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# Graphical Abstracts/J. Fluorine Chem. 144 (2012) v–xii

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## Interionic cross relaxation and tunable color luminescence in $KY_3F_{10}:Tb^{3+}$ nano/microcrystals synthesized by hydrothermal approach

Jinsu Zhang[a], Baojiu Chen[a], Zuoqiu Liang[a], Xiangping Li[a], Jiashi Sun[a], Ruixia Zhong[b], Lihong Cheng[a], Haiyang Zhong[a]

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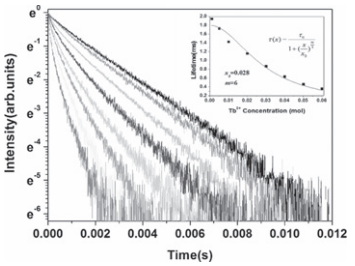


► The hydrothermal (HT) approach is applied to synthesize $KY_3F_{10}:Tb^{3+}$ phosphor. ► Emitting colors can be tuned from blue to green by increasing $Tb^{3+}$ concentration. ► Luminescence dynamical process is detailedly analyzed. ► Electronic dipole–dipole interaction governs the dynamic CR process.

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## Tribological properties of fluorinated nanocarbons with different shape factors

N. Nomède-Martyr[abc], E. Disa[ab], P. Thomas[c], L. Romana[c], Jean-Louis Mansot[cd], M. Dubois[ab], K. Guérin[ab], W. Zhang[abe], A. Hamwi[ab]

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[b]*CNRS, UMR 6296, 63170 Aubière, France*
[c]*Groupe de Technologie des Surfaces et Interfaces (GTSI, EA 2432), Faculté des Sciences Exactes et Naturelles, Université des Antilles et de la Guyane, 97159 Pointe à Pitre Cedex, France*
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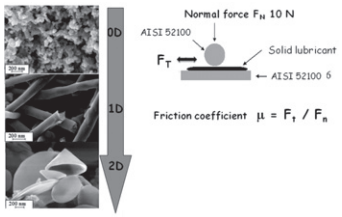
[e]*Ecole Centrale de Pékin, Beijing University of Aeronautics and Astronautics (BUAA), Road 37, HaiDian District, Beijing 100191, China*




► Nanocarbonaceous materials with different shape factors were fluorinated using pure $F_2$ gas with similar fluorine contents. ► Structure and C—F bonding are similar at given fluorine content. ► The tribological properties of the fluorinated nanocarbons have been investigated and compared according to the shape factor.

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## Quantum chemistry calculations of branched fluorocarbon systems

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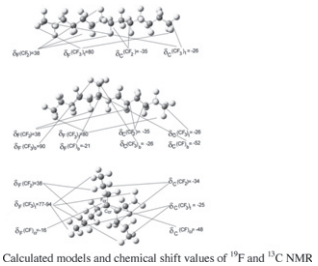
[b]*A.A. Baikov Institute of Metallurgy and Material Science RAS, Leninsky pr. 49, Moscow 119334, Russia*


Calculated models and chemical shift values of $^{19}F$ and $^{13}C$ NMR

► The processes of branch formation in the fluorocarbon chain molecules are studied by results of quantum-chemical calculations. ► The methods HF and DFT we used to calculate $C_nF_{2n+2}$ molecules. ► The features of $^{13}C$ and $^{19}F$ NMR spectra to identify $CF_3$ branches, cross-linking and intersecting formations of the chains are revealed. ► The possible structures of branched entities were found.

doi:10.1016/S0022-1139(12)00336-3

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## The first fluorous biphase hydrogenation catalyst incorporating a perfluoropolyalkylether: $[RhCl(PPh_2(C_6H_4C(O)OCH_2CF(CF_3)(OCF_2CF(CF_3))_nF))_3]$ with $n$ = 4–9

Chadron M. Friesen[a], Craig D. Montgomery[a], Sebastian A.J.U. Temple[b]

