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^{19}F NMR applications in chemical biology

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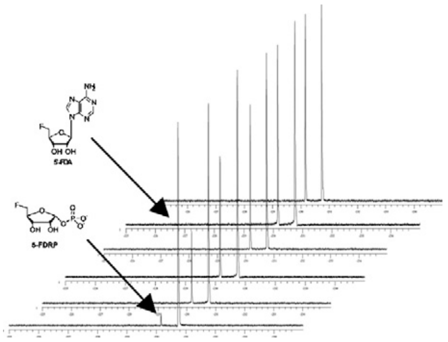
Analysis of organofluorine compounds by ^{19}F NMR was largely confined to synthetic chemists but this technique is finding increasing applications in biological systems. In this paper we review the recent literature highlighting the exploitation of ^{19}F NMR in a range of research areas at the interface of chemistry and biology.



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Facile allylboration of ketones with β-benzyloxy-γ,γ-difluoroallylboronate: Preparation of *gem*-difluorinated homoallylic *tert*-alcohols

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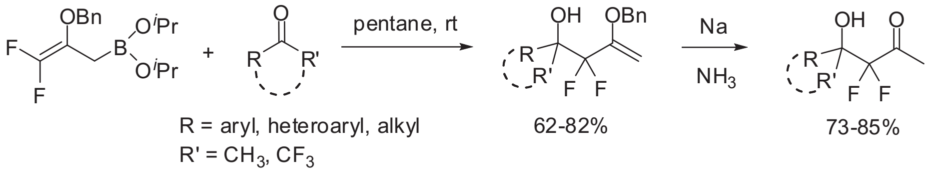

The reaction of β-benzyloxy-γ,γ-difluoroallylboronate, at room temperature and in the absence of catalysts, with a variety of aromatic and aliphatic ketones of varying sterics and electronic requirements furnishes fluorinated homoallylic *tert*-alcohols in 62–82% yields. Representatives of these alcohols were converted to their corresponding α,α-difluoro-β-hydroxy ketones in 73–85% yields.

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[2 + 2] Photodimerization and photopolymerization of diphenylhexatriene crystals utilizing perfluorophenyl–phenyl stacking interactions

Yoriko Sonoda[a], Midori Goto[b], Seiji Tsuzuki[c], Haruhisa Akiyama[a], Nobuyuki Tamaoki[a]

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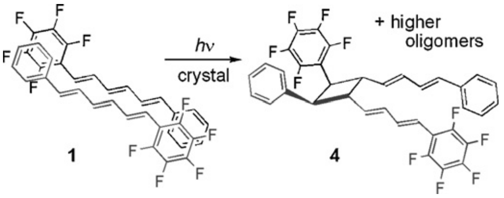

The perfluorophenyl–phenyl stacking interactions were effectively utilized to control the photoreactions of diphenylhexatrienes in the crystalline state.

doi:10.1016/S0022-1139(09)00009-8

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Synthesis and upconversion luminescence properties of $YF_3:Yb^{3+}/Tm^{3+}$ octahedral nanocrystals

Guofeng Wang[a], Weiping Qin[a], Guodong Wei[a], Lili Wang[ab], Peifen Zhu[a], Ryongjin Kim[a], Daisheng Zhang[ac], Fuheng Ding[a], Kezhi Zheng[a]

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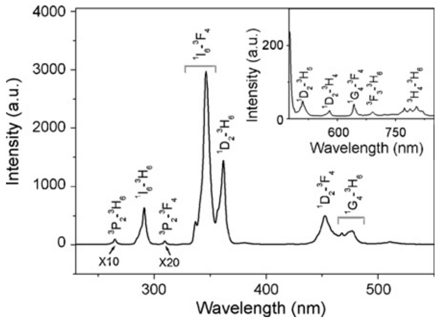

UC luminescence spectrum of $YF_3:Yb^{3+}(20\%)/Tm^{3+}(2\%)$ nanocrystals under 980-nm excitation. Inset: magnification of the spectrum in the range of 475–850 nm.

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The effect of fluorine atoms on gas transport properties of new polynorbornene dicarboximides

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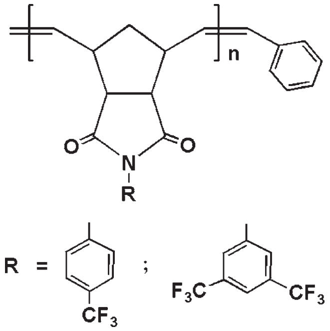
The synthesis and ring opening metathesis polymerization (ROMP) of the new *N*-4-trifluoromethylphenyl-norbornene-5,6-dicarboximide (**2a**) and *N*-3,5-bis (trifluoromethyl) phenyl-norbornene-5,6-dicarboximide (**2b**) mixtures of *exo* and *endo* monomers were performed. The gas transport properties of the corresponding polymer (**Poly-2a**) were determined and found to be one of the largest reported to date in glassy polynorbornene dicarboximides.



