

WFC 2017

Robert Syvret, *Program Chair* and Markus Etzkorn, *Program Co-chair*

Plenary Lecture designated (PL) and Invited Lecture designated (IN)

SUNDAY EVENING

Clearwater Hilton
Foyer DEFG

Welcoming reception 5:00 to 7:00 p.m.

Foyer DEFG

Poster Session I **7:00 - 9:00**

R. G. Syvret, Organizer, Presiding

1. C–F and C–H activation reactions of fluorinated molecules at rhodium-silyl complexes. **C.N. von Hahmann**
2. Functionalization by C–F bond activation of fluorocarbons using germylium- and silylium-like surface species. **G. Meissner**, T. Braun, E. Kemnitz
3. Synthesis of a heptapeptide containing trifluoromethyl- λ^6 -tetrafluorosulfanyl groups. **A. Capellan**, A. Ikeda, J.T. Welch
4. Improving access to aromatic sulfur pentafluorides by direct fluorination of disulfides. **J. Ajenjo**, P. Beier
5. Synthesis and chemistry of SF₅N< and SF₅CF₂-containing heterocycles. **S.P. Belina**, A.V. Matsnev, J.S. Thrasher
6. Reactivity of SF₅ oganyls towards transition metals. **C. Berg**, T. Braun, R. Laubenstein, B. Braun
7. Synthesis and characterization of SF₅-containing fullerene derivatives. **S. Qing**, N.J. DeWeerd, A.V. Matsnev, S.H. Strauss, O.V. Boltalina, J.S. Thrasher
8. Recent developments in the preparation of monofluoroalkenes from 3-fluoro-3-halopropenes. **J. Hamel**, M. Cloutier, M. Drouin, J. Paquin
9. Hydrogen-bond-promoted Friedel-Crafts reaction of secondary propargylic fluorides. **J. Hamel**, M. Beaudoin, M. Cloutier, J. Paquin

10. Sugar-based isoxazoles with perfluoroalkylmethyl moiety as antibacterial candidates. **A. Mohammed**
11. Sensitive detection of protein function via perfluoro-*tert*-butyl amino acids. **N.J. Zondlo**
12. Amine-catalyzed decarboxylative chlorination of α -fluoro- β -keto carboxylic acids. **K. Kitahara**, A. Naruse, S. Iwasa, K. Shibatomi
13. Recent findings and trends in the chemistry of tetrafluoridobromates(III). **S.I. Ivlev**, A.J. Karttunen, R.V. Ostvald, D. Kraus
14. Chiral fluoride anion generators in asymmetric catalytic reactions. **S. Park**, S. Paladhi, C. Song
15. Investigation on Cl-F exchange mechanism occurring at C(sp²) and C(sp³) orbitals of halogenated cyclopentene. **H. Quan**, C. Zhang, M. Tamura
16. New polyfluorinated polyethers and synthesis of their hypothetical epoxide intermediates. **C. Liu**, X. Liu, A.V. Matsnev, J.S. Thrasher
17. Through-space arene activation by anchimeric assistance from fluorine: A different method of directing electrophilic substitution. **M. Holl**, T. Lectka
18. Investigation of nucleophilic difluoromethylation using the Ruppert-Prakash reagent. **S. Krishnamoorthy**, S.G. Prakash
19. Surface activities of bivalent and trivalent salts of perfluorooctanoic acid and perfluorobutanoic acid in water and in organic liquids. **Z. Xiao**, H. Xing, Z. Dou, J. Xiao
20. Surface activity and interfacial activity of amine oxide type fluorinated surfactant and its mixture with anionic hydrocarbon surfactant in strong acidic solution. **Z. Xiao**, H. Xing, Z. Dou, J. Xiao
21. New perfluoroalkoxyl co- and terpolymers with tetrafluoroethylene (TFE). **C.A. Parrish**, D. Hercules, A.R. Scavuzzo, E.G. Burns, A.V. Matsnev, J.S. Thrasher
22. Preparation of ultra-thin two-dimensional semifluorinated polymer films at liquid-liquid interface
. **J.H. Kramer**, **S. Mao**
23. 3-difluoroalkyl-3-hydroxy-isoindolin-1-ones: Improved synthesis of a versatile scaffold. **S.B. Munoz**, V. Krishnamurti, G.A. Olah, S.G. Prakash
24. Biological evaluation of both enantiomers of fluoro-thalidomide: Comparative case study using human myeloma cell line H929. **E. Tokunaga**, N. Shibata

