# Full RMRM2020 Program (updated Oct. 26<sup>th</sup>)

Color codes: Invited speaker; Guest speaker; Post Doc; Grad; Undergraduate

1. Noon purple Plenary and award speakers, one is 45 min with 5 min Live Q&A follow the presentations; others are 25 min live presentations – 5 min Live Q&A follow the presentations

2. Purple session invited speakers, most are 25 min live presentations – 5 min Live Q&A follow the presentations

**3.** Brown guest speakers with variable times of recorded talks – these presentations are spread around the program and Live Q&A follow the cluster of presentations (3-5 talks)

4. Red Postdoctoral pre-recorded presentations, 9 min recorded talk – Live Q&A follow the cluster of presentations (3-5 talks)

**5. Blue Graduate pre-recorded presentations, 6 min recorded talk – Live Q&A follow the cluster of presentations (3-5 talks)** 

6. Green Undergraduate pre-recorded presentations, 3 min recorded talk – Live Q&A follow the cluster of presentations (3-5 talks)

# RMRM2020 Nov. 11, 13 and 14

Debbie Crans, Program Chair

Kateryna Kostenkova, Assistant Program Chair

#### **TUESDAY AFTERNOON**

### **Pre-meeting Icebreaker Mixer**

3:00-4:00 pm Information on meeting details and getting to know your coattendees

#### THURSDAY MORNING

## Welcome Room

8:00 -9:00 am Information and welcome bag

### (1) Pikes Peak Opening Ceremony

8:45 Welcoming Words and Information on Symposium

Debbie C. Crans, Carlos Oligo Delgado and Dean Janice Nerger, Colorado State University

(1) Pike's Peak

# Young Talent in the Rocky Mountain Region

Young Investigator Symposium

D. C. Crans, *Organizer, Presiding* C. J. Olivo-Delgado, G. G. Stanley, *Presiding* 

**9:00** Introduction to Young Talent in Rocky Mountain Region.

**9:01 1.** Effects of a dynamic local environment on the properties of chemical systems. **R. Noriega** 

**9:31 2.** Toward noninvasive biomedical thermometry with cobalt-59 molecular NMR thermometers. **J. Zadrozny** 

**10:01 3.** Manipulating flux in living cells with biocompatible catalysis. **D. Domaille** 

**10:31 4.** Coupled lipid miscibility and phosphotyrosine-driven protein condensation on membranes. **J.K. Chung**, W. Huang, C. Carbone, L.M. Nocka, A.N. Parikh, R.D. Vale, J.T. Groves

**11:01 5.** Elucidating the action of abused volatile organic solvent, toluene on the central reward pathway. **A. Apawu**, S.P. Callan, T.A. Mathews, S.E. Bowen

**11:31 6.** Partitioning of lead in plants, birds and arthropods found on the Colorado Smelter superfund site in Pueblo, Colorado, **J. Carsella**, E.K. Petersen, T. Schiffer, S. Staples, C. Varian-Ramos, M. Diawara

#### Durango

ACS Workshops

8:00 am Opportunities for Chemists in the Federal Government 10:00 am Careers in Industrial Chemistry: Identifying Your Role in the Industrial Value Chain

**Devils Backbone** 

# **ACS Workshop**

8:00 am Leadership: Fostering Innovation

#### THURSDAY AFTERNOON

(1) Pike's Peak

# **Lunch Plenary**

#### Safety in the Rockies

D. C. Crans, Organizer, Presiding

12:00 Introduction

12:05 7. Creating a culture of safety in academic laboratories. P.K. Dorhout

**12:50 8.** Standardizing risk management in laboratory and pilot plant facilities: A model. **K. Johnson** 

**1:25 9.** Critical aspects of a robust potent compound containment program. **A.K. Doane**, R.I. Livingston

(1) Pike's Peak

# Sustainability Symposium

In Rocky Mountains Region and Beyond

G. G. Stanley, *Organizer, Presiding* E. Y. Chen, *Presiding* 

**2:00 10.** Towards a circular plastics economy: Design principles and synthetic methodologies for sustainable plastics with tunable properties and chemical circularity. **E.Y. Chen** 

**2:30 11.** Strong Lewis acids slow heterogeneous electron transfer to heterobimetallic ruanyl complexes. **J.D. Blakemore** 

