novel catalyst for the synthesis of polyhydroquinoline derivatives via unsymmetrical Hantzsch reaction

Rajendra Surasani^{a,c}, Dipak Kalita^a, A.V. Dhanunjaya Rao^a, Kaviraj Yarbagi^b, K.B. Chandrasekhar^c^aCustom Pharmaceuticals Services, Dr. Reddy's Laboratories Ltd., Bollaram Road, Miyapur, Hyderabad 500049, India^bAnalytical Research, Dr. Reddy's Laboratories Ltd., Bollaram Road, Miyapur, Hyderabad 500049, India^cDepartment of Chemistry, Institute of Science and Technology, JNT University of Anantapur, Anantapur 515002, India

An efficient and one-pot protocol for the synthesis of polyhydroquinoline derivatives promoted by FeF₃ is described.



J. Fluorine Chem., 135 (2012) 97

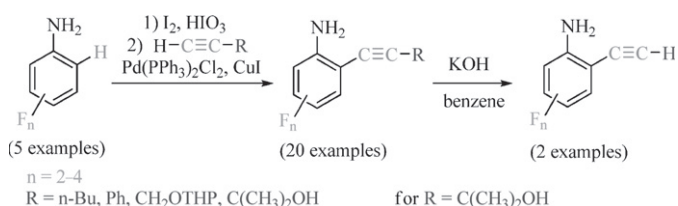
Synthesis of polyfluorinated *ortho*-alkynylanilines

Larisa V. Politanskaya^a, Igor P. Chuikov^a, Ekaterina A. Kolodina^b,
Mark S. Shvartsberg^b, Vitalij D. Shteingarts^a

^aN.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry, Siberian Branch of Russian Academy of Sciences, Acad. Lavrentiev Avenue 9, 630090 Novosibirsk, Russian Federation

^bA.A. Kovalsky Institute of Chemical Kinetics and Combustion, Siberian Branch of Russian Academy of Sciences, Institutskaya Str. 3, 630090 Novosibirsk, Russian Federation

A series of polyfluorinated *ortho*-alkynylanilines have been synthesized by the Sonogashira reaction of polyfluorinated *ortho*-iodanilines with terminal alkynes.

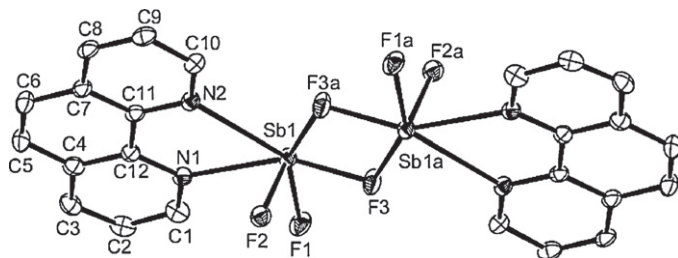
*J. Fluorine Chem.*, 135 (2012) 108

Synthesis and structures of antimony trifluoride complexes with N-heterocyclic ligands

Sophie L. Benjamin, Jennifer Burt, William Levason, Gillian Reid, Michael Webster

School of Chemistry, University of Southampton, Southampton SO17 1BJ, UK

The crystal structures of SbF₃ complexes with heterocyclic nitrogen ligands show a pyramidal SbF₃ core with longer bonds to the neutral ligand and longer Sb...F contacts typically completing a distorted seven-coordination at Sb.

*J. Fluorine Chem.*, 135 (2012) 114

Reactions of fluoroalk-1-en-1-yltrifluoroborate and perfluoroalk-1-yn-1-yltrifluoroborate salts and selected hydrocarbon analogues with hydrogen fluoride and with halogenating agents in aHF and in basic solvents

Vadim V. Bardin^a, Nicolay Yu. Adonin^{ab}, Hermann-Josef Frohn^c

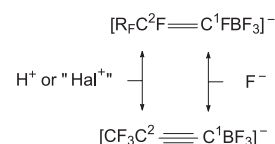
^aN.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry, SB RAS, Acad. Lavrentjev Avenue 9, 630090 Novosibirsk, Russian Federation

^bG.K. Borekov Institute of Catalysis, SB RAS, Acad. Lavrentjev Avenue 5, 630090 Novosibirsk, Russian Federation

^cInorganic Chemistry, University of Duisburg-Essen, Lotharstrasse 1, D-47048 Duisburg, Germany

The electrophilic halofluorination of K[R_FCF=CFBF₃] and K[R_FCHal=CFBF₃] or K[R_FC≡CFBF₃] with NCS or NBS in aHF yielded K[R_FCFHal-CF₂BF₃] and K[R_FCHalCF₂-CF₂BF₃] (Hal = Cl, Br), respectively. K[CF₃C≡CFBF₃] in aHF solution added slowly HF and formed K[CF₃CH₂CF₂BF₃] besides protodeboration (CF₃C≡CH and K[BF₄]). In the presence of traces of water K[CF₃CH₂-C(O)BF₃] was obtained as a by-product. K[*trans*-C₄F₉CF=CFBF₃] reacted with Cl₂ in MeOH to give K[C₄F₉CFCl-C(O)BF₃].

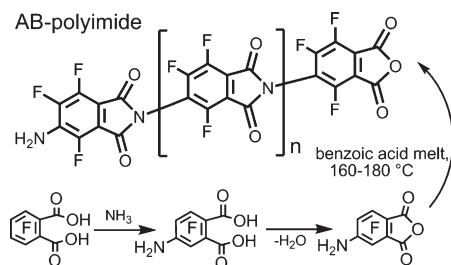
Alternatives to electrophilic deboration reactions:
Addition of the electrophile to C².