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Activation of hydrocinnamic acids with pentafluorophenol *versus* pentafluorothiophenol: Reactivity towards hexylamine

Fernanda M.F. Roleira[a], Fernanda Borges[b], Lourdes C.R. Andrade[c], José A. Paixão[c], Maria J.M. Almeida[c], Rui A. Carvalho[d], Elisiário J. Tavares da Silva[a]

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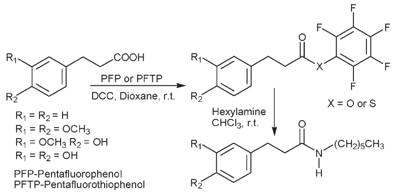
[c]*CEMDRX, Department of Physics, Faculty of Sciences and Technology, Coimbra University, 3004-516 Coimbra, Portugal*
[d]*CNC, Department of Biochemistry, Faculty of Sciences and Technology, Coimbra University, 3004-516 Coimbra, Portugal*



Synthesis of hexylamides using fluorine derivatives as intermediate active esters.

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Preparation of donor–acceptor substituted fluorostilbenes and crystal chemistry of fluorinated (*E*)-4-(4-halogeno-styryl)-benzonitriles

Raúl Mariaca[a], Gaël Labat[a], Norwid-Rasmus Behrnd[a], Michel Bonin[a], Fabien Helbling[a], Patrick Eggli[a], Gaëtan Couderc[a], Antonia Neels[b], Helen Stoeckli-Evans[b], Jürg Hulliger[a]

[a]*Department of Chemistry and Biochemistry, University of Berne, Freiestrasse 3, CH-3012 Berne, Switzerland*
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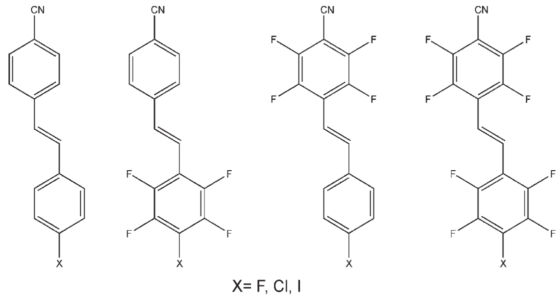

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Synthesis and characterization of Cu(II) paddlewheel complexes possessing fluorinated carboxylate ligands

Alexander N. Wein[a], Rebekah Cordeiro[a], Natalie Owens[a], Hillary Olivier[a], Kenneth I. Hardcastle[b], Jack F. Eichler[a]

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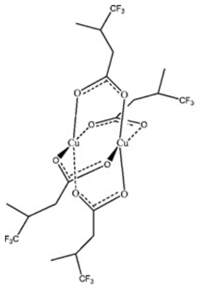
[b]*Department of Chemistry, Emory University, 1515 Dickey Drive, Atlanta, GA 30022,USA*

A series of copper(II) paddlewheel complexes possessing fluorinated carboxylate ligands have been structurally characterized and a qualitative relationship between the ^{19}F NMR line broadening and the distance between the Cu(II) ions and ^{19}F atoms has been established.



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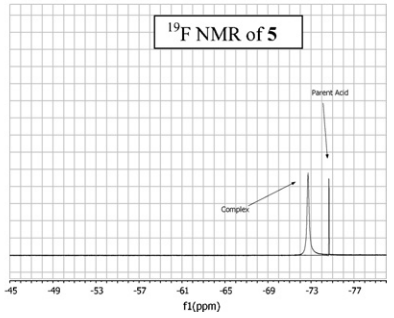

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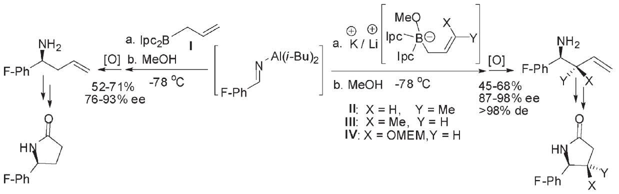
γ-Fluorophenyl-GABA derivatives from fluorobenzonitriles in high diastereomeric and enantiomeric excess