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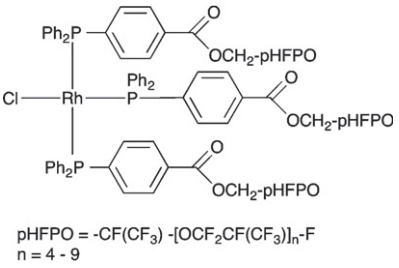


► A triarylphosphine ligand that incorporates the perfluoropolyalkylether. ► Polyhexafluoropropylene oxide with a –C(O)$OCH_2$– spacer is synthesized. ► A Wilkinson's catalyst derivative is synthesized with this ligand. ► The catalyst is employed as a Fluorous Biphase Catalyst for the hydrogenation of 2-cyclohexen-1-one. ► Turnover frequencies as well as partition coefficients and Rh leaching studies are reported.

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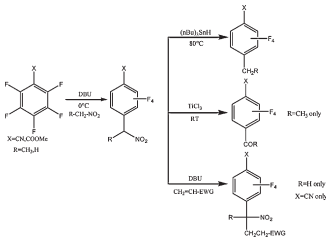
## Reaction of nitroalkanes with polyfluoroaromatic compounds

R. Vaidyanathaswamy, K. Radha, M. Dharani, T.S. Raguraman, Rajdeep Anand

*Projects and R&D, SRF Ltd., Manali Industrial Area, Manali, Chennai 600068, India*



► Nucleophilic substitution of nitroalkyl carbanion occurs at para position of pentafluorobenzonitrile and methyl pentafluorobenzoate. ► The nitro compounds thus formed undergo tin hydride reduction and Nef reaction to give valuable products. ► In presence of base, the nitro compounds add on to Michael acceptors.

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## Hydrogen bonding interactions in two isomers of fluorobenzoylthioureas and their absorption spectra

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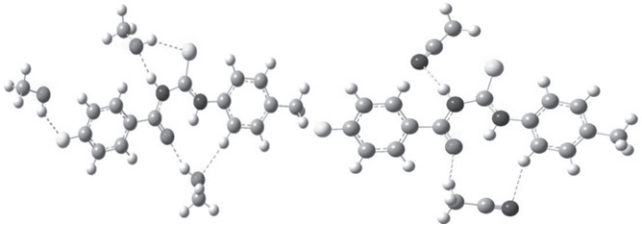

► Crystal structures of two benzoylthiourea isomers were determined by X-ray diffraction method. ► Intra- and intermolecular hydrogen bonds affect each other in the crystals. ► The intramolecular hydrogen bonds broaden the UV absorption bands of n → π* transition. ► The intermolecular hydrogen bonds cause to unusual blue shifts of the UV absorption band for π → π* transition.

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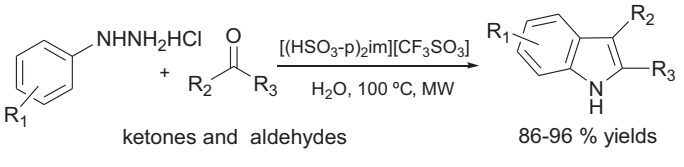
## Novel $SO_3H$-functionalized ionic liquids catalyzed a simple, green and efficient procedure for Fischer indole synthesis in water under microwave irradiation




Bai Lin Li[a], Dan-Qian Xu[b], Ai Guo Zhong[a]

[a]*Department of Pharmaceutical and Chemical Engineering, Taizhou College, Linhai Zhejiang 317000, PR China*
[b]*State Key Laboratory Breeding Base of Green Chemistry Synthesis Technology, Zhejiang University of Technology, Hangzhou 310032, PR China*

► The whole process was performed in water without using any organic solvents. ► The reaction–separation–recycle process was quite convenient. ► The catalytic system of $[(HSO_3\text{-}p)_2im][CF_3SO_3]/H_2O$ could be reused directly.