25. Toward fluorinated isoindene dimers and heterocyclic, fluorinated *anti*-bisarene scaffolds. M. Etzkorn, **J. Franklin**, V. Wait
26. Cobalt-catalyzed aryl C–F bond borylation. **D. Song**, E. Lee
27. Synthesis and application of new perfluoro(alkoxyalkyl)-substituted heteroarenes. **M. Noro**, Y. Takahira, N. Miyake, D. Jomuta, T. Nakano, Y. Matsukawa, Y. Morizawa
28. A flexible, iterative strategy for synthesizing fluorinated bioactive molecules. **A.M. Ahmed**, L. Hunter
29. Nitrogen-doped single-walled carbon nanotubes prepared from fluorinated SWCNTs. K. Yokoyama, Y. Sato, M. Yamamoto, T. Nishida, **Y. Sato**
30. General and GMP-compliant method for radiofluorination of electron-rich aromatic compounds using copper triflate. **T. Morley**, V. Carroll, C. Papin, M. Zheng, d. alagille, R.M. Baldwin, G.D. Tamagnan
31. Low cost deoxyfluorination reaction with methanesulfonyl fluoride / DBU system. **K. KURIHARA**, A. Harada, Y. NAKAMURA
32. Synthesis, characterisation, and computational study of fluorido(imido)tungsten(VI) complexes. **D. Turnbull**, S.D. Wetmore, M. Gerken
33. Difluoro(imidazolium)sulfuranes. **S. Lim**, E. Lee
34. Exploring adducts of SF₄ and [SF₃]⁺ with various oxygen-bases. **D. Stuart**, D. Turnbull, S.D. Wetmore, M. Gerken
35. Nafion-H@SPIONs as a robust perfluoro-tagged nanocatalyst for the synthesis of AT-130 analogous in a microreactor. **A. Khosropour**
36. Crystal engineering with polyfluoroarenes: Anion- π , lone pair- π , and π - π interactions, and halogen bonding. **G.C. Saunders**, H. Althagbi, D. Bernstein, C. Crombie, D. McQuiston, M. Oosterwijk, W. Zou
37. Efficient process for the synthesis of trifluoromethylated spiro[indoline[1,3]oxazino[3,2a]quinolin]-2-ones. G. Liu, **Y. Wu**, X. Sun, J. Han, J. Chen, H. Zhang, W. Cao
38. Exploiting the fluorine *gauche* effect for applications in medicinal and supramolecular chemistry. **A. Ariawan**, L. Hunter
39. Xenon trioxide and its coordination chemistry. **J.T. Goettel**, V. Haensch, H. Mercier, G.J. Schrobilgen