**2:50 12.** Replacing non-renewable carbon with bio-derived alternatives. **A.D. Sutton** 

**3:20 13.** Systematic investigation of graft copolymers as compatibilizers in a poly(styrene)-poly(lactic acid) model system. **O.N. Manahan**, G. Miyake **CANCELED** 

3:40 14. Plastics upcycling – benefits in manufacturing. N. Rorrer

**4:10 15.** Bifunctional nickel and copper electrocatalysts for CO<sub>2</sub> reduction and the oxygen evolution reaction. **H. Pan**, C. Barile

**4:30 16.** Extrinsic atom effects on the anodic properties of one-dimensional TiS2-xSex solid solutions. **R. Weeks**, E.J. Miller, L. Whittaker-Brooks canceled

**4:30 17.** Highly active cationic Co(II) bisphosphine hydroformylation catalysts. **G.G. Stanley** 

(2) Estes

#### Senior Chemists Symposium

Celebrating Senior Chemists in the Rocky Mountains and Flash Presentations

D. C. Crans, *Organizer* M. B. Jacobs, R. Noriega, H. Zhao, *Presiding* 

2:00 Introduction of Session.

**2:02 18.** Reflections on a career built on the foundations of chemistry: From polysaccharides to dementia. **J.R. Bamburg** 

**2:32 19.** Consensus structures of the Mo(V) sites of sulfite-oxidizing enzymes derived from variable frequency pulsed EPR spectroscopy, isotopic labelling and DFT calculations. **J. Enemark** 

**3:02 20.** Porphene: A heterocyclic analog of graphene. T. Magnera, P. Dron, M. Jovanovic, J. Bozzone, E. Miller, W. Bu, **J. Michl** 

**3:32 21.** New two-dimensional organic frameworks for membrane separations. **B.A. Parkinson**, J.O. Hoberg, K. Li

**4:02 22.** Dynamics and structure of molecular fluids - a tribute to Branka M. Ladanyi. **N.E. Levinger** 

**4:32** Introduction to Flash Presentations.

**4:33 23.** Demonstration of the use of NMR spectroscopy for the measurement of vapor-liquid equilibria. **J. Widegren**, C. Suiter, V. Malavé, E. Garboczi, M. McLinden

**4:39 24.** Rapid vapor collection method for vapor pressure measurements of low-volatility compounds. M. Harries, **C.N. Beuning**, B.L. Johnston, T.M. Lovestead, J. Widegren

**4:48 25.** Investigation of plasma modified zeolite catalyst on hydrothermal liquefaction of chlorella powder. B. Jang, **T.M. Haque**, M.P. Jaimes, E. Cardenas, K. Largent

**4:54 26.** Spatio-temporal super-resolution microscopy. **M. Dunlap**, D.P. Ryan, P.M. Goodwin, P. Bourdin, J.A. Hollingsworth, J.H. Werner, M.P. Gelfand, A.K. Van Orden

5:00 Discussion.

**5:07 27.** Investigating the shape of aerosol-OT reverse micelles and the impact of force field. **C. Gale**, M.D. Molayousefi, N.E. Levinger

**5:13 28.** Aerogels doped with nanomaterials show improved mechanical strength and potential for expanded application integration with printed structures. **C.J. Hanson**, S.L. Edwards, M.F. Beaux, D.R. Vodnik, C.E. Hamilton

**5:19 29.** Effect of molecular structure on the properties of self-assembled reverse bilayer vesicles. **O. Villanueva**, A.F. Cozzolino, S. Moaven

#### 5:25 Discussion.

**5:32 30.** Modeling of unimolecular dissociation constants and reaction energies of ionic liquids: Applications in electrospray propulsion. **J. Deyanova**, B.D. Prince

**5:38 31.** Bond dissociation energies of transition metal borides. **D. Merriles**, C. Nielson, E. Tieu, M.D. Morse

5:44 32. Can infrared laser break the chemical bonds in viruses?. C. Yu

**5:47 33.** Nature of formal hydride transfer reactivity in mo-dependent formate dehydrogenase. **J. Lepluart**, M.L. Kirk

5:53 Discussion.