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## Buckminsterfullerene derivatives bearing a fluoroalkyl group for use in organic photovoltaic cells

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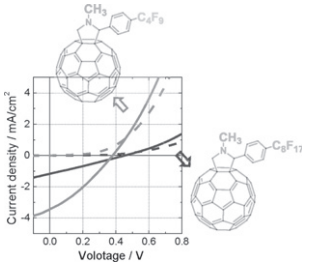
► We synthesized six novel fluoroalkyl fullerene derivatives. ► Photovoltaic cells using the fullerene derivatives were characterized. ► The cell performances were notably affected by the substituents on the fullerenes. ► This is the first example of the use of fluoroalkyl fullerenes for the solar cells.




J. Fluorine Chem., 144 (2012) 59

## Morpholine sulfur trifluoride: Vibrational spectra, conformational properties and crystal structure

Andrea Flores Antognini[a], Norma L. Robles[a], Edgardo H. Cutin[a], Eduard Bernhardt[b], Markus Hirschberg[b], Xiaoqing Zeng[b], Helge Willner[b], Heinz Oberhammer[c]

[a]*INQUINOA (CONICET-UNT) Instituto de Química Física, Facultad de Bioquímica, Química y Farmacia, Universidad Nacional de Tucumán, San Lorenzo 456, (4000) Tucumán, Argentina*
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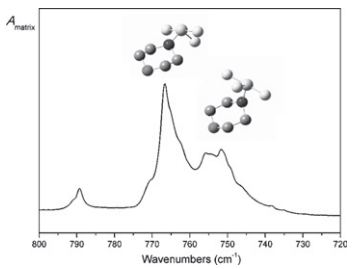
[c]*Institut für Physikalische und Theoretische Chemie, Universität Tübingen, 72076 Tübingen, Germany*

► Morph-$SF_3$ exists in the gas phase as a mixture of two conformers: equatorial and axial. ► Ar matrix IR spectra show an unexpected temperature independent conformational equilibrium. ► The equatorial conformer is the only form present in the crystal (X-ray crystallography).

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## Boron difluoride complexes of carbamoyl Meldrum's acids

Natalia Pawelska[a], Łukasz Ponikiewski[b], Sławomir Makowiec[a]

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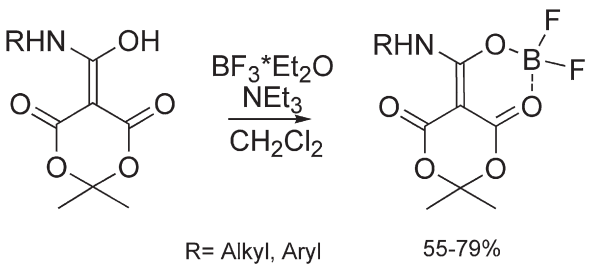
[b]*Department of Inorganic Chemistry, Faculty of Chemistry, Gdańsk University of Technology, Narutowicza 11/12, 80-233 Gdańsk, Poland*

► The new type of carbamoyl Meldrum's acids derivatives have been revealed. ► The structure of the new compounds were confirmed with X-ray crystallography. ► Prepared complexes are stable and easily isolable. ► Other derivatives of Meldrum's acids was examined.



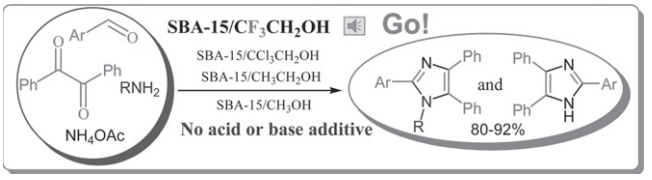

J. Fluorine Chem., 144 (2012) 69

## SBA-15/TFE (SBA-15/2,2,2-trifluoroethanol) as a suitable and effective metal-free catalyst for the preparation of the tri- and tetra-substituted imidazoles via one-pot multicomponent method

Sadegh Rostamnia, Ali Zabardasti

*Organic and Nano Group (ONG), Department of Chemistry, University of Maragheh, P.O. Box 14115-175, Maragheh, Iran*

► Un-functionalized SBA-15 mesoporous and 2,2,2-trifluoroethanol (SBA-15/TFE). ► Imidazole production via 3-CR is reported. ► A reusable porous catalyst system using commercially available fluorinated alcohol was employed. ► Represents advantages, operational simplicity, higher yield and with easy workup.