*J. Fluorine Chem.*, 135 (2012) 129

Synthesis and characterization of the first perfluoroaromatic polyimide of the AB-type

Tamara A. Vaganova, Inna K. Shundrina, Soltan Z. Kusov, Elena V. Karpova, Irina Yu. Bagryanskaya, Evgenij V. Malykhin

N. N. Vorozhtsov Novosibirsk Institute of Organic Chemistry, Siberian Branch of the Russian Academy of Sciences, Lavrentiev Avenue 9, 630090 Novosibirsk, Russian Federation

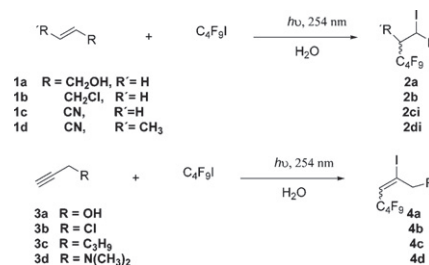


J. Fluorine Chem., 135 (2012) 137

Light-induced iodoperfluoroalkylation reactions of carbon-carbon multiple bonds in water

M. Slodowicz^a, S. Barata-Vallejo^b, A. Vázquez^b, N. Sbarbati Nudelman^b, A. Postigo^a^aFaculty of Science-University of Belgrano-Villanueva 1324 CP 1428-Buenos Aires, Argentina^bDepartamento de Química Orgánica-Facultad de Ciencias Exactas y Naturales-Universidad de Buenos Aires-Pabellón II, 3er piso-Ciudad Universitaria-CP 1428-Buenos Aires, Argentina

Radical iodoperfluorobutylation (Halogen Atom-transfer reactions) of alkenes and alkynes is achieved in water in yields ranging from 58 to 97%. The reaction products are obtained in higher yields in water than in previously studied media.

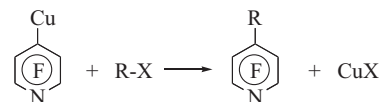


J. Fluorine Chem., 135 (2012) 144

Preparation of *p*-substituted tetrafluoropyridyl derivatives via the tetrafluoropyridylcopper reagent

Ba Van Nguyen, Donald J. Burton

Department of Chemistry, The University of Iowa, Iowa City, IA 52242, USA

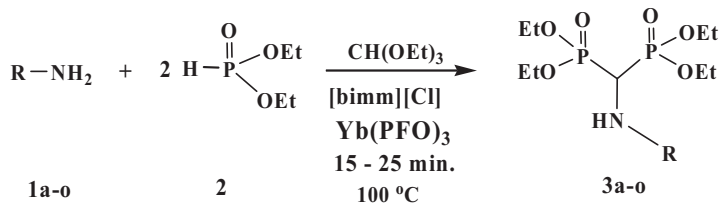
 R = allylic, vinyl, aryl, acetylenic, acyl, propargyl X = I, Br, Cl, OTs

J. Fluorine Chem., 135 (2012) 155

A facile synthesis of aminomethylene bisphosphonates catalyzed by ytterbium perfluorooctanoate under ionic liquid condition

Mudumala Veera Narayana Reddy^a, Jongsik Kim^b, Yeon Tae Jeong^a^aDepartment of Image Science and Engineering, Pukyong National University, Busan 608-737, Republic of Korea^bDepartment of Chemistry, Dong-A University, Busan 604-714, Republic of Korea

An efficient and one-pot protocol for the synthesis of aminomethylene bisphosphonates promoting by ytterbium perfluorooctanoate [$Yb(PFO)_3$] under ionic liquid conditions is described.

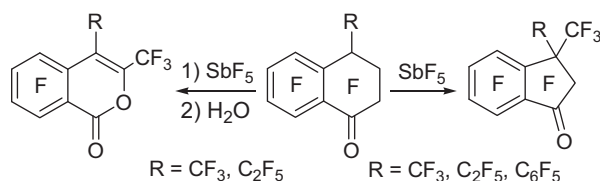


J. Fluorine Chem., 135 (2012) 159

Synthesis and skeletal rearrangements of perfluorinated 4-alkyl- and 4-phenyl-tetralin-1-ones under the action of antimony pentafluoride

Yaroslav V. Zonov, Victor M. Karpov, Vyacheslav E. Platonov

N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry, Novosibirsk 630090, Russia



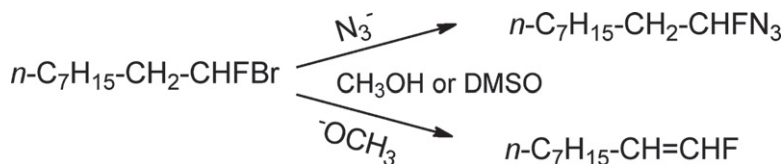
J. Fluorine Chem., 135 (2012) 167

Impact of fluorine substituents on the rates of nucleophilic aliphatic substitution and β -elimination

Henry Martinez, Adele Rebeyrol, Taylor B. Nelms, William R. Dolbier Jr

Department of Chemistry, PO Box 117200, University of Florida, Gainesville, FL 32611-7200, United States

α, α or γ -Fluorine substitution can have a profound effect upon the rates of substitution or elimination of an alkyl halide.