(3) Horsetooth

#### Young Talent in the Rocky Mountain Region

#### Young Talent in Rocky Mountains and Flash Presentations

D. C. Crans, *Organizer* C. C. Aldrich, C. J. Burrows, J. A. Latham, J. E. Sabol, *Presiding* 

**2:00** Introduction to Biomedical, Nanoscinece, Bioanalytical Science and Protein Modifications.

**2:01 34.** Synthesis, characterization, biological activity against *Trypanosoma cruzi* and metallomics of novel heteroleptic oxidovanadium(V) compounds. **G. Scalese**, I. Machado, L. Perez, D. Gambino

**2:10 35.** Investigation of decomposition kinetics and anti-cancer activities and of mixed-ligand vanadium complexes. **C. Yigit**, H. Murakami, A. Levina, P.A. Lay, D.C. Crans

**2:19 36.** Multinuclear NMR studies of anticancerous Non-Innocent Vanadium Schiff Base Complexes showing isomer formation. **A.C. Bates**, H. Murakami, D.C. Crans

**2:25 37.** In-silico evaluation of DNAJB1-PRKACA fusion proteins binding site. **S. Cabrera** 

**2:31 38.** Automated construction of fragment-based pharmacophores to elucidate novel GPCR ligands. **G.L. Szwabowski**, A.L. Parrill-Baker, D.L. Baker

2:37 Discussion; Nanoscience.

**2:47 39.** Synthesis and characterization of gold nanoparticles prepared with the flavonoid quercetin. **A. Holm**, M. Watzky

**2:50 40.** Preparation of gold nanoparticles in novel thioether-functionalized ionic liquids. **E. Kulesus**, **H. Leloup**, M. Watzky, H. Zhao

**2:53 41.** STM and XPS studies of co nanoparticles on reducible CeO<sub>2</sub>(111) thin films. **L. Du**, D.L. Braedt, J. Miao, J. Zhou

**2:59** Discussion: Nanoscience and Bioanalytical studies continued.

**3:05 42.** Nanoconfinement raises the barrier to hydrogen atom exchange between water and glucose. **S.L. Miller** 

**3:11 43.** Direct carbon-carbon bond formation between single-wall carbon nanotubes: Fact or artifact?. **P.S. Senanayake**, M. Talipov

**3:17 44.** Development of chemical strategies prepare synthetic lasso peptides and their isomers. **L. Digal**, A. Ghorai, M. Mifflin, A.G. Roberts

**3:23** Discussion: Bioanalytical Methods continued.

**3:31 45.** Preparation of apolipoprotein C III peptide antigens for display on virus like particles to combat cardiovascular disease. **N.R. Lopez**, N. Lee

**3:34 46.** Mapping electrostatic protein-membrane interactions of Slp-4 C2 domains using molecular phylogenetic analysis and structure prediction. **N. Chon**, S. Tran, C. Miller, H. Lin, J.D. Knight

**3:43 47.** Electroanalytical tools and molecular-based assays to measure the impact of noise on dopamine neurotransmission in the central auditory pathway. **P. Wilson**, A. Apawu

**3:49 48.** Detection of intracellular HNO delivery via a thiol-functionalized indicator with capillary zone electrophoresis. **A.N. Amarakoon**, D. Plewa, M. Han, N. Ke, C. Janczak, K.M. Miranda, C.A. Aspinwall

**3:55 49.** Statistical analysis of protein-protein comparison methods. **C. Dyer**, A.L. Parrill-Baker, D.L. Baker

**4:01** Discussion: Bioanalytical Studies Continued.

**4:10 50.** Light-activated quantum dot potentiation of antibiotics to treat drugresistant biofilms. **D.F. Stamo**, A. Chatterjee

**4:16 51.** Optimization of the attachment of a base labile fluorescence quencher in designing a triazabutadiene probe to image mosquito larval gut proteins. **W.N. Wijetunge**, L.E. Guzman, J.C. Jewett

**4:22 52.** Direct visualization of dimethyl sulfoxide permeation in live rice callus cells by coherent anti-Stokes Raman scattering (CARS) microscopy. **F.M. Samuels**, N.E. Levinger, G. Volk

**4:28 53.** Self-docking and cross-docking simulations of G protein-coupled receptor-ligand complexes: analysis of ligand type and receptor activation state. **B. Thomas**, A.L. Parrill-Baker, D.L. Baker

**4:34 54.** Investigating the relationship between receptor aggregation and signaling by luteinizing hormone receptor, a G protein-coupled receptor. D. Althumairy, **X. Zhang**, N. Baez, B. Barisas, D. Roess, G.R. Bousfield, D.C. Crans

4:40 Discussion: Bioanalytical Studies and Protein modification.