P. Veeraraghavan Ramachandran, G. Venkat Reddy, Debanjan Biswas

Department of Chemistry, Purdue University, 560 Oval Drive, West Lafayette, IN 47907-2084, United States



An enantioselective synthesis of α-fluoroaryl homoallylic amines in 52–71% yields and 76–93% enantioselectivities has been achieved *via* the allylboration of the corresponding fluorinated *N*-aluminobenzaldimines with *B*-allyldiisopinocampheylborane in the presence of methanol, followed by alkaline hydrogen peroxide workup. Crotylboration of these aluminobenzaldimines with potassium *B*-methoxy *B-E-* or *-Z*-crotyldiisopinocampheylborinate provided the corresponding β-*anti*- or -*syn*-methyl α-fluoroarylhomoallylamines, respectively in high de and ee. Similarly, alkoxyallylboration with lithium *B*-methoxy *B*-γ-OMEMallyldiisopinocampheylborinate provided the corresponding β-*syn*-alkoxyhomoallylamines in excellent de and ee. Representatives of these amino alkenes were converted to the corresponding optically active *N*-Boc-protected fluorinated amino alcohols *via* hydroboration-oxidation. Further chromium-mediated oxidation provided *N* Boc-protected γ-fluorophenyl-γ-aminobutyric acids, which upon deprotection provided the corresponding γ-lactams.

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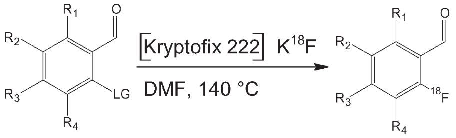
Nucleophilic substitution of nitro groups by [^{18}F]fluoride in methoxy-substituted *ortho*-nitrobenzaldehydes—A systematic study

Bin Shen[a], Dirk Löffler[a], Gerald Reischl[a], Hans-Jürgen Machulla[a], Klaus-Peter Zeller[b]

[a]*Radiopharmacy, PET Centre, Eberhard Karls University Tübingen, Germany*
[b]*Institute of Organic Chemistry, Eberhard Karls University Tübingen, Germany*

As model reactions for the introduction of fluorine-18 into aromatic amino acids via S_NAr, the replacement of NO_2 by [^{18}F]fluoride ion in mono- to tetra-methoxy-substituted 2-nitrobenzaldehydes was investigated systematically.



LG = NO_2, Br
R_1/ R_2/ R_3/ R_4 = H or OMe

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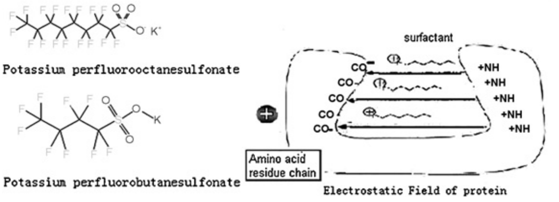
Study on the Langmuir aggregation of fluorinated surfactants on protein

Ling Li, Zu Shun Xu, Gong Wu Song

Ministry-of-Education Key Laboratory for the Synthesis and Application of Organic Function Molecules, Hubei University, Xueyuan Road 11#, Wuchang, Wuhan City, Hubei Province 430062, People's Republic of China



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Investigation of CF_2 carbene on the surface of activated charcoal in the synthesis of trifluoroiodomethane via vapor-phase catalytic reaction

Guang-Cheng Yang[a], Shi Lei[a], Ren-Ming Pan[a], Heng-Dao Quan[b]

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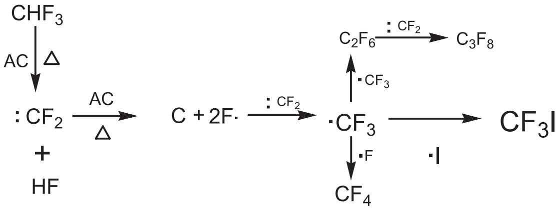
[b] *National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8565, Japan*



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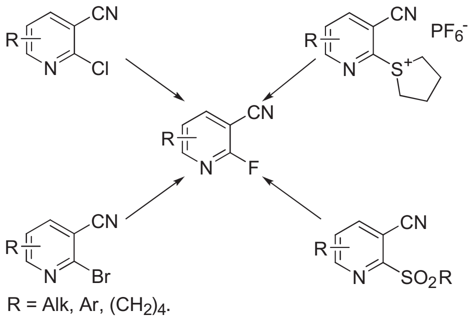
Synthesis of 3-cyano-2-fluoropyridines