J. Fluorine Chem., 135 (2012) 176

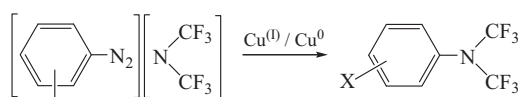
A convenient synthesis of *N,N*-bis(trifluoromethyl)anilines

M.E. Hirschberg^a, N.V. Ignat'ev^b, A. Wenda^a, H.-J. Frohn^c, H. Willner^a

^aInorganic Chemistry, Bergische Universität Wuppertal, Gaußstr. 20, D-42097 Wuppertal, Germany

^bPM-ABE, Merck KGaA, Frankfurter Str. 250, D-64293 Darmstadt, Germany

^cInorganic Chemistry, Universität Duisburg-Essen, D-47048 Duisburg, Lotharstr. 1, Germany



J. Fluorine Chem., 135 (2012) 183

Aryldiazonium bis(trifluoromethyl)imides

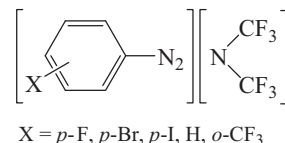
M.E. Hirschberg^a, N.V. Ignat'ev^b, A. Wenda^a, H.-J. Frohn^c, H. Willner^a

^aInorganic Chemistry, Bergische Universität Wuppertal, Gaußstr. 20, D-42097 Wuppertal, Germany

^bPM-ABE, Merck KGaA, Frankfurter Str. 250, D-64293 Darmstadt, Germany

^cInorganic Chemistry, Universität Duisburg-Essen, D-47048 Duisburg, Lotharstr. 1, Germany

$[\text{ArN}_2][\text{N}(\text{CF}_3)_2]$ are the first examples of diazonium salts with this type of anion. Their properties will be compared to $[\text{ArN}_2][\text{N}(\text{SO}_2\text{CF}_3)_2]$.

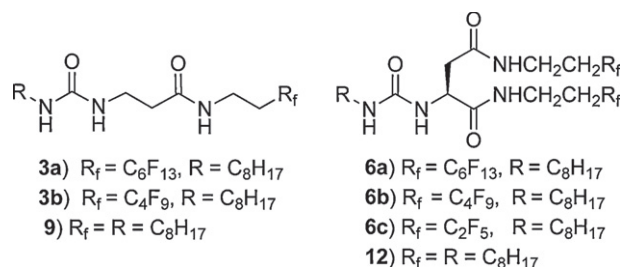


J. Fluorine Chem., 135 (2012) 187

Hydrophobic and oleophobic surface modification using gelling agents derived from amino acids

Anilkumar Raghavanpillai, Vincent A. Franco, Walter E. Meredith

DuPont Central Research & Development, Experimental Station, Wilmington, DE 19880, United States



J. Fluorine Chem., 135 (2012) 195

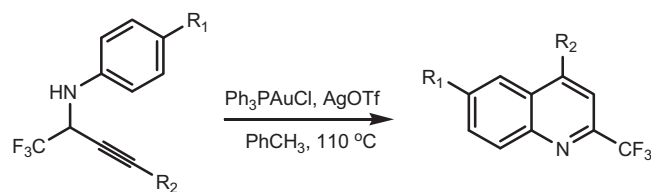
An efficient synthesis of 2-trifluoromethyl quinolines via gold-catalyzed cyclization of trifluoromethylated propargylamines

Mei Zhu^a, Weijun Fu^a, Guanglong Zou^b, Chen Xun^a, Dongsheng Deng^a, Baoming Ji^a

^aCollege of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471022, PR China

^bSchool of Chemistry and Environmental Science, Guizhou University for Nationalities, Guiyang 550025, PR China

A highly efficient cyclization reaction of trifluoromethylated propargylamines leading to 2-trifluoromethyl-4-aryl quinolines was developed by using gold(I) as a catalyst under.



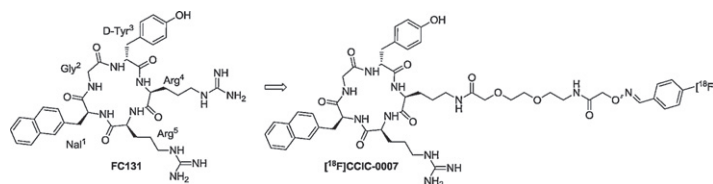
J. Fluorine Chem., 135 (2012) 200

¹⁸F-labelling of a cyclic pentapeptide inhibitor of the chemokine receptor CXCR4

Ola Åberg, Federica Pisaneschi, Graham Smith, Quang-De Nguyen, Elizabeth Stevens, Eric O. Aboagye

Comprehensive Cancer Imaging Centre, Department of Surgery and Cancer, Faculty of Medicine, Imperial College London, Hammersmith Hospital, Du Cane Road, London W12 0NN, UK

The ¹⁸F-labelled cyclic pentapeptide, [¹⁸F]-CCIC-0007 designed to bind to the extracellular domains of chemokine receptor CXCR4, was synthesised via conjugation of [¹⁸F]fluorobenzaldehyde with the corresponding aminooxy functionalised cyclopentapeptide. Tissue pharmacokinetic studies in mice demonstrated rapid blood clearance, together with biliary and renal elimination.



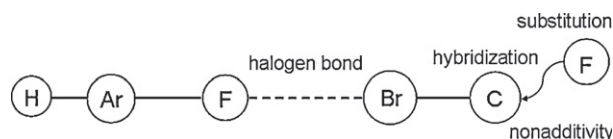
J. Fluorine Chem., 135 (2012) 207

The structure, properties, and nature of C–Br...F halogen bond involving HArF: Substitution, hybridization, and nonadditivity

Qing-Zhong Li*, Ran Li, Shu-Na Jiang, Wen-Zuo Li, Jian-Bo Cheng

The Laboratory of Theoretical and Computational Chemistry, School of Chemistry and Chemical Engineering, Yantai University, Yantai 264005, PR China

The F substitution, hybridization, nonadditivity, and electrostatic nature of halogen bond with HArF as the halogen acceptor and C–Br as the halogen donor have been evaluated.