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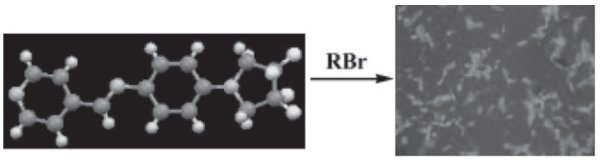
## Pyridinium-based ionic liquid crystals with terminal fluorinated pyrrolidine

Jingqi Tao[a], Junwen Zhong[a], Peilian Liu[a], Stelck Daniels[c], Zhuo Zeng[ab]

[a]*College of Chemistry & Environment, South China Normal University, Guangzhou 510006, China*
[b]*Key Laboratory of Organofluorine Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai 200032, China*
[c]*Department of Chemistry, University of Idaho, Moscow, ID 83844-2343, USA*




**Ionic Liquid Crystals with Fluorinated Pyrrolidine**

► Novel pyridinium-based fluorinated ionic liquid crystals were synthesized. ► These compounds show a wide mesophase range and are stable to high temperatures. ► The mesophase behavior is affected by the configuration of the heterocycle. ► Fluorinated azepine causes the liquid crystal properties to disappear.

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## Siloxane based syntheses of fluorous ethenes and their tandem Heck reactions with aryl iodides

Ágnes Csapó, József Rábai

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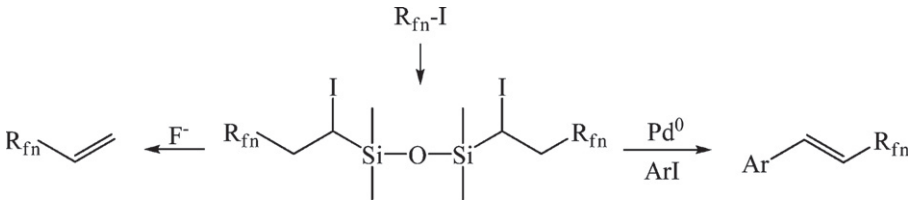


► Perfluoroalkyl-ethenes are formed by the TBAF·3$H_2O$ or KF/$NEt_3$/$H_2O$ treatment of organosilicons in DMF. ► Tandem-Heck coupling reactions using fluorous silanes as olefin precursors were performed. ► A silica supported 'perfluorooctyl-ethene surrogate' was synthesized and applied for a Heck coupling reaction.

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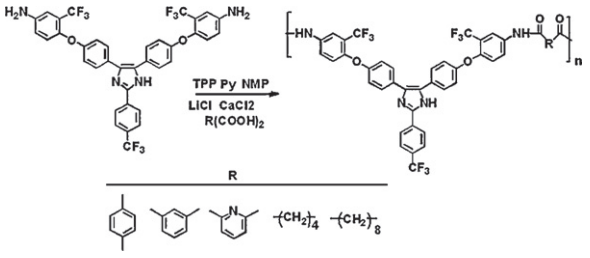
## Novel para-linked and $CF_3$-substituted poly(amide-ether-imidazole)s: Solubility, optical and thermal properties

Mousa Ghaemy, Farshad Rahimi Berenjestanaki

*Polymer Chemistry Research Laboratory, Department of Chemistry, Mazandaran University, Babolsar, Iran*




► New class of poly(amide-ether-imidazole)s containing $CF_3$ groups were prepared by direct polycondensation. ► The fluoropolymers were characterized and their properties such as viscosity, solubility, thermal and photophysical were investigated. ► These polymers with different functional groups in the backbone showed fluorescence emission with excellent solubility and suitable thermal stability.

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## Dipole (hyper)polarizabilities of fluorinated benzenes: An ab initio investigation

Andrea Alparone

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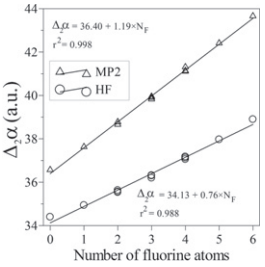


► We computed dipole moments and (hyper)polarizabilities of fluorobenzenes. ► Polarizability anisotropy is linearly related to the number of fluorine atoms. ► Hyperpolarizability differences among isomers are elucidated using density analyses.

