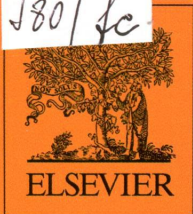


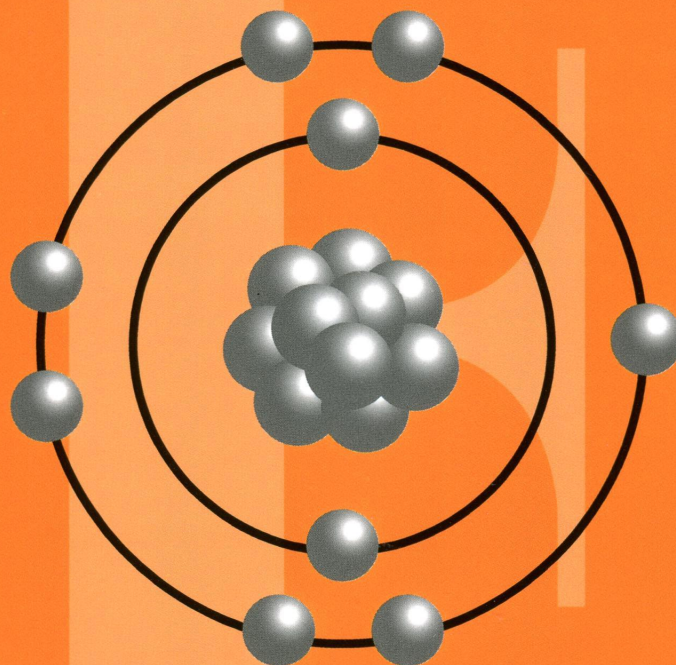
TW  
J80/sc

Volume 168, December 2014

ISSN 0022-1139



# JOURNAL OF FLUORINE CHEMISTRY



*J. Fluorine Chem.*

Available online at [www.sciencedirect.com](http://www.sciencedirect.com)

**ScienceDirect**



## Contents

Graphical Abstracts .....	v
<b>Full Length Articles</b>	
Microwave-assisted TsOH/SiO <sub>2</sub> -catalyzed one-pot synthesis of novel fluoro-substituted coumarin hydrazones under solvent-free conditions G.-Y. Yang, J.-T. Yang, C.-X. Wang, S.-F. Fan, P.-H. Xie and C.-L. Xu .....	1
The influence of inorganic materials on the pyrolysis of polytetrafluoroethylene. Part 2: The common oxides of Al, Ga, In, Zn, Cu, Ni, Co, Fe, Mn, Cr, V, Zr and La G.J. Puts and P.L. Crouse .....	9
Synthesis and biological evaluation of 7-trifluoromethylpyrazolo[1,5- <i>a</i> ]pyrimidines as anti-inflammatory and antimicrobial agents R. Aggarwal, E. Masan, P. Kaushik, D. Kaushik, C. Sharma and K.R. Aneja .....	16
Theoretical study on dynamics of the gas phase reactions of CF <sub>3</sub> CF <sub>2</sub> CH <sub>2</sub> OCHF <sub>2</sub> with OH radicals L. Wang, T. Zhang, J. Wen, H. He and J. Zhang .....	25
Use of fluoroform as a source of difluorocarbene in the synthesis of <i>N</i> -CF <sub>2</sub> H heterocycles and difluoromethoxypyridines C.S. Thomason, L. Wang and W.R. Dolbier .....	34
Unexpected formation of <i>N,N',N''</i> -trialkylguanidinium bis(trifluoromethylsulfonyl)imide salts from carbodiimides and bis(trifluoromethylsulfonyl)imide B.A. Shainyan and L.L. Tolstikova .....	40
Zinc promoted asymmetric propargylation of <i>N</i> -(2-chlorotetrafluoroethanesulfin)imines L.-J. Liu and J.-T. Liu .....	44
Visible-light-mediated trifluoroethylation of 2-isocyanobiaryl with trifluoroethyl iodide: Synthesis of 6-trifluoroethyl-phenanthridines W. Fu, M. Zhu, C. Xu, G. Zou, Z. Wang and B. Ji .....	50
BrF <sub>3</sub> -KHF <sub>2</sub> : An air-stable fluorinating reagent T. Shishimi and S. Hara .....	55
Piperidine and 3,3,4,4,5,5-hexafluoropiperidine as terminal groups: Syntheses and properties as new liquid crystals F. Hong, H. Li, D. Zhu, Z. Xia, H. Zhang, H. Wang and Z. Zeng .....	61
Compatibility of container materials with Cr in molten FLiNaK salt J. Qiu, Y. Zou, G. Yu, H. Liu, Y. Jia, Z. Li, P. Huai, X. Zhou and H. Xu .....	69
Synthesis of new bis(3-perfluoroalkyl-1 <i>H</i> -pyrazole) polyoxyethylene N.H. Mekni.....	75
Accurate equations of state for CF <sub>4</sub> , CF <sub>4</sub> -Ar, and CF <sub>4</sub> -CH <sub>4</sub> fluids using two-body and three-body intermolecular potentials from molecular dynamics simulation M. Abbaspour and M. Sheykh .....	81
High-symmetry compact structures are preferred equilibrium configurations of Li <sub><i>n</i></sub> F <sub><i>n</i>+1</sub> <sup>-</sup> ( <i>n</i> = 2–5) superhalogen anions D. Wileńska, P. Skurski and I. Anusiewicz .....	99
Synthesis of fluorine-containing 1,3-thiazine derivatives from primary polyfluoroalkanethioamides S.S. Mykhaylychenko, N.V. Pikun, E.B. Rusanov and Y.G. Shermolovich .....	105
Hydrodeboration of potassium polyfluoroaryl(fluoro)borates with alcohols N.Yu. Adonin, A.Yu. Shabalin and V.V. Bardin .....	111
Synthesis and anticancer activity evaluation of 3,4-mono- and bicyclosubstituted <i>N</i> -(het)aryl trifluoromethyl succinimides E.L. Luzina and A.V. Popov .....	121