40. Nanoscale Lewis acidic aluminium chlorofluoride (ACF) in the activation of small molecules. **B. calvo**
41. Facile, single-step method for functionalization of hetero-PAHs with perfluorinated alkyl or aromatic rings. **K. Rippy**, N.J. DeWeerd, Y. Chen, O.V. Boltalina, S.H. Strauss
42. Radical fluorination of sp^3 C-H and C-C bonds employing transition metals, radical initiators, and photochemistry: Methods, mechanisms, and advances in selectivity. **C.R. Pitts**, T. Lectka
43. HF addition reactions across $C\equiv N$ and $C=O$ bonds. **A. Baxter**, J. Hegge, R.M. Haiges, K.O. Christe
44. New trifluoromethylated organics: A photochemical approach. **T. Mathew**, K. Belligund, S.G. Prakash, G.A. Olah
45. Direct trifluoromethylation from fluoroform with dimsyl-K. **S. Qing**, A.V. Matsnev, G. Lin, C. Liu, Y. Chen, J.S. Thrasher
46. Olefin insertion into a Pd-F bond: Catalyst reactivation following β -F elimination in ethylene/vinyl-fluoride copolymerization. **S. Wada**, R.F. Jordan
47. Atmospheric chemistry of $(CF_3)_2CHOCH_3$: Kinetics of the gas-phase reactions with OH radicals, atmospheric lifetime, and global warming potentials. **S. Qin**, D. Liu, W. Li, Q. Zhang
48. Efficient process for the synthesis of perfluoroalkylated tetrahydro-4*H*-chromenes. X. Yan, J. Han, J. Chen, H. Zhang, **W. Cao**
49. Efficient process for the synthesis of perfluoroalkylated pyrazolopyridines. D. He, J. Han, J. Chen, H. Zhang, **W. Cao**
50. Efficient one-pot three-component process for the synthesis of perfluoroalkylated indolizines. D. He, J. Han, J. Chen, H. Zhang, **W. Cao**

Clearwater Hilton

Starfish

Hospitality Room 9:00 – 11:00 p.m.

Co-sponsored by SynQuest Laboratories and Apollo Scientific

MONDAY MORNING

Clearwater Hilton
Salons EF

Fluorine Chemistry Session I

Sponsored by Arkema Inc. Fluorochemicals

R. G. Syvret, *Organizer, Presiding*

7:50 Introductory Remarks. Plenary (PL), Invited (IN)

8:00 51. (PL) Xenon(II) oxide chemistry, and the coordination chemistry of XeF₆, XeO₃, and NgF₂ (Ng = Kr, Xe). J.T. Goettel, J. DeBackere, V. Haensch, M.R. Bortolus, M. Ivanova, J. Haner, K. Matsumoto, H. Mercier, **G.J. Schrobilgen**

8:30 52. (IN) Fluoronium ions and hypervalent fluorine. **K.O. Christe**, R.M. Haiges, M. Rahm, D.A. Dixon

9:00 53. (IN) Generation of a symmetrical fluoronium ion in solution: From theoretical interest to potential practical applications. **T. Lectka**

9:30 54. (IN) Nanoscopic luminescent alkaline earth metal fluorides doped with rare earth metal fluorides. **E. Kemnitz**, T. Krahl, B. Ritter

10:00 Intermission. *Co-sponsored by ACS Division of Fluorine Chemistry and Beijing Yuji Science and Technology Co. Ltd.*

Clearwater Hilton
Salons EF

Fluorine Chemistry Session II

Co-sponsored by 3M Company and ExFluor Research Corporation

J. T. Welch, *Presiding*

10:20 55. (IN) Nano-CoF₃ as electrode material for Li-ion battery; synthesis, characterizations and electrochemical properties. **A. Tressaud**, H. Groult, S. Neveu, S. Leclerc, A. Porras-Gutierrez, C. Julien, E. Durand, C. Labrugere

10:50 56. Breaking C-F bonds for electricity: design, synthesis, and characterization of new fluorinated carbon materials for high capacity cathodic materials. **H. Sun**

11:10 57. (IN) Fluorocarbon-assisted dynamic self-assembly: Applications in materials sciences and medicine. **M. Krafft**

11:40 58. Selective synthesis of perfluorinated E-1-propenyl amines. **W.M. Lamanna**, A. Monteil, S. Smith, M.J. Bulinski, M.G. Costello, J.G. Owens

12:00 Lunch.