**4:49 55.** Towards de novo sequencing of the human milk glycome: Highresolution cyclic ion mobility separations. **G. Nagy** 

**4:55 56.** Analysis of *Cannabinoids* in natural and synthetic samples. J. Chavez, **D. Spurlin**, R.M. Hyslop, C.E. Brown

**4:58 57.** Redox potentials of truncated menaquinone analogues in soybean phosphatidylcholine liposomes are sensitive to odd- or even-length of isoprene chain. **K. Doucette**, B. Heritage, C. Beuning, D.C. Crans

**5:04 58.** Improving enzymatic transesterification activity in functionalized ionic liquid. **C. Toe**, H. Zhao

**5:07 59.** Substituted decavanadate (V<sub>9</sub>Mo) inhibits the growth of *Mycobacterium Smegmatis*. **Z. Arhouma**, K. Kostenkova, D.C. Crick, D.C. Crans

**5:13** Discussion: Protein Modification and Processing.

**5:21 60.** Elucidating the role of the axial cysteine residue in NHase catalysis and the enzyme maturation. **I. Ogutu** 

**5:30 61.** Determining co-modification of 5hmC-DNA and protein structure through mammalian evolution. **R.S. Czarny** 

**5:36 62.** Non-enzymatic post-translational modification of lysine clusters in C2 domains. **C.C. Beauchamp-Perez**, C. Michel, R. Reisdorph, N. Reisdorph, K. Fritz, C. Shearn, J.D. Knight

**5:42 63.** Efficiency and selectivity of RNAse A cleaving RNA containing 8-oxo-7, 8-dihydroguanosine. **C. Phillips** 

**5:45 64.** Evaluating changes in reactive oxygen species (ROS) as a plausible mechanism underlying the effect of noise on dopamine system in the hub for central auditory processes. **B. Doe** 

5:51 Discussion.

(4) Red Rocks

# Workshop: Empowering Academic Researchers to Strengthen Safety Culture

1:00 – 4:00 pm Safety workshop organized by Jessica Martin (University of Connecticut) for graduate students. The American Chemical Society is sponsoring a program to help educate graduate students about lab safety culture and opportunities for promoting safety. The participants will be awarded a certificate for completion of the course (can be added on resumes). This three-hour workshop will be led by Sarah Zim (University of Chicago) and Jessica DeYoung (University of Iowa). The purpose of this workshop is to help develop individualized plans for the creation or improvement of student safety

programs. You can read more about the results of previous workshops in this Journal of Chemical Health and Safety (K. A. Miller and K. I. Tyler, Journal of Chemical Health and Safety, 2019, 1871-

5532; <u>https://pubs.acs.org/doi/10.1021/acs.chas.8b26309</u>). Other key topics include hazard assessment, risk management, safety management practices, and complementary top-down approaches. This workshop is primarily directed at graduate student issues, but faculty and staff are encouraged to participate.

# Mixer programming 6:00 pm – 8:00 pm

# Hosts Carlos Olivo-Delgado (IT) & Debbie C. Crans (introductions)

6:00-6:30 pm mixer 6:30 pm ACS President Elect H. N. Chen, Welcome ACS National Board Chair John Adams, Historial Highlights ACS Regional Past Chair Donivan Porterfield, Regional Highlights Past ACS President, Bonnie Charpentier, Safety in Chemistry ChemClub Colorado State University Chair, Benjamin Reynolds

7:10 pm Distribution into Specialty Rooms

- 1. Meet the ACS National Board Members
- 2. Meet the ACS Regional Board Members
- 3. Colorado ACS Future Communications Interactive Discussion (Helen Gerhard and Michael Jacobs)
- 4. NSF Program officer Mike Adams and Shing Ho
- 5. Do you want to improve your presentation skills? Susan Morris
- 6. Ensuring laboratory Safety. James Kaufman

#### FRIDAY MORNING

(1) Pike's Peak

# **Senior Chemists Symposium**

#### Celebrating the Contributions of Senior Chemists in the Rocky Mountains Region

D. C. Crans, Organizer

E. L. Clennan, M. H. Rakowsky, H.Gerhard Presiding

9:00 Introduction.