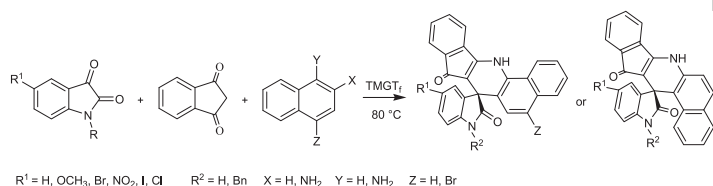
J. Fluorine Chem., 135 (2012) 213

Tetramethylguanidinium triflate: An efficient catalyst solvent for the convergent synthesis of fused spiro[1,4-dihydropyridine-oxindole] compounds

Kurosh Rad-Moghadam, Leila Youseftabar-Miri

Chemistry Department, University of Guilan, P.O. Box 41335-19141 Rasht, Iran

The ionic liquid *N,N,N,N*-tetramethylguanidinium triflate was found an efficient catalyst solvent for promoting the synthesis of spiro[dihydropyridine-oxindole] compounds. This catalyst provided a quick method for sole production of the desired spiro-compounds from readily available and simple starting materials.



R¹ = H, OCH₃, Br, NO₂, I, Cl R² = H, Bn X = H, NH₂ Y = H, NH₂ Z = H, Br

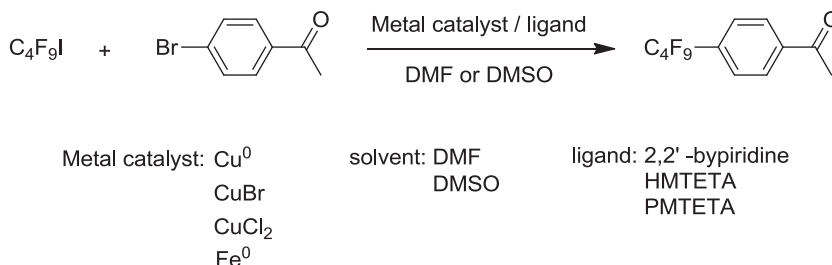
J. Fluorine Chem., 135 (2012) 220

Optimization of the synthesis of 4'-nonafluorobutylacetophenone by metal catalysed cross-coupling reaction

Flavio Ceretta^a, Alessandro Zaggia^a, Lino Conte^a, Bruno Ameduri^b

^aUniversity of Padua, Department of Chemical Processes of Engineering, via Marzolo 9, 35131 Padua, Italy

^bIngénierie & Architectures Macromoléculaires, Institut Charles Gerhardt, UMR 5253, ENSCM 34296 Montpellier Cedex, France

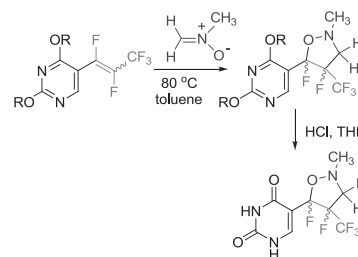
*J. Fluorine Chem.*, 135 (2012) 225

Synthesis of 5-fluorovinyl derivatives of pyrimidines via Suzuki–Miyaura coupling and their 1,3-dipolar cycloaddition reactions with nitrones

Hanna Wójtowicz-Rajchel, Henryk Koroniak

Adam Mickiewicz University, Department of Chemistry, Grunwaldzka 6, 60-780 Poznań, Poland

A simple synthesis of a new class of fluorinated isoxazolidinyl derivatives of pyrimidine is described.

*J. Fluorine Chem.*, 135 (2012) 231

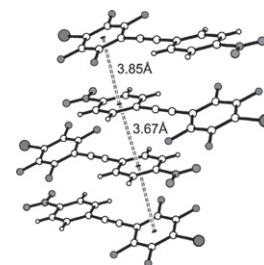
Specific interaction modes in the crystal structures of oligofluorinated tolans featuring additional electron donor and acceptor groups

Mario Stein^a, Ricarda Berger^a, Wilhelm Seichter^b, Jürg Hulliger^a, Edwin Weber^b

^aDepartment of Chemistry and Biochemistry, University of Berne, Freiestrasse 3, CH-3012 Berne, Switzerland

^bInstitute of Organic Chemistry, Technische Universität Bergakademie Freiberg, Leipziger Straße 29, D-09596 Freiberg, Sachsen, Germany

Fluorinated tolans with *para*-substituted electron donor and acceptor groups have been synthesized and studied regarding their modes of packing in crystalline state.

*J. Fluorine Chem.*, 135 (2012) 240

Synthesis and anti-cancer, anti-metastatic evaluation of some new fluorinated isocoumarins and 3,4-dihydroisocoumarins

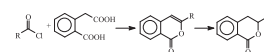
Obaid-ur-Rahman Abid^a, Muhammad Khalid^a, Muhammad T. Hussain^b, Muhammad Hanif^a, Ghulam Qadeer^a, Nasim H. Rama^a, Alexander Kornienko^c, Khalid M. Khan^d

^aDepartment of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan

^bDepartment of Applied Sciences, National Textile University, Faisalabad 37610, Pakistan

^cDepartment of Chemistry, New Mexico Tech, Socorro, NM 87801, Mexico

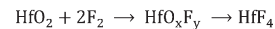
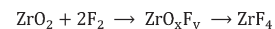
^dH. E. J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi 75270, Pakistan



Synthesis of a new series of dihalophenylisocoumarin and 3,4-dihydroisocoumarin derivatives is reported. Synthesized compounds were evaluated for antimetastatic activity and anti-cancer activity against breast cell line (MCF-7).

J. Fluorine Chem., 135 (2012) 246

A thermogravimetric study of the fluorination of zirconium and hafnium oxides with fluorine gas

Oduetse S. Monnahela^a, Bernard M. Vilakazi^a, Jacobus B. Wagener^a, Andreas Roodt^b, Pieter A.B. Carstens^a, Willem L. Retief^a^aApplied Chemistry Department, South African Nuclear Energy Corporation Limited, P.O. Box 582, Pretoria 0001, South Africa^bDepartment of Chemistry, University of the Free State, P.O. Box 339, Bloemfontein 9300, South AfricaThermogravimetric investigation of the fluorination of ZrO₂ and HfO₂ using fluorine gas.