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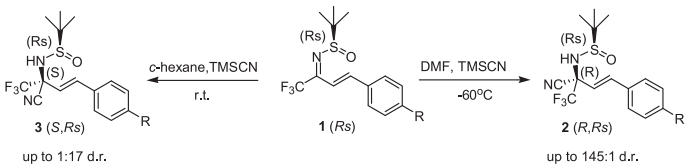
## The Regio-specific solvent controlled asymmetric Strecker reaction of trifluoromethyl α,β-unsaturated *N-tert*-butanesulfinyl ketimines with trimethylsilyl cyanide

Xiao-Ming Yuan[a], Jian Xu[a], Zhen-Jiang Liu[c], Xian-Jin Yang[ab], Li-Min Wang[ab], Yan Zhang[a], Xue-Yan Yang[a], Xiao-Peng He[a], Jin-Tao Liu[b]

[a]*Key Laboratory for Advanced Materials and Institute of Fine Chemicals, East China University of Science and Technology, 130 Meilong Road, Shanghai 200237, China*
[b]*Key Laboratory of Organofluorine Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, Shanghai 200032, China*
[c]*School of Chemical and Environmental Engineering, Shanghai Institute of Technology, 100 Haiquan Road, Shanghai 201418, China*




► The reaction of chiral *N-tert*-butanesulfinyl ketimines with TMSCN was studied. ► Different diastereoselectivities were obtained in terms of the solvents used. ► In *c*-hexane, d.r. (2a:3a) of the addition products is up to 1:17. ► In DMF, a reversed diastereoselectivity was observed with up to 145:1 d.r. (2a:3a).

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## New structural units in molybdenum oxyfluoride chemistry

David W. Aldous, Philip Lightfoot

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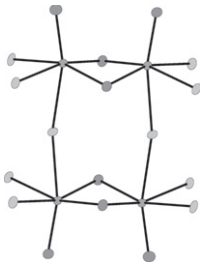

► A facile route to novel reduced molybdenum oxyfluorides. ► New dimer and tetramer units containing Mo—Mo bonds. ► First example of a reduced, infinitely extended molybdenum oxyfluoride.

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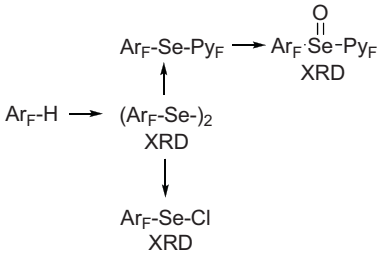
## New polyfluorinated aromatic and aza-aromatic diselenides, selenyl chlorides, non-symmetric selenides and selenoxides

Arkady G. Makarov, Alexander Yu. Makarov, Irina Yu. Bagryanskaya, Makhmut M. Shakirov, Andrey V. Zibarev

*Institute of Organic Chemistry, Russian Academy of Sciences, 630090 Novosibirsk, Russia*




► New polyfluorinated ArSeSeAr synthesized in 3 steps in one-pot reaction from ArH. ► New ArSeCl were obtained from corresponding ArSeSeAr with use of $Cl_2$. ► Highly reactive [$ArSe^-Na^+$] generated *in situ* and reacted with $C_6F_5N$ to give $ArSePy_F$. ► $ArSePy_F$ were oxidized with $KMnO_4$ to chiral $ArSe(=O)Py_F$.