9:02 65. Chemistry at the environmental water-air interfaces. V. Vaida

9:32 66. Redox revolutions on Earth and beyond. A. Anbar

**10:02 67.** Plasma assisted catalysis: New approaches focused on fundamental chemistry. **E.R. Fisher** 

**10:32 68.** Effects of luteinizing hormone receptor expression level on receptor aggregation and function. D. Althumairy, J.M. Pace, D.A. Roess, **B. Barisas** 

**11:01 69.** From boron hydrides to lanthanides and nuclear reactors to in vivo imaging. **G.R. Eaton** 

**11:30 70.** Heli-acenes as templates for a torque-lock-propagate approach for the synthesis of configurationally-pure twisted-acenes. **E.L. Clennan**, J. Weber, S. Tannir

(2) Estes

# **Medicinal Chemistry Symposium**

#### Medicinal and Biological Chemistry: Oral and Flash Presentations

D. C. Crans, *Organizer* M. B. Jacobs, A. C. Smith, A. J. Wiemer, *Presiding*  **9:00** Introduction to the Biomedical and Biological Symposium.

**9:03 71.** "Water-mimicking" ionic liquids for lipase activation and enzymatic polymerization. **H. Zhao** 

**9:28 72.** Directly observing cell-nanoparticle interactions by 3D localization microscopy in live flowing cells. **L.E. Weiss**, Y. Shalev Ezra, S. Goldberg, B. Ferdman, O. Adir, A. Schroeder, O. Alalouf, Y. Shechtman

**9:37 73.** Development of novel spiroligomer carbohydrate binding molecules. **S. Chepyshev**, C.E. Schafmeister

**9:43 74.** Inhibition of an iron-sulfur cluster biogenesis pathway towards development of novel antibiotics. **A. Boncella**, E. Sabo, C. Gladfelter, C. Morrison

**9:49 75.** Open questions on the biological roles of first-row transition metals. **K. Kostenkova**, D.C. Crans

#### 9:55 Discussion.

**10:04 76.** Modular synthesis and characterization of diffusible signal factor analogs for the study of structure activity relationships and mechanism of action. **R. Wiley**, D.L. Baker

**10:10 77.** <sup>1</sup>H NMR study of menaquinone-2 interactions in a phosphatidylcholine liposome membrane model. **G. Bublitz**, K. Doucette, D.C. Crans

**10:16 78.** Bacterial inhibition with liposoluble extracts of *Padina gymnospora*. **P.N. Gines Velez**, **P.A. Balbuena**, **G.** Peña Hurtado

**10:19 79.** Stimuli-activated quantum dots clear *Salmonella* intracellular infections in preosteoblast cells. **K. Eller**, C. McCollum, M. Levy, P. Nagpal, A. Chatterjee

#### 10:25 Discussion.

**10:36 80.** Synthesis and characterization of novel non-innocent vanadium Schiff base complexes with anti-cancer properties superior to cisplatin. **H. Murakami**, C. Yigit, J.T. Koehn, D.J. Gaebler, A. Bates, A. Levina, P.A. Lay, D.C. Crans

**10:42 81.** Evaluation of N-(9'-acridinyl)-O-phenylhydroxylamines. **J. Forster**, M.D. Mosher Canceled

**10:42 82.** Transcriptome-based design of PNA inhibitors re-sensitizes CRE E. coli to carbapenems. **T. Aunins**, K. Erickson, A. Chatterjee

**10:48 83.** Elucidating the neurochemical basis for the effect of chronic toluene inhalation on accumbal dopamine release. **K. Reiser**, A. Apawu

#### 10:54 Discussion.

**11:04 84.** Discovery of novel fadd32 inhibitor of mycobacterium tuberculosis with improved drug properties. **J. Sethiya**, R. Scott, G. Majeres, L. Dieckman, E. North

**11:10 85.** Ligand binding site location comparison across class A GPCR complexes. **M. Griffing**, A.L. Parrill-Baker, D.L. Baker

**11:16 86.** Stereoselective synthesis of the potential 5-HT<sub>2A</sub> agonist (2*S*,7*S*)-2-(4-bromo-2,5-dimethoxybenzyl)-7-(2-methoxyphenyl)azepane. **J. Talbert** 

#### 11:19 Discussion.

**11:25 87.** Receptor pharmacophore benchmarking: The role of ligand function in model development. **P. Castleman**, G.L. Szwabowski, D. Bowman, J. Cole, A.L. Parrill-Baker, D.L. Baker

**11:31 88.** Finding small molecule inhibitors that target DUSP5 using virtual screening: Applications in computational chemistry. **J. Grajeda**, M. Talipov

11:34 89. Bacterial inhibition with liposoluble extracts of *Mentha pulegium*. P.N. Gines Velez, N. Cabrera, L. Rivera, G. Peña CANCELED

11:37 Discussion.