Self-assembled monolayers on gold generated from terminally perfluorinated alkanethiols bearing propyl vs. ethyl hydrocarbon spacers O. Zenasni, A.C. Jamison, M.D. Marquez and T.R. Lee .....	128
Reaction of (2,2,3,3-tetrafluoropropyl)sulfonyl chloride with ethyl acrylate as a route to functionalized enamines and ring substituted 3,4-dihydro-2H-thiazine-1,1-dioxides S.A. Siry, V.M. Ogurok and Y.G. Shermolovich .....	137
Fluorous bis(oxazolines) ligand: Synthesis and application in Kabachnik-Fields reaction H. Wang, T. Deng and C. Cai .....	144
Chemoselective trifluoromethylation of the C=N group of $\alpha$ -iminoketones derived from arylglyoxals E. Objalska, M.K. Kowalski, G. Mlostoń, A. Linden and H. Heimgartner .....	151
Synthetic utility of dizinc reagents derived from 1,4-diiodo- and 1,4-dibromooctafluorobutane P.T. Kaplan, B. Chen and D.A. Vicić .....	158
Structure control at the nanoscale in fluorinated graphitized carbon blacks through the fluorination route Y. Ahmad, E. Disa, K. Guérin, M. Dubois, E. Petit, A. Hamwi, P. Thomas and J.-L. Mansot .....	163
A new synthesis of trifluoromethyl sulfides utilizing thiocyanates and fluoroform S. Potash and S. Rozen .....	173
A (Fluoroalkyl)Guanidine Modulates the Relaxivity of a Phosphonate-Containing T <sub>1</sub> -Shortening Contrast Agent X. Wu, A.C. Dawsey, B.N. Siriwardena-Mahanama, M.J. Allen and T.J. Williams .....	177
Synthesis, crystal structure and ion mobility in the complex fluorides of antimony (III) with the lithium cation N.V. Makarenko, A.A. Udovenko, L.A. Zemnukhova, V.Ya. Kavun and M.M. Polyantsev .....	184
Chemical composition and magnetic property modifications of Na <sub>2</sub> Ti <sub>2</sub> Sb <sub>2</sub> O using PTFE as an alkali-metal ion extraction reagent T.C. Ozawa, T. Naka, A. Matsushita, S.M. Kauzlarich and T. Sasaki .....	189
1:1 and 2:1 cocrystallizations of alkoxy-substituted naphthalene derivatives with octafluoronaphthalene through arene-perfluoroarene interactions A. Hori, H. Takeda, J.R. Premkumar and G.N. Sastry .....	193
Ion mobility and phase transitions in heptafluorodiantimonates(III) Cs <sub>(1-x)</sub> (NH <sub>4</sub> ) <sub>x</sub> Sb <sub>2</sub> F <sub>7</sub> and K <sub>0.4</sub> Rb <sub>0.6</sub> Sb <sub>2</sub> F <sub>7</sub> according to NMR and DSC data V.Ya. Kavun, M.M. Polyantsev, L.A. Zemnukhova, A.B. Slobodyuk and V.I. Sergienko .....	198