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## Effect of fluorine–oxygen mixed gas treated graphite fibers on electrochemical behaviors of platinum–ruthenium nanoparticles toward methanol oxidation

Soo-Jin Park[a], Yongju Jung[b], Seok Kim[c]

[a]*Department of Chemistry, Inha University, 253, Yonghyun-dong, Nam-gu, Incheon 402-751, South Korea*
[b]*Department of Applied Chemical Engineering, Korea University of Technology and Education, 307, Gajeon-ri, Byeongcheon, Cheonan-si, Chungnam-do 330-708, South Korea*
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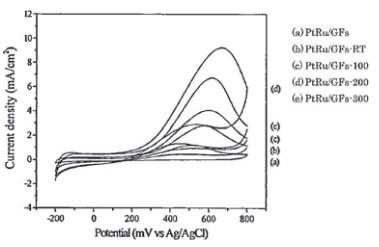


► PtRu particles were deposited on fluorine–oxygen mixed gas-treated graphite nanofibers. ► Gas treatment temperature was changed to modify surface characteristics. ► The catalyst showed the improved activity using treated graphite nanofibers. ► Activity was dependent on particle size and specific surface area of catalysts.

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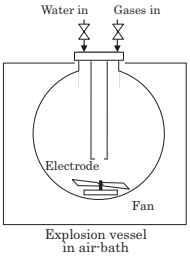
## Effects of temperature and humidity on the flammability limits of several 2L refrigerants

Shigeo Kondo, Kenji Takizawa, Kazuaki Tokuhashi

*National Institute of Advanced Industrial Science and Technology (AIST), Central 5, 1-1-1, Higashi, Tsukuba, Ibaraki 305-8565, Japan*

► Effects of temperature and humidity on the flammability limits of 2L refrigerants were investigated. ► Temperature effect on $NH_3$, R32, and R143a is explainable by White's rule, but not for 1234yf and -ze. ► Humidity does not affect the flammability limits of $NH_3$, R32, and R143a. ► Flammability of 1234yf and -ze is markedly enhanced by humidity due to catalytic effect.

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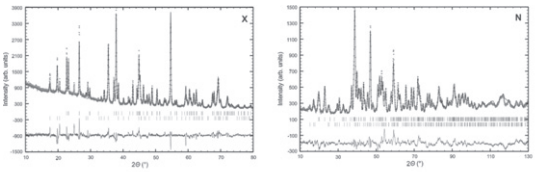
## The study of the system $Na_3AlF_6$–$FeF_3$

František Šimko[a], Ondrej Prítula[a], Aydar Rakhmatullin[b], Catherine Bessada[b]

[a]*Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dúbravská cesta 9, 845 36 Bratislava, Slovakia*

[b]*Conditions Extrêmes et Matériaux: Haute Température et Irradiation CNRS, 1D av. de la Recherche Scientifique, 450 71 Orléans, France*

► $FeF_3$ dissolves in the $Na_3AlF_6$ melt in the form of various solid solutions. ► System with 25 mol% $FeF_3$ contains crystalline phases in weight ratio: 64.8 ± 2.8% of $Na_3(Al_xFe_y)F_6$ and 35.2 ± 2.7% of $Na_5(Al_xFe_y)_3F_{14}$, respectively. ► Non-ferrous unique volatile product originates in the system $Na_3AlF_6$–$FeF_3$. ► It confirms $Fe^{3+}/Al^{3+}$ substitution but not the traditional view of forming $FeF_6^{3-}$ species in $AlF_6^{3-}$ melts.




Rietveld fits for the calculations with the X-ray (X) and the neutron (N) diffraction patterns

Sample $Na_3AlF_6$ + 25 mol% $FeF_3$: Crystalline phases of solid solutions in weight ratio (64.8±2.8)% of $Na_3(Al_xFe_y)F_6$ and (35.2±2.7)% of $Na_5(Al_xFe_y)_3F_{14}$, respectively.

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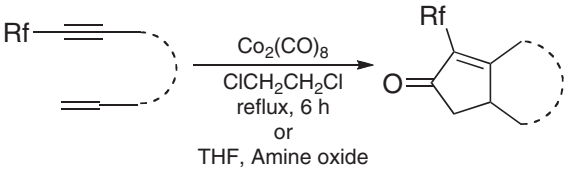
## A novel synthesis of fluorine-containing cyclopentenones *via* Pauson–Khand reaction

Tsutomu Konno, Takumi Kida, Akinori Tani, Takashi Ishihara

*Department of Chemistry and Materials Technology, Kyoto Institute of Technology, Matsugasaki, Sakyo-ku, Kyoto 606-8585, Japan*

► *Intermolecular* PKR was done by using fluoroalkylated alkynes with 2-norbornene. ► Reaction at the reflux gave the cyclopentenones as a diastereomeric mixture. ► *Intramolecular* PKR was carried out by using teminal enyne compounds. ► Reaction proceeded smoothly in the presence of amine oxide. ► Allyl $CF_3$-propargyl ethers afforded adducts as a single isomer.