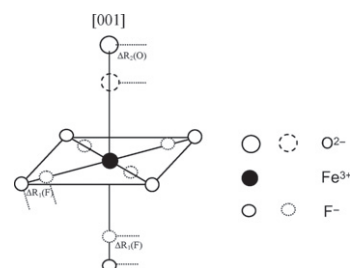
J. Fluorine Chem., 135 (2012) 250

Zero-field splitting of the ground state and local lattice distortions for Fe³⁺ ions at the tetragonal FeF₅O cluster center in Fe³⁺:KMgF₃ crystals

Zi-Yuan Yang

Department of Physics and information technology, Baoji University of Arts and Science, Baoji 721007, Shaanxi, China

The theoretical ZFS parameter D , $(a + 2F/3)$, and the energy level separations Δ_1 and Δ_2 of the ground state for Fe³⁺ ion in Fe³⁺:KMgF₃ crystals yield a good agreement with experiment findings when the five F ions moves toward the center ion Fe³⁺ by $|\Delta R_1(\text{F})| = 6.4 \times 10^{-4}$ nm and the O²⁻ ion toward the center ion Fe³⁺ by $|\Delta R_2(\text{O})| = 10.55 \times 10^{-3}$ nm.

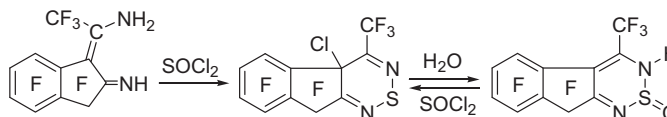


J. Fluorine Chem., 135 (2012) 254

Fluorinated dihydroindeno[2,1-c][1,2,6]thiadiazines: The first synthesis, structural characterization and reactivity

Victor M. Karpov, Vyacheslav E. Platonov, Tatjana V. Rybalova, Yuri V. Gatilov, Makhmut M. Shakirov

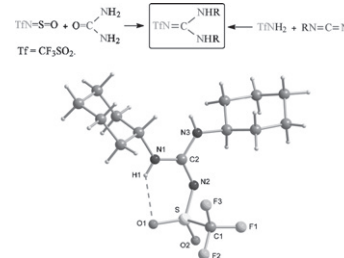
N.N. Vorozhtsov Novosibirsk Institute of Organic Chemistry, Novosibirsk 630090, Russia



J. Fluorine Chem., 135 (2012) 261

Simple methods for the preparation of N-triflyl guanidines and the structure of compounds with the CF₃SO₂NCN fragmentBagrat A. Shainyan^a, Ljudmila L. Tolstikova^a, Uwe Schilde^b^aA. E. Favorsky Irkutsk Institute of Chemistry, Siberian Division of Russian Academy of Sciences, 1 Favorsky Street 664033, Irkutsk, Russia^bChemisches Institut der Universität Potsdam, P.O. Box 69 15 53, D-14415 Potsdam, Germany

Two novel and simple approaches to N-triflyl guanidines are elaborated. The formally double C=N bond in TfN=C(NHHex-c)₂ is longer than the formally single N-C bonds.



J. Fluorine Chem., 135 (2012) 265

Synthesis, physical–chemical properties and *in vitro* photodynamic activity against oral cancer cells of novel porphyrazines possessing fluoroalkylthio and dietherthio substituents

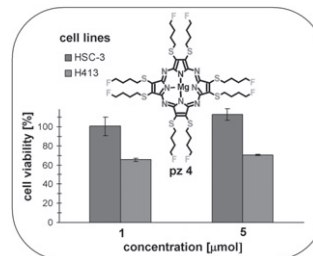
Jaroslav Piskorz^a, Paulina Skupin^a, Sebastian Lijewski^b, Maciej Korpusinski^b, Mateusz Sciepora^b, Krystyna Konopka^c, Stanislaw Sobiak^b, Tomasz Goslinski^b, Jadwiga Mielcarek^a

^aDepartment of Inorganic and Analytical Chemistry, Poznan University of Medical Sciences, Grunwaldzka 6, 60-780 Poznan, Poland

^bDepartment of Chemical Technology of Drugs, Poznan University of Medical Sciences, Grunwaldzka 6, 60-780 Poznan, Poland

^cDepartment of Biomedical Sciences, University of the Pacific, Arthur A. Dugoni School of Dentistry, San Francisco, USA

The photochemical properties and biological activity of the series of novel porphyrazines possessing fluoroalkylthio and dietherthio peripheral substituents are presented.



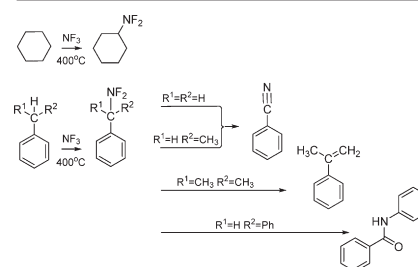
J. Fluorine Chem., 135 (2012) 272

Ab initio study of the mechanisms of reactions of NF₃ with aliphatic and benzylic substrates

Randolph K. Belter^a, Cheri A. McFerrin^b

^aY-Not Chemical Consulting, Zachary, LA 70791, USA

^bDept. of Chemistry, Louisiana State University, Baton Rouge, LA 70803, USA

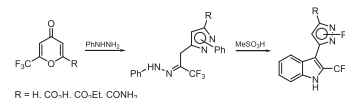


J. Fluorine Chem., 135 (2012) 278

Regioselective synthesis of trifluoromethylated 3-(pyrazolyl)indoles on the basis of 6-(trifluoromethyl)comanic acid

Boris I. Usachev, Dmitrii L. Obydenov, Vyacheslav Ya. Sosnovskikh

Department of Chemistry, Ural Federal University, pr. Lenina 51, 620083 Ekaterinburg, Russia



J. Fluorine Chem., 135 (2012) 285

Investigation of superhalogen properties of RhF_n (*n* = 1–7) clusters using quantum chemical method