MONDAY AFTERNOON

Clearwater Hilton
Salons EF

Fluorine Chemistry Session III
Sponsored by Peach State Labs
G. Sandford, *Presiding*

1:30 59. (PL) Recent studies in the area of fluoroalkylations and fluorinations. **S.G. Prakash**

2:00 60. (IN) A new version of Umemoto reagents as practically useful electrophilic trifluoromethylating agents. **T. Umemoto**

2:30 61. (IN) Sustainable concepts for late-stage fluoroalkyl(thiol)ations. **L.J. Goossen**

3:00 62. (IN) New approaches in the direct introduction of CF₃S and CF₃S(O) motifs. **D. Cahard**

3:30 Intermission. *Co-sponsored by ACS Division of Fluorine Chemistry and Beijing Yuji Science and Technology Co. Ltd.*

Clearwater Hilton
Salons EF

Fluorine Chemistry Session IV
Sponsored by Beijing Yuji Science & Technology Co. Ltd
S. G. Prakash, *Presiding*

3:50 63. (IN) Recent advances in hydrogen bond-controlled nucleophilic halogenation. **G.B. Hammond**

4:20 64. (IN) Selectively fluorinated heterocyclic systems. **G. Sandford**

4:50 65. Azidoperfluoroalkanes – neglected, stable and useful fluorinated synthons. **P. Beier**

5:10 66. Difluorinated ketones as under-studied fluorinated building blocks. **G. Pattison**

5:30 67. From fluoroalkylation to fluorination: Deoxyfluorination of alcohols with 3,3-difluoro-1,2-diarylcyclopropenes (CpFluors). L. Li, C. Ni, F. Wang, **J. Hu**

Clearwater Hilton
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Hospitality Room 9:00 – 11:00 p.m.

Co-sponsored by SynQuest Laboratories and Apollo Scientific

TUESDAY MORNING

Clearwater Hilton
Salons EF

Fluorine Chemistry Session V
Sponsored by Galaxy Chemicals, LLC
G. J. Schrobilgen, *Presiding*

8:00 68. (PL) Computational approaches to the study of fluorine containing molecules. **D.A. Dixon**

8:30 69. (IN) Metallocenes and oxidative fluorine reagents. **K. Seppelt**, M. Malischewski

9:00 70. (IN) Fluorinated precursors as catalysts for exciting transformations. **H.W. Roesky**

9:30 71. (IN) Fluorine-rich fluorides: New insights into the chemistry of polyfluoride anions and beyond. **S. Riedel**

10:00 Intermission. *Co-sponsored by ACS Division of Fluorine Chemistry and Beijing Yuji Science and Technology Co. Ltd.*

Clearwater Hilton
Salons EF

Fluorine Chemistry Session VI
Co-sponsored by Merck KGaA and TCI Chemicals America
J. Hu, *Presiding*

10:20 72. (IN) Pentafluoroethyl derivatives of sulfur(IV) fluorides. N. Kostiuik, P. Hazendonk, S.D. Wetmore, **M. Gerken**

10:50 73. (IN) Chemistry of halogen and uranium fluorides. **D. Kraus**

11:20 74. (IN) Protonation and addition reactions of nitriles, azides and isocyanates with anhydrous HF. **R.M. Haiges**, T. Saal, A. Baxter, K.O. Christe

11:50 FLUO Division Business Meeting 11:50 to 12:00.

12:00 Lunch.

TUESDAY AFTERNOON

Clearwater Hilton
Salons EF

Fluorine Chemistry Session VII
Sponsored by Arkema Inc. Fluorochemicals
M. Gerken, *Presiding*

1:30 75. (IN) Activation of SF₆ at rhodium complexes. **T. Braun**, L. Zámotná, C. Berg

2:00 76. (IN) Reactions of fluorocarbons with late transition metal complexes. **J. Love**

2:30 77. (IN) Green hydrofluoroalkene synthesis via base-metal complex mediation or catalysis.
R.T. Baker

3:00 78. (IN) Organocatalytic C-F bond activation with alanes and gallanes. A.D. Jaeger, R. Walter, **D. Lentz**

3:30 Intermission. *Co-sponsored by ACS Division of Fluorine Chemistry and Beijing Yuji Science and Technology Co. Ltd.*

Clearwater Hilton
Salons EF

Fluorine Chemistry Session VIII
Sponsored by Peach State Labs
T. Braun, *Presiding*

3:50 79. (IN) New reagents for difluoromethyl and difluoromethylene transfer. **D.A. Vicic**, L. Xu, P.T. Kaplan