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## Controllable synthesis, upconversion luminescence, and paramagnetic properties of $NaGdF_4$:$Yb^{3+}$,$Er^{3+}$ microrods

Zhe Chen, Zhenyu Liu, Ye Liu, Kezhi Zheng, Weiping Qin

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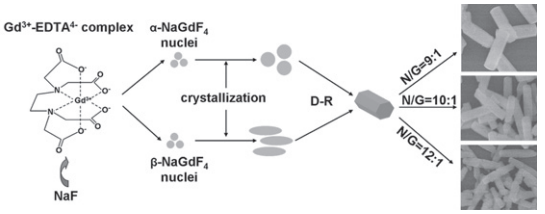
► Well-shaped single-crystal $NaGdF_4$ microrods are first prepared. ►The effects of varied reaction conditions on products are all studied in detail. ► Size-dependent upconversion luminescence is discussed. ► Paramagnetic properties of microrods with different size are also discussed.



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## Enhanced dispersion stability and photocatalytic activity of $TiO_2$ particles fluorinated by fluorine gas

Jae-Ho Kim[a], Fumihiro Nishimura[a], Susumu Yonezawa[b], Masayuki Takashima[b]

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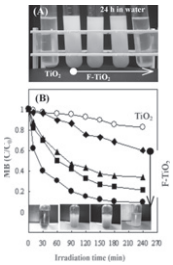


► Fluorinated $TiO_2$ (F-$TiO_2$) particles were prepared using fluorine gas. ► F-$TiO_2$ particles indicated good dispersion stability better than pure $TiO_2$ particles in various solvents. ► Degradation ratio of methylene blue (MB) with F-$TiO_2$ was much higher than that of untreated $TiO_2$. ► Absorption wavelength range of F-$TiO_2$ particles expanded to 500 nm.

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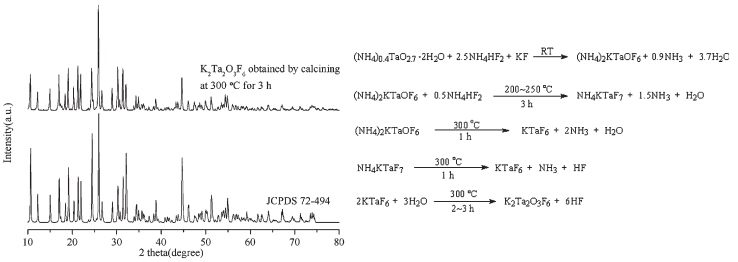
## Low-temperature synthesis of $K_2Ta_2O_3F_6$

Cuihua Lin, Heng Jiang, Hong Gong, Tingting Su, Zhengyi Zhang, Wenguang Liu

*School of Chemistry and Materials Science, Liaoning Shihua University, Fushun 113001, China*




► $K_2Ta_2O_3F_6$ can be obtained by fluorination reaction at 300 °C. ► The intermediates are assumed to be $(NH_4)_2KTaOF_6$ and $NH_4KTaF_7$. ► Their thermal decomposition resulted in KTaF6. ► Hydrolysis of $KTaF_6$ produces $K_2Ta_2O_3F_6$.