Shamoon Ahmad Siddiqui^a, Anoop Kumar Pandey^b, Tabish Rasheed^c, Mahima Mishra^d

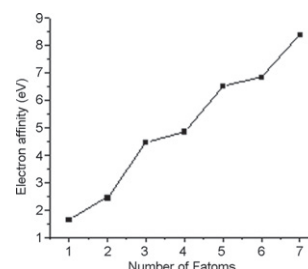
^aCentre for Advanced Materials and Nanoengineering, Najran University, Najran, Saudi Arabia

^bDepartment of Physics, Lucknow University, Lucknow, India

^cDepartment of Applied Sciences, School of Engineering and Technology, Sharda University, Plot No. 32-34, Knowledge Park III, Greater Noida 201306, N.C.R., U.P., India

^dDepartment of Applied Science, S.I.T.M., Lucknow, India

Graphical abstract shows a graph between electron affinity (EA) and number of Fluorine atoms. EA rises from 1.5 eV to 9.0 eV as the number of Fluorine atoms increases from 1 to 7. The EA of RhF₇ (9.0 eV) is much higher than Cl atom, which has highest EA among all elements in the periodic table. Hence, we can conclude that



J. Fluorine Chem., 135 (2012) 292

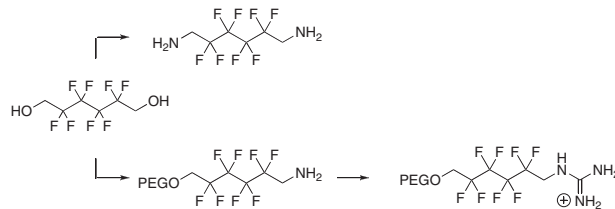
Synthesis and phosphonate binding of guanidine-functionalized fluorinated amphiphiles

Xinping Wu^a, Emine Boz^a, Amy M. Sirkis^a, Andy Y. Chang^b, Travis J. Williams^a

^aLoker Hydrocarbon Research Institute, Department of Chemistry, University of Southern California, Los Angeles, CA 90089-1661, USA

^bThe Saban Research Institute of Children's Hospital of Los Angeles, 4650 Sunset Boulevard, Los Angeles, CA 90027-6062, USA

We report convenient procedures for the use of highly fluorinated α,ω -diols as building blocks for the rapid assembly of amphiphilic materials containing a fluororous phase region.



J. Fluorine Chem., 135 (2012) 303

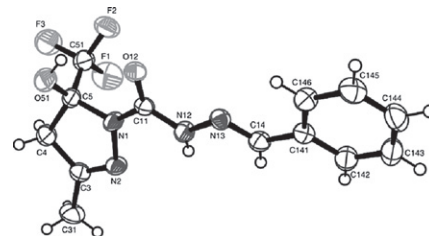
New trifluoromethyl-containing (*E*)-*N'*-arylidene-[3-alkyl(aryl/heteroaryl)-4,5-dihydro-1*H*-pyrazol-1-yl]carbohydrazides: Synthesis, crystal structure and antimicrobial/antioxidant activity

Helio G. Bonacorso^a, Susiane Cavinatto^a, Patrick T. Campos^a, Liliane M.F. Porte^a, Jussara Navarini^a, Gisele R. Paim^a, Marcos A.P. Martins^a, Nilo Zanatta^a, Caroline Z. Stuker^b

^aNúcleo de Química de Heterociclos – NUQUIMHE, Departamento de Química, Universidade Federal de Santa Maria, 97105-900 Santa Maria, RS, Brazil

^bNúcleo de Pesquisas de Produtos Naturais – NPPN, Departamento de Química, Universidade Federal de Santa Maria, 97105-900 Santa Maria, RS, Brazil

The regioselective synthesis and structural study via X-ray diffraction of a series of twenty-seven new (*E*)-*N'*-arylidene-(5-trifluoromethyl-5-hydroxy-4,5-dihydro-1*H*-pyrazol-1-yl)carbohydrazides with ability to capture DPPH free radical, but showing a weak fungistatic and bacteriostatic activity, is described.



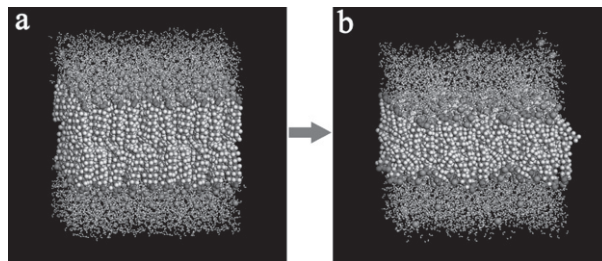
J. Fluorine Chem., 135 (2012) 315

Lyotropic liquid crystal phases of lithium perfluorinated fatty acid salts in aqueous solutions and molecular dynamics study of the lamellar phase

Panfeng Long, Hui Yan, Xiaohui Guo, Jingcheng Hao

Key Laboratory of Colloid and Interface Chemistry (Shandong University) and Key Laboratory of Special Functional Aggregated Materials, Ministry of Education, Jinan 250100, China

Anisotropic lyotropic liquid crystal (LLC) of lithium perfluorinated fatty acids (PFL/M-Li) were investigated in aqueous solutions, and NVT molecular dynamics simulations have been carried out to investigate the mechanism for the formation of lamellar LLC phases and their properties.