Phase transitions in fluoride KFe <sub>2</sub> F <sub>6</sub> with tetragonal tungsten bronze structure M.V. Gorev, I.N. Flerov, A. Tressaud, M.S. Molokeev, A.V. Kartashev, E.I. Pogoreltsev and O.A. Bayukov .....	204
Effects of chronic fluoride intake on the antioxidant systems of the liver and kidney in rats F.G. Iano, M.C. Ferreira, G.B. Quaggio, M.S. Fernandes, R.C. Oliveira, V.F. Ximenes and M.A.R. Buzalaf .....	212
Fluorination of steroid estrogens with Selectfluor®: Elucidation of regio- and stereoselectivity R.P. Bogautdinov, A.F. Fidarov, S.N. Morozkina, A.A. Zolotarev, G.L. Starova, S.I. Selivanov and A.G. Shavva .....	218
Synthesis and conformational study of new S-polyfluoroalkyl dithiocarbamates I. Chniti, M.A.K. Sanhoury, D. Merlet and I. Chehidi .....	223
Synthesis of polyfluoroaryl-containing 1,2,3-triazoles by reaction of polyfluoroarenes, sodium azide and active methylene ketones/esters J. Wu, D. Fu and S. Cao .....	230
A DFT computational study on the molecular mechanism of the nitro group migration in the product derived from 3-nitro-2-(trifluoromethyl)-2H-chromene and 2-(1-phenylpropylidene)malononitrile A. Łapczuk-Krygier, V.Yu. Korotaev, A.Yu. Barkov, V.Ya. Sosnovskikh, E. Jasińska and R. Jasiński .....	236
Stereoselective synthesis of $\beta$ -fluoroenyne by the reaction of gem-difluoroalkenes with terminal alkynes G. Jin, J. Zhang, W. Wu and S. Cao .....	240
Heat capacity, entropy, dielectric properties and T-p phase diagram of (NH <sub>4</sub> ) <sub>3</sub> TiF <sub>7</sub> E.I. Pogoreltsev, I.N. Flerov, A.V. Kartashev, E.V. Bogdanov and N.M. Laptash .....	247
Easy access to <sup>19</sup> F-labeled nanoparticles for use as MRI contrast probes via self-assembly of fluorinated copolymers synthesized by sequential RAFT polymerization P.I.R. Muraro, A.G.O. de Freitas, S.G. Trindade, F.C. Giacomelli, J.-J. Bonvent, V. Schmidt, F.P. dos Santos and C. Giacomelli .....	251
<b>Short Communication</b>	
Synthesis and property of novel phthalocyanine having a 3,5-bis-pentafluorosulfanylphenyl group on the $\alpha$ -peripheral position N. Iida, E. Tokunaga, N. Saito and N. Shibata .....	93
The influence of inorganic materials on the pyrolysis of polytetrafluoroethylene. Part 1: The sulfates and fluorides of Al, Zn, Cu, Ni, Co, Fe and Mn G.J. Puts and P.L. Crouse .....	260