



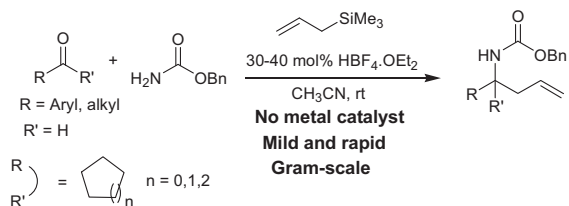
Graphical Abstracts/J. Fluorine Chem. 166 (2014) v–x

HBF₄·OEt₂: An efficient fluorinated acid catalyst for the one-pot synthesis of secondary and tertiary N-homoallylic carbamates

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- HBF₄·OEt₂ is used as a catalyst for the first time in this reaction.
- HBF₄·OEt₂ is used as superior alternative to metal triflates and other catalysts.
- The broad substrates compatibility of HBF₄·OEt₂ makes this method more useful.
- This method is operationally simple and easily scalable.
- A mechanism is also proposed by showing the catalytic involvement of HBF₄·OEt₂.

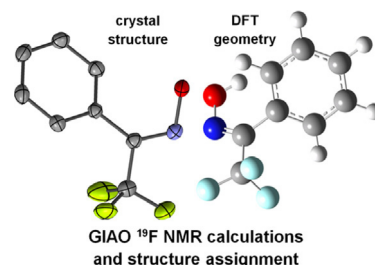


J. Fluorine Chem., 166 (2014) 1

Quantum chemical calculation of ¹⁹F NMR chemical shifts of trifluoromethyl diazirine photoproducts and precursors

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- Quantum chemical prediction of ¹⁹F NMR spectra.
- E/Z assignment of oximes via ¹⁹F NMR spectroscopy.
- ¹⁹F NMR reference table of CF₃ groups associated with photoaffinity labeling.

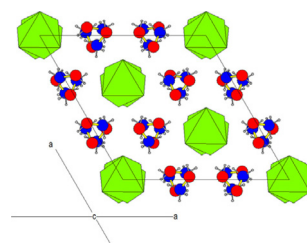


J. Fluorine Chem., 166 (2014) 8

Synthesis and characterization of new hydroxylammonium fluoromanganates and fluoroscandates

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- New hydroxylammonium fluorometallates with the formulas (NH₃OH)₂MnF₄ and (NH₃OH)₃ScF₆, were prepared in aqueous HF.
- (NH₃OH)₂MnF₄ crystallizes monoclinic, P2₁/c, the structure consisting of [MnF₂]_n anionic layers perpendicular to *a* axis.
- (NH₃OH)₃ScF₆ crystallizes trigonal, R3c, with isolated ScF₆ octahedra, surrounded by hydroxylammonium cations.
- Both compounds decompose during thermal analysis in several steps, yielding corresponding fluorides (MnF₂ and ScF₃).



J. Fluorine Chem., 166 (2014) 15

Surface fluorination effects on TiAl particle oxidation resistance

J. Fluorine Chem., 166 (2014) 22

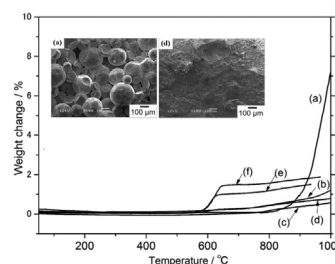
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● Surface fluorination of TiAl alloy particles was conducted at 25–200 °C with F₂ gas. ● Below 125 °C, an oxyfluoride layer on TiAl particles was made from the oxide layer. ● At more than 150 °C, the fluoride layer on TiAl was made from the oxyfluoride layer. ● Fluorinated TiAl oxidation resistance can be 10 times that of untreated material.



Studies of the products from the reactions of co-acids containing concentrated HF and dilute HNO₃ with Zircaloy-4

J. Fluorine Chem., 166 (2014) 28

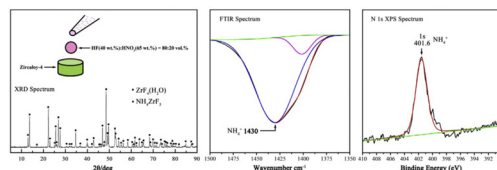
H.F. Gu^{ab}, L.F. Zhang^{ab}, M.Y. Li^{ab}, L. Wang^c, X.N. Li^c, S.Q. Wu^{ab}, S. Peng^c, B. Gao^c, G.P. Li^a

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● The co-acid containing HF (40 wt.%) and HNO₃ (65 wt.%) with four volume ratios, 100:0, 94:6, 89:11 and 80:20, was used. ● The products from the reactions of HF–HNO₃ system with Zircaloy-4 were identified by XRD, FTIR and XPS synthetically. ● The usage of concentrated HF solution leads to the formation of crystalline ZrF₄(H₂O). ● The usage of co-acids containing HF and HNO₃ leads to the formation of crystalline ZrF₄(H₂O) and NH₄ZrF₅.



Coupling of trifluoromethyl isocyanide ligands in binuclear iron carbonyl complexes

J. Fluorine Chem., 166 (2014) 34

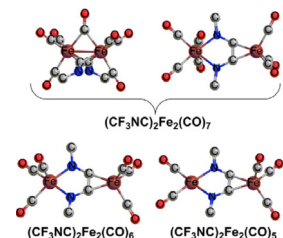
Guoliang Li^{ab}, Lihua Liu^a, Jing Wang^a, Qian-shu Li^a, Yaoming Xie^c, R. Bruce King^{ac}

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● (CF₃NC)₂Fe₂(CO)_n (n = 7, 6, 5) and (CF₃NC)Fe(CO)_n (n = 4, 3) have been studied by DFT. ● Coupling of CF₃NC ligands is predicted to occur in (CF₃NC)₂Fe₂(CO)_n (n = 6, 5). ● (CF₃NC)Fe(CO)₄ has nearly degenerate equatorial and axial trigonal bipyramidal isomers.



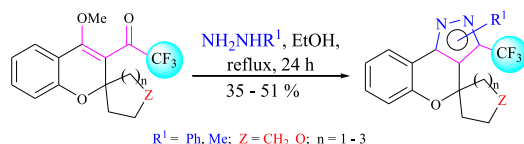
Regioselective synthesis and through-space ¹³C–¹⁹F spin–spin coupling NMR of new tetracyclic 3-(trifluoromethyl)-spiro(chromen[4,3-c]pyrazole-4,1'-cycloalkanes)

J. Fluorine Chem., 166 (2014) 44

Helio G. Bonacorso, Fábio D. Garcia, Chaiene R. Belo, Aniele Z. Tier, Clarissa P. Frizzo, Marcos A.P. Martins, Nilo Zanatta

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● TFAA in the acylation of spiro[chromen-2,1'-cycloalkan]-4-ones (Kebbe's adducts). ● 3-(Trifluoromethyl)-spirochromen[4,3-c]pyrazole-4,1'-cycloalkanes are synthesized. ● Through-space ¹³C–¹⁹F spin–spin coupling NMR is presented and discussed. ● Structures solved by ¹H, ¹³C and ¹⁹F NMR (spin–spin coupling), MS and X-ray data. ● ¹⁹F NMR assigned the trifluoromethyl group position at pyrazole derivatives.



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