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## Soluble copoly(aryl ether ether ketone ketone)s containing xanthene and hexafluoroisopropylidene moieties

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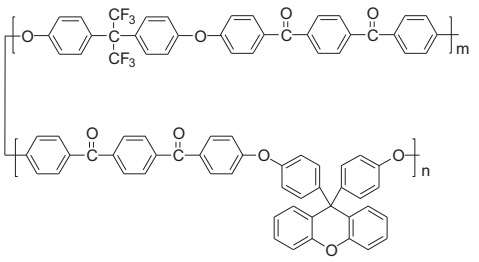


► Four new PEEKK copolymers containing xanthene and hexafluoroisopropylidene moieties were synthesized. ► These PEEKKs exhibited good solubilities, mechanical and thermal properties, especially higher glass transition temperatures. ► Introduction of hexafluoroisopropylidene units into the polymers afforded them low dielectric constants and high optical transparency.

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## The nonisothermal crystallization kinetics of surface fluorinated polypropylene/polypropylene blend

Weihong Guo[a], Lei Gao[a], Guanlong Chen[a], Yan Zhang[a], Haoming He[c], Tian Xie[c], Sanke Yang[c], Shimin Ding[a], Xianjin Yang[abc]

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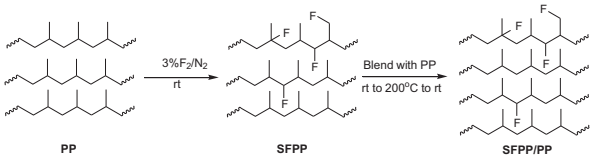
[b]*Key Laboratory of Organofluorine Chemistry, Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, 345 Lingling Road, Shanghai 200032, China*
[c]*Wengfu Group Co. Ltd., Guizhou 550000, China*




► The surface fluorinated polypropylene/PP blend was prepared. ► The nonisothermal crystallization kinetics properties of the blend were studied. ► DSC shows the incompatibility of surface fluorinated polypropylene and PP is good. ► Introducing fluorine into PP leads to its $T_0$, $T_c$ and $\Delta E$ increasing. ► Mo equation supplies a reasonable description for its crystallization behavior.

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## FSG-Hf($NPf_2$)$_4$ catalyzed, environmentally benign synthesis of 1,8-dioxo-decahydroaridines in water–ethanol

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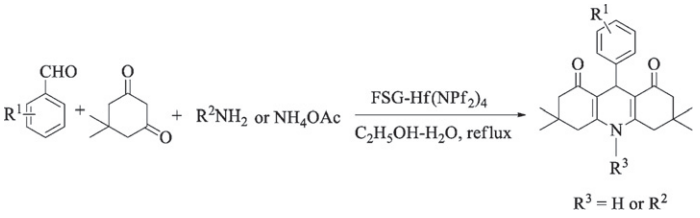
► Fluorous silica gel supported Hf($NPf_2$)$_4$ was prepared. ► 1,8-Dioxo-decahydroacridines were synthesized in the presence of FSG-Hf($NPf_2$)$_4$. ► FSG-Hf($NPf_2$)$_4$ can be recovered and reused without significant loss of activity.

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## New approach to 3,3-difluoroallyl alcohol

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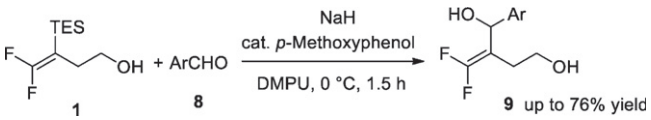
[a]*Faculty of Pharmaceutical Sciences, Setsunan University, 45-1, Nagaotoge-cho, Hirakata 573-0101, Japan*

[b]*Department of Chemistry, The University at Albany – SUNY, 1400 Washington Ave., Albany, NY 12222, United States*




► This is the first synthesis of 4,4-difluoro-3-(triethylsilyl) but-3-en-1-ol (**1**). ► **1** generates 2,2-difluorovinylanion by treatment of **1** with NaH. ► The generated 2,2-difluorovinylanion attacks to aldehydes. ► **1** serves good building block for introducing 2,2-difluorovinyl unit.

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## A novel system for the Suzuki cross-coupling reaction catalysed with light fluorous palladium–NHC complex

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► A novel Pd–NHC catalyst containing fluorous tags was prepared and characterized. ► Suzuki reactions were carried out in co-solvent and high yields were obtained. ► The catalyst could be reused three times without significant loss of activity.