**11:42 90.** Synthesis and evaluation of the rhodamine- and biotin- probes for detection of cysteine containing proteins. **S.H. Nguyen**, **K.M. Okin**, **J.E. Ward** 

**11:45 91.** Study of near infrared DNA damage and photo-cytotoxicity by a brominated 4-quinolinium dicarbocyanine dye (ESS2-2-4). **Y. Waku Kouomou**, E. Ahoulou, K.B. Grant, M. Henary, O. Taratula

11:48 92. Virus-like particles (VLPs) as a vaccine platform. E. Sohn, N. Lee

**11:51 93.** Synthesis and duplex stability of N2-Alkyl 8-Oxo-2'-deoxyguanosine oligonucleotides for use as substrate analogs for DNA repair protein MutY. **M. Bright**, R.P. Van Ostrand, S.S. David

11:54 Discussion.

(3) Horsetooth

# Young Talent in the Rocky Mountain Region

#### Young Investigator and Flash Presentations

D. C. Crans, *Organizer* A. M. Morey, S. S. Rocks, G. G. Stanley, A. K. Van Orden, *Presiding* 

9:00 Introduction by session chair.

**9:02 94.** New synthetic methodology enabled by base-promoted proton, electron and halogen transfer processes. **J. Bandar** 

**9:32 95.** Synthesis, characterization and reactivity of N-alkylated organic photocatalysts. **N.A. Swisher**, D. Corbin, G. Miyake

9:41 96. Total synthesis of indolizidine and quinolizidine alkaloids. J. Renner

**9:47 97.** "On water" synthesis of fluorosulfonyl 1,2,3-Triazoles. **A.L. Nazarova**, J. Thomas, V.V. Fokin

**9:56 98.** One-pot alkylation via traceless dearomatized pyridyl phosphonium ylides. **P. Fricke**, A. McNally

**10:02** Questions for 3 presentations: Introduction of Flash Presentations.

This presenation should be removed 10:11 99. Synthesis of configurationally twisted acenes by the torque, lock, and propagate approach: The mallory and dione routes. M. McConnell, J. Weber, S. Tannir, E.L. Clennan - Canceled

**10:14 100.** Exploratory syntheses of truncated, partially saturated menaquinone derivatives. **M. Braasch-Turi**, D.C. Crans

**10:20 101.** Synthesis of 2,4'-bipyridines via a unique radical coupling of cyanopyridines and heteroaryl phosphonium salts. **J. Greenwood**, J. Koniarczyk, J. Alegre-Requena, R.S. Paton, A. McNally

**10:26 102.** Synthesis of functionalized ionic liquids for coal dissolution and pretreatment. **M. Franklin**, H. Zhao

**10:32 103.** Synthesis of novel ionic liquids towards enzymatic ring-opening polymerization to polyesters. **C. Martin**, H. Zhao

10:35 Discussion and Questions.

**10:43 104.** Multivariate approach in designing chiral metal organic frameworks. **T. Ericson**, B. Tahmouresilerd, A.F. Cozzolino

**10:49 105.** Core-extended *N*,*N*-diaryl dihydrophenazine photoredox catalysts: Structure-property relationships and advantages in organocatalyzed atom transfer radical polymerization. **M. Price**, G. Miyake

**10:55 106.** Mechanistic insights into organocatalyzed birch reduction driven by visible light. **M. Kudisch**, J. Cole, **D.** Chen, R.M. Pearson, C. Lim, G. Miyake

**11:01 107.** Understanding the reactivity of tertiary amines and in situ generated ammoniums under reductive metal catalysis. **C.I. Nwachukwu**, T.P. McFadden, A.G. Roberts

**11:07 108.** Computational study of the torque, lock, and propagate approach to make configurationally stable twisted heli-thiopentacenes and helidithiopentacenes. **S. Tannir**, E.L. Clennan

11:16 Discussion and Questions.