J. Fluorine Chem., 135 (2012) 323

Synthesis, characterization and fungicidal activities of novel fluorinated 3,5-disubstituted-4*H*-1,2,4-triazol-4-amines

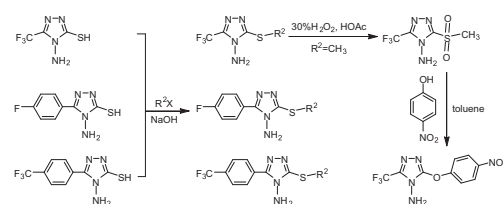
Min Chen^{ab}, Xian-Feng Wang^{ab}, Si-Si Wang^{bc}, Yi-Xiao Feng^c, Feng Chen^c, Chun-Long Yang^{abc}

^aKey Laboratory of Monitoring and Management of Crop Diseases and Pest Insects, Ministry of Agriculture, Nanjing Agricultural University, Nanjing 210095, PR China

^bJiangsu Key Laboratory of Pesticide Science, Nanjing Agricultural University, Nanjing 210095, PR China

^cDepartment of Chemistry, College of Science, Nanjing Agricultural University, Nanjing 210095, PR China

Fifteen 3,5-disubstituted-4*H*-1,2,4-triazol-4-amines were designed, synthesized and characterized, two of them were confirmed by X-ray diffraction crystallography. These title compounds showed certain fungicidal activities against the plant pathogens.



J. Fluorine Chem., 135 (2012) 330

Amino-ethoxilated fluorinated amphiphile: Synthesis, self-assembling properties and interactions with ssDNA

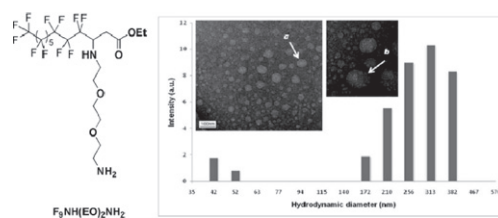
Nicolas Dupuy^a, Andreea Pasc^a, Stéphane Parant^b, Stéphane Fontanay^c, Raphaël E. Duval^c, Christine Gérardin^a

^aLERMAB – EA 4370, Nancy-Université, BP 70239, F-54506 Vandoeuvre-lès-Nancy, France,

^bUMR 7565 SRSMC, Nancy-Université, BP 70239, 54506 Vandoeuvre-lès-Nancy, France,

^cGEVSM, SRSMC, UMR UHP-CNRS 7565, Nancy-Université, Faculté de Pharmacie, 5 rue A. Lebrun, B.P. 80403, 54001 Nancy Cedex, France

A monocatenar surfactant, noted $F_9NH(EO)_2NH_2$ and consisting of (i) a fluorinated hydrophobic tag responsible of self-assembling, (ii) an ethylenoxide moiety sufficiently hydrophilic to avoid precipitation of the lipid-ODN complex and (iii) a protonated at physiological pH primary amine responsible of binding, was synthesized and its surface chemical properties were examined with the aim to have a highly water-soluble surfactant spontaneously forming vesicles entrapping drug or gene carriers.



J. Fluorine Chem., 135 (2012) 339

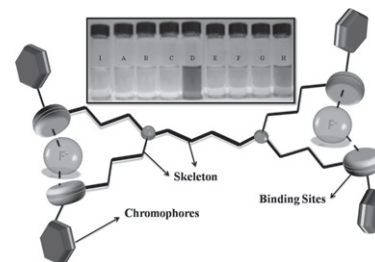
DAB-Am-4 based colorimetric receptors for fluoride and pyrophosphate anions

Manish Khandelwal^a, In-Chul Hwang^b, Prakash Chandran R. Nair^c

^aDepartment of Chemistry, Florida Institute of Technology, 150 West University Blvd., Melbourne, FL 32901, USA

^bCenter for Superfunctional Materials, Department of Chemistry, Pohang University of Science and Technology, Pohang 790-784, Republic of Korea

^cAmrita School of Biotechnology, Amrita Vishwa Vidyapeetham University, Amritapuri, Clappana P.O., Kollam, Kerala 690 525, India



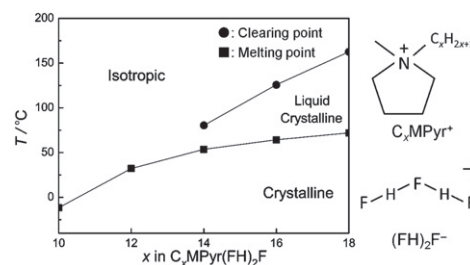
J. Fluorine Chem., 135 (2012) 344

Effects of alkyl chain length on properties of N-alkyl-N-methylpyrrolidinium fluorohydrogenate ionic liquid crystals

Fei Xu, Shohei Matsubara, Kazuhiko Matsumoto, Rika Hagiwara

Graduate School of Energy Science, Kyoto University, Sakyo-ku, Kyoto 606-8501, Japan

A series of N-alkyl-N-methylpyrrolidinium fluorohydrogenate salts ($C_xMPyr^+(FH)_2F$, $x = 10, 12, 14, 16$, and 18) have been characterized by infrared spectroscopy, thermal analysis, polarized optical microscopy, X-ray diffraction, and anisotropic ionic conductivity measurements. The liquid crystalline mesophase of $C_{14}MPyr(FH)_2F$ exhibits large anisotropy in ionic conductivity.

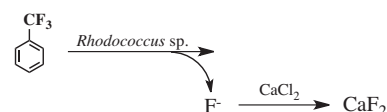


J. Fluorine Chem., 135 (2012) 350

Retransformation of fluoride ion generated from the biodegradation of benzotrifluoride to calcium fluoride

Noritaka Iwai, Yosuke Watanabe, Tomoya Kitazume

Graduate School of Bioscience and Biotechnology, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-ku, Yokohama 226-8501, Japan



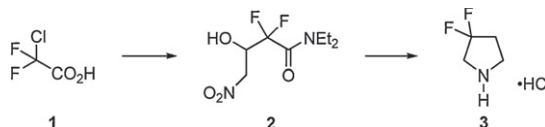
J. Fluorine Chem., 135 (2012) 354

An efficient synthesis of 3,3-difluoro-pyrrolidine hydrochloride starting with 2-chloro-2,2-difluoroacetic acid

Lulin Wei^a, Teresa M. Makowski^a, Jennifer L. Rutherford^b^aChemical Research and Development, Pfizer Worldwide Research and Development, Eastern Point Road, PO Box 8013, Groton, CT 06340-8013, USA^bLafayette College, Department of Chemistry, Hugel Science Center, Easton, PA 18042, USA

A facile and fluorination-free synthesis of 3,3-difluoropyrrolidine hydrochloride

(3), an important synthon in the synthesis of biologically active compounds, is reported. The seven-step synthesis starts from the commercially available 2-chloro-2,2-difluoroacetic acid (1) in a three-step telescoped process that produces crystalline *N,N*-diethyl-2,2-difluoro-3-hydroxy-4-nitrobutanamide (2). A convenient and high-yielding reductive nitromethylation of 2 followed by a catalytic hydrogenation/cyclization sequence and borane reduction affords 3 in good yield and purity.