4:20 80. Carbon-fluorine bond activation induced by silver particles. **G.C. Saunders**, H. Thomas, A. Marr, F. Lorenzini, Y. Wang

4:50 81. Structures and hydration/dehydration dynamics of M₂(H₂O)_nB₁₂F₁₂: M⁺ = Li⁺-Cs⁺, Ag⁺; n = 0-4. **S.H. Strauss**, D.V. Peryshkov, E.V. Bukovsky, H. Wu, W. Zhou, **W. tang**, W. Jones, M. Lozinsek, T.C. Folsom, D. Heyliger, T. Udovic

5:20 82. Fluorinated and other halogenated CB₁₁ carborane anions and radicals. A. Wahab, F. Šembera, J. Ludvík, J. Klíma, R. Crespo, M. Piqueras, Z. Janoušek, **J. Michl**

5:50 83. Fluorination of fullerenes: From curiosity-driven research to real-world applications.
O.V. Boltalina

Wednesday Morning

Clearwater Hilton
Foyer DEFG

Fluorine Chemistry Poster Session II, exposition and buffet breakfast
R. G. Syvret, *Organizer, Presiding*

8:00 - 10:00 a.m.

Clearwater Hilton

Starfish

Hospitality Room 9:00 – 11:00 p.m.

Co-sponsored by SynQuest Laboratories and Apollo Scientific

THURSDAY MORNING

Clearwater Hilton
Salons EF

Fluorine Chemistry Session IX
Sponsored by Galaxy Chemicals, LLC.
H. Koroniak, *Presiding*

8:00 84. (PL) An enzymatic method for C-¹⁸F bond formation for PET. **D. O'Hagan**

8:30 85. (IN) Fluorine-18 radiochemistry in drug development and clinical research. **N. Vasdev**

9:00 86. Hypervalent Iodine based radiofluorination for the preparation of PET radiopharmaceuticals. **S.H. Liang, N. Vasdev**

9:30 87. (IN) A challenge to fluorine gas generation by electrolysis at ambient temperature. **K. Matsumoto, T. Inoue, S. Tawa, T. Sugimoto, R. Hagiwara**

10:00 Intermission. *Co-sponsored by ACS Division of Fluorine Chemistry and Beijing Yuji Science and Technology Co. Ltd.*

Clearwater Hilton
Salons EF

Fluorine Chemistry Session X
Sponsored by Arkema Inc. Fluorochemicals.
K. Matsumoto, *Presiding*

10:20 88. (IN) Strategic incorporation of fluorine into bioactive compounds for chemical biology and drug discovery. **I. Ojima**

10:50 89. (IN) Synthesis of fluorinated aminophosphonates *via* stereocontrolled heterocycles ring opening. K. Margas-Musielak, P. Mrowiec, M. Skibinska, M. Rapp, T. Cytlak, M. Kubicki, **H. Koroniak**

11:20 90. Fluorobenzene derivatives as multifunctional tools for medicinal chemistry and modification of biomolecules. **F. Diness**, M. Meldal, C.B. Jacobsen, A. Embaby

11:40 91. Enantioselective Friedel-Crafts alkylation reaction of indoles with beta-aryl-beta-trifluoromethyl nitroalkene. **T. Akiyama**, I. Ibáñez Sánchez

12:00 Lunch.

THURSDAY AFTERNOON

Clearwater Hilton
Salons EF

Fluorine Chemistry Session XI
Sponsored by Peach State Labs
D. O'Hagan, Presiding

1:30 92. (IN) SF₅ enolates in Ti(IV)-mediated aldol reactions. M.V. Ponomarenko, S. Grabowsky, R. Pal, A.A. Fokin, **G. Roesenthaler**

2:00 93. (IN) Methods for the synthesis of CF₃- and SF₅-containing molecules using a building-block approach. **J. Paquin**

2:30 94. (IN) Reactivity of fluorine substituted ester enolates. **G. Haufe**, A. Dreier, B. Beutel, P. Dudzinski, F. Friese, A.V. Matsnev, J.S. Thrasher