**11:25 109.** Architectural analysis of branched polymers via soret contraction factor. **M. Toney**, K.R. Williams

**11:31 110.** Total THM-NOW: A low-cost online analyzer for total trihalomethanes in drinking water. **M. Alfonso**, N. Boppana, M.A. Brown, P.S. Simone, G.L. Emmert

#### 11:37 111. Modeling pollutant levels. P. Johnson, K. Johnson, L. Huang

**11:40 112.** Measuring arsenic levels in the Fountain Creek watershed based on uptake by the bryophyte *Hygrohypnum ochraceum*. **A. Chavez**, **N. Gasparovic**, D.C. Crans, J. Carsella

**11:46 113.** Infrared spectrum and atmospheric chemistry of 1,1,2,3,3,4,4 heptafluorobut-1-ene. **R. Sapkota**, G. Rawling, P. Marshall

**11:52** Discussion of papers.

#### FRIDAY AFTERNOON

(1) Pike's Peak

### Lunch Plenary

Iota Sigma Pi - Meitnerium Chapter and WCC Session

D. C. Crans, *Organizer, Presiding* M. Braasch-Turi, J. K. Chung, B. A. Hernandez-Sanchez, *Presiding* 

12:00 Session Introduction by Debbie Crans.

12:05 114. Reflections in water: Musings on my favorite molecule. N.E. Levinger

12:40 115. Vignettes from a career in medicinal chemistry. G.I. Georg

**1:10 116.** Anion coordination: Size, charge, and nexus with water. S. Pramanik, S. Kaur, S. Brunclik, V.W. Day, **K. Bowman-James** Monitoring motion with electron spins. T. Ngendahimana, W. Moore, L. Woodcock. G. R. Eaton, and **S. S. Eaton** 

**1:40** Panel Introduction by Maggi Braasch-Turi and Bernadette Hernandez-Sanchez.

**1:45** Iota Sigma Pi and WCC Panel. Academia: Nancy Levinger, Gunda Georg and Sandra S. Eaton; Industry Helen Gerhard and Jennifer McLauchlan and National Lab: Jaqueline Kiplinger

(1) Pike's Peak

# **Medicinal Chemistry Symposium**

#### Medicinal and Bioinorganic Chemistry

D. C. Crans, Organizer, Presiding C. C. Aldrich, Presiding C. I. Georg, Presiding

#### 2:30 Introduction.

2:32 117. Design of antibiotics to overcome resistance in mycobacteria. C.C. Aldrich

**3:02 118.** Inhibition of geranylgeranyl diphosphate synthesis by triazole bisphosphonates. A. Fairweather, D.B. Goetz, C.M. Schroeder, N.H. Bhuiyan, M.L. Varney, S.L. Haney, S.A. Holstein, **D.F. Wiemer** 

**3:32 119.** Cellular kinetics of phosphoantigen prodrug forms. C.C. Hsiao, X. Huang, M. Schladetsch, N.A. Lentini, D.F. Wiemer, **A.J. Wiemer** 

**4:02 120.** Inhibition of methyl transferases: The present and future. **M.A. Brown**, D.C. Crans

**4:30 121.** Small-molecule modulation of gene expression via DNA quadruplex structures. **C.J. Burrows**, A.M. Fleming

**5:00 122.** Optimization of the leads and synthesis of a ketohexokinase inhibitor clinical candidate. **A.C. Smith** 

**5:30 123.** Discovery and development of BET bromodomain inhibitors for male non-hormonal contraception. **G.I. Georg** 

(2) Estes

# **General Papers**

#### **Oral and Flash Presentations**

D. C. Crans, Organizer K. Kitzmiller, N. E. Levinger, C. J. Olivo-Delgado, M. Weinrich, Presiding

#### 2:30 Chemical Education.

**2:33 124.** Artificial intelligence tool for accessible chemistry education. J. Watters, F. Jiang, A.A. Hill, **M. Weinrich** 

**3:03 125.** Designing a culturally inclusive STEM and health research training program for Native American students. **N. Lee**, J. Lee

**3:33 126.** Tracking information literacy in science students: A longitudinal study of skills retention through the chemistry curriculum. **J.D. Knight**, M. Bruehl, D. Pan

**3:53 127.** Can students learn chemistry without midterm exams?. **D.J. Weiss**, P. McGuire, W. Clouse, R. Wrobel

3:59 128. Multiple ways to virtually engage students in chemistry labs. A.S. Smeltzer Schwab

4:05 Introduction to Flash Presentations.