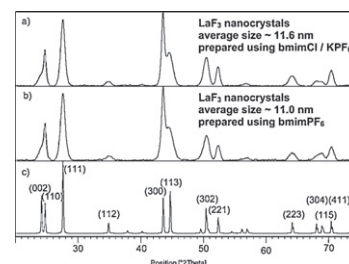


J. Fluorine Chem., 135 (2012) 358

Lanthanum trifluoride nanoparticles prepared using ionic liquids

Vilém Bartůňek^a, Vít Jakeš^a, Vladimír Král^b, Jakub Rak^b^aDepartment of Inorganic Chemistry, Faculty of Chemical Technology, Institute of Chemical Technology, Technická 5, 166 28 Prague 6, Czech Republic^bDepartment of Analytical Chemistry, Faculty of Chemical Engineering, Institute of Chemical Technology, Technická 5, 166 28 Prague 6, Czech Republic

Fine LaF₃ nanocrystals were prepared using ionic liquid bmimPF₆ (used both as solvent and as fluorination agent) with liquid La(NO₃)₃ as source of lanthanum and using bmimCl as solvent and KPF₆ as fluorination agent, respectively. Prepared nanocrystals formed nonordered agglomerates. Although nanocrystals prepared by both ways are of very similar size, the sizes of their agglomerates differ significantly. Reactions were performed at 200 °C for 90 min.

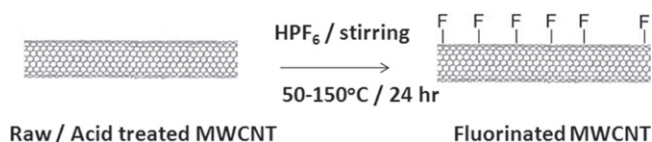


J. Fluorine Chem., 135 (2012) 362

Fluorination of multiwall carbon nanotubes by a mild fluorinating reagent HPF₆

Jatindranath Maiti, Nitul Kakati, Seok Hee Lee, Young Soo Yoon

Energy and Sensor Laboratory, School of Materials Science and Engineering, Yonsei University, 134 Shinchon Dong, Seoul 120-749, South Korea

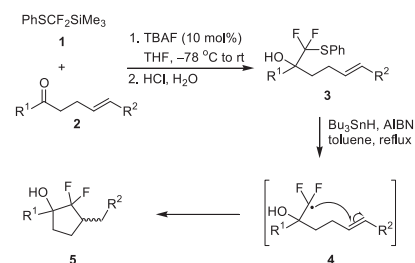


J. Fluorine Chem., 135 (2012) 367

α,α -Difluoro- α -phenylsulfanyl- α -trimethylsilylmethane as “CF₂–” synthetic building block for the preparation of gem-difluoromethylenated cyclopentanols

Krisana Peewasan, Chutima Kuhakarn, Darunee Soorukram, Patoomratana Tuchinda, Vichai Reutrakul, Manat Pohmakotr

Center of Excellence for Innovation in Chemistry (PERCH-CIC) and Department of Chemistry, Faculty of Science, Mahidol University, Rama VI Road, Bangkok 10400, Thailand



J. Fluorine Chem., 135 (2012) 373

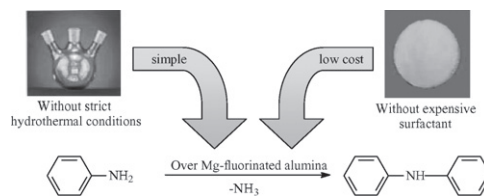
Low cost and non-surfactant synthesis of fluorinated alumina modified with magnesium for condensation of aniline to diphenylamine

Chunming Zheng^a, Xiaohong Sun^b

^aState Key Laboratory of Hollow-fiber Membrane Materials and Membrane Processes, School of Environmental and Chemical Engineering, Tianjin Polytechnic University, Tianjin 300160, PR China

^bKey Laboratory of Advanced Ceramics and Machining Technology, Ministry of Education, School of Materials Science and Engineering, Tianjin University, Tianjin 300072, PR China

Fluorinated alumina modified with magnesium was synthesized via a simple, non-corrosive and non-synthetic organic surfactant needed method instead of H-beta zeolite as effective solid acid catalyst for condensation of aniline to diphenylamine.

*J. Fluorine Chem.*, 135 (2012) 379

Nucleophilic activation of a nitrile group: Synthesis of trifluoromethyl substituted 4H-1,3,5-dioxazines

Kostiantyn V. Turcheniuk, Igor V. Shevchenko

Institute of Bioorganic Chemistry and Petrochemistry of NAS of Ukraine, Murmanskaya str. 1, 02660 Kiev, Ukraine

The negatively charged carbon atom of phosphorus ylides activates the nucleophilicity of the adjacent nitrile group. Such nitriles can add two equivalents of hexafluoroacetone to the CN triple bond to give 4H-1,3,5-dioxazines. Depending on the substituents at phosphorus atom this reaction can go stereoselectively with the formation of only one isomer.