3:00 95. (IN) Recent progress in the chemistry of SF₅CX₂- and SF₅N-containing compounds. **A.V. Matsnev**, S.P. Belina, S. Qing, C.A. Parrish, J.S. Thrasher, P. Dudzinski, G. Haufe

3:30 Intermission. *Co-sponsored by ACS Division of Fluorine Chemistry and Beijing Yuji Science and Technology Co. Ltd.*

Clearwater Hilton
Salons EF

Fluorine Chemistry Session XII
Co-sponsored by Halocarbon Products Corporation and Chemours
J. Paquin, Presiding

3:50 96. (IN) Further exploitation of photoredox catalysis in the generation and use of difluoromethyl radicals to prepare molecules of synthetic interest. **W.R. Dolbier**, Z. Zhang, H. Martinez

4:20 97. (IN) Advances in the preparation and reactions of trifluoromethyl tetrafluoro- λ^6 -sulfany compounds. A. Ikeda, A. Capellan, N.B. Breen, L. Zhong, **J.T. Welch**

4:50 98. (IN) Cycloaddition reactions of perfluoroacyl isothiocyanates. **V. Petrov**

5:20 99. (IN) Challenges in the successful synthesis of oligo(hexafluoropropylene oxide) perfluoroisopropenyl ether (PIPE). T.J. Burgess, A. Pasiuk, B.J. Jelier, **C. Friesen**

5:50 100. New 3-fluorocyclobutyl amines and amino acids: synthesis and physical chemical properties. **I. Kondratov**, I.A. Feskov, A.V. Chernykh, D. Radchenko, N.A. Tolmachova, G. Haufe

**Clearwater Hilton
Salons EF**

Banquet reception 7:00 – 7:30 p.m.

Banquet dinner 7:30 – 9:00

Starfish

Hospitality Room 9:00 – 11:00 p.m.

Co-sponsored by SynQuest Laboratories and Apollo Scientific

FRIDAY MORNING

Clearwater Hilton
Salons EF

Fluorine Chemistry Session XIII

Co-sponsored by ACS Division of Polymer Chemistry and Solvay Chemicals, Inc.

R. M. Haiges, *Presiding*

8:00 101. (IN) Preparation of *meta*- and *para*-SF₅-substituted pyridines. **N. Shibata**

8:30 102. (IN) Synthesis of organofluorine compounds using difluorocarbene. **A.D. Dilman**, V. Levin

9:00 103. Selected synthetic aspects of fluoro-isoindenone chemistry: How much fluorine is too much?. **M. Etzkorn**, J. Franklin, V. Wait, J. Spinaris

9:30 104. Ruthenium-catalyzed cross-metathesis with highly fluorinated olefins. **Y. Takahira**, T. Usuda, Y. Morizawa, N. Otozawa

9:50 105. Gold(I) activating C-F bond: Catalysis and mechanism. **J. Zhang**, J. Hu

10:10 Intermission. *Co-sponsored by ACS Division of Fluorine Chemistry and Beijing Yuji Science and Technology Co. Ltd.*

Clearwater Hilton
Salons EF

Fluorine Chemistry Session XIV

Sponsored by Beijing Yuji Science & Technology Co. Ltd.

M. Etzkorn, Presiding

10:30 106. NHC nickel-catalyzed derivatization of polyfluoroarenes. **U. Radius**

10:50 107. Transverse relaxation (T₂) time and peak width at half-height measurements for support of di-radical intermediates during the reaction of chlorosulfonyl isocyanate with electron-rich monofluoroalkenes. **D.F. Shellhamer**, Z.J. Beavis, S.L. Elwin, L. Gomez, s. Van Horne

11:10 108. Structural elucidation of fluorosurfactants by NMR. **H. Liu**

11:30 109. Which nonmetal, which halogen, is the strongest oxidant? A study with sysematics and surprises. M. Ponikvar-Svet, D.N. Zeiger, **J.F. Liebman**

11:50 Closing Remarks – R.G. Syvret, Conference Chair.