Anatoliy M. Shestopalov[a], Ludmila A. Rodinovskaya[a], Alexander E. Fedorov[a], Victor E. Kalugin[a], Kirill G. Nikishin[a], Alexandr A. Shestopalov[a], Andrei A. Gakh[b]

[a] *N.D. Zelinsky Institute of Organic Chemistry, 119991, Leninsky Pr. 47, Moscow, Russia*

[b] *Oak Ridge National Laboratory, Oak Ridge, TN 37831-6242, USA*

The paper presents the synthesis of 3-cyano-2-fluoropyridines from readily available precursors via nucleophilic substitution of a leaving group in the 2-postion with KF or Bu_4NF in polar aprotic solvents such as DMF and DMSO.



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Synthesis and molecular structures of heptafluoroisopropylated fullerenes: $C_{60}(i\text{-}C_3F_7)_8$, $C_{60}(i\text{-}C_3F_7)_6$, and $C_{60}(CF_3)_2(i\text{-}C_3F_7)_2$

Tatyana Mutig[a], Stanislav M. Avdoshenko[b], Erhard Kemnitz[a], Sergey I. Troyanov[ab]

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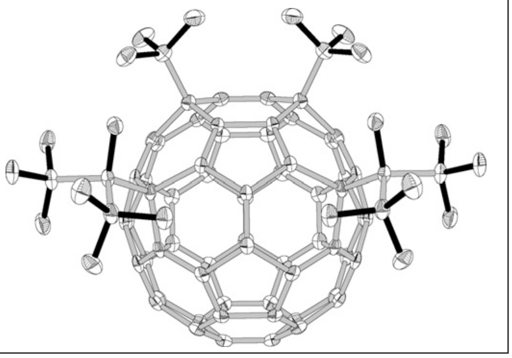
[b] *Chemistry Department, Moscow State University, Leninskie Gory, 119991 Moscow, Russia*

One isomer of $C_{60}(i\text{-}C_3F_7)_8$, three isomers of $C_{60}(i\text{-}C_3F_7)_6$, as well as the first mixed perfluoroalkylated compound, C_s-$C_{60}(CF_3)_2(i\text{-}C_3F_7)_2$, were synthesized from C_{60} and $i\text{-}C_3F_7I$ by heating in the ampoule, isolated by HPLC, and structurally characterized by X-ray single crystal diffraction.



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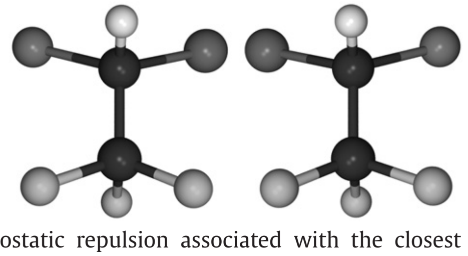
Molecular association in 2-bromo-2-chloro-1,1,1-trifluoroethane (Halothane)

Anna Olejniczak[a], Andrzej Katrusiak[a], Pierangelo Metrangolo[b], Giuseppe Resnati[b]

[a] *Faculty of Chemistry, Adam Mickiewicz University, Grunwaldzka 6, 60-780 Poznan, Poland*

[b] *Nanaostructured Fluorinated Materials Laboratory, DCMIC, Politecnico di Milano, 7, via Mancinelli, I-20131 Milano, Italy*



Single crystal of a general anesthetic Halothane, $BrClCHCF_3$, have been grown by isochoric freezing and its structure determined by X-ray diffraction at 1.85(5) GPa. The electrostatic repulsion associated with the closest intermolecular contacts in this structure is consistent with the lower freezing and boiling points and higher vapor pressure of Halothane compared to its analogues anesthetics without fluorine atoms.

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The preparation of perfluoroalkenyl allenes (trienes) and pentafluorophenyl allenes

Donald J. Burton, Greg A. Hartgraves

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

$$R_FCu + HC{\equiv}CCR^1R^2X \xrightarrow[RT]{DMF} R_FCH{=}C{=}CR^1R^2$$

$X = Cl, OTs$

$R^1 = H, CH_3$

$R^2 = CH_3, CH_3$

$R_F = F_2C{=}CF,$

$(Z)\text{-}CF_3CF{=}CF,$

C_6F_5

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Enantioselective α-hydrazination of α-fluoro-β-ketoesters catalyzed by chiral nickel complexes

Joo Yang Mang, Dae Gil Kwon, Dae Young Kim

Department of Chemistry, Soonchunhyang University, Asan, Chungnam 336-745, Republic of Korea