**4:10 129.** Analysis of the impacts of student sense of social belonging on student outcomes in STEM. **J.D. Edwards**, R. Frey, R. Barthelemy

**4:16 130.** Comparison of online content homework with metacognitive training homework in general chemistry courses. **N. Ellis**, H. Wiegreffe, A. Hefzalla, E. Heider

**4:19 131.** Task analysis of undergraduate biology and chemistry laboratory activities. **A. Reid**, J. Heath, J. Velasco

**4:22 132.** Instructional behaviors in undergraduate biology and chemistry laboratory courses. **J. Heath**, A. Reid, M. Painter, J. Velasco

4:25 133. Chemistry of indigenous peoples. M. Gomes da Silva CANCELED

**4:28** Questions to 4 papers: Introduction to Session:General Papers.

**4:37 134.** Encapsulating metal-organic framweorks (MOFs) within mesoporous silica for use in heterogenous catalysis. **S.E. Massimi**, B.G. Trewyn

**4:43 135.** Visible-light-promoted reactions via intermolecular charge transfer using (thiol)phenols as electron donors. **B. Liu**, C. Lim, G. Miyake

**4:52 136.** Intra- and inter-ligand charge transfers in a new donor-acceptor complex. **S. Gao**, **J. yang**, **M.L. Kirk** 

**4:58** Cancel#**137.** Shining a new light on catalysis: Light responsive molecular dyads for direct control of redox switchable-catalysts. C. J. Aviles Martin. E. Pinkhassik. Canceled **170.** "Exploring environmentally sensitive bezothiadiazole and their uses" **C. Warner**, S. Norris, B Lampkn, P. Bouc, A. Thooft, J lukesh, S. I, Suarez, H. Brown-Harding, B. VanWeller

**5:04 138.** Visible light driven synthesis of remdesivir precursor. **A. Green**, C. Lim, G. Miyake

**5:10** Discussion; after that Electrochemical papers.

**5:20 139.** Photoredox catalyst design for proton coupled electron transfer. **C. Chrisman**, G. Miyake

**5:26 140.** Improved photoelectrochemical water oxidation catalysis via atomic layer deposition of alumina: Passivating surface trap states on a tin-oxide, phosphonate-functionalized perylene diimide plus CoO<sub>x</sub> system. **C. Jewell**, R. Finke

**5:32 141.** Impacts of performing electrolysis during organocatalyzed atom transfer radical polymerization. **D. Corbin**, B. McCarthy, G. Miyake

**5:38 142.** Altering non-innocent anti-cancer compounds: How the addition of CI to VO[HSHED] catecholates can change their electrochemistry. **A. Haase**, J. Hagan, H. Murakami, C.N. Beuning, P.A. Lay, D.C. Crans

**5:44 143.** Multimodal spectroscopic investigation of the conformation and local environment of biomolecules at an electrified interface. **S. Moonitz**, N. Shepard, R. Noriega

5:50 Discussion.

(3) Horsetooth

## **General Papers**

Oral, Flash, and Safety Presentations

D. C. Crans, Organizer

J. Carsella, R. Noriega, G. G. Stanley, H. Zhao, Presiding

**2:30** Flash Presentations in Inorganic, Physical and Analytical Chemistry;Career enhancement strategies.

**2:32 144.** Quantitative analysis of diffusible signaling factors using negative ion liquid chromatography electrospray ionization mass spectrometry (HPLC-ESI-MS). **B. Hoffman**, D.L. Baker

**2:38 145.** Complementary pairs from clashing forces throughout chemistry: Visualizing the pauli exclusion principle and its far-reaching implications. **J.P. Joyce**, A.K. Rappe, M.P. Shores

**2:44 146.** Frustrated Lewis pairs with applications in hydrogen storage. **G. Russell-Parks**, B.G. Trewyn, T. Gennett

2:50 147. Chromophoric photonic crystals. L. Garcia Alzate - Canceled

2:50 Physical-Inorganic Chemistry - General papers Questions.

**3:00 148.** Studies of the formation and infrared spectrum of formyl fluoride. **G. Rawling**, R. Sapkota, P. Marshall

**3:06 149.** Entropy and enthalpy of the hemoglobin-fluoride complex redox reactions ( $Fe^{3+}/Fe^{2+}$ ) at pH 5 reveal significant heme-pocket structural changes with temperature. **K.G. Flanders**, T. Mada, J. Cerda

**3:09 150.** Earth abundant transtion metal effects on methane concerted metalation-deprotonation, a DFT study. **W.M. Grumbles**, K. Melancon, T.R. Cundari

**3:15 151.** Crystallographcially observed mechanistic conversion of lanthanide nitrates by hexamethylenetetramine (HMTA) to ceramic oxide materials. **P.C. Reuel**, T.J. Boyle, R.E. Cramer

**3:18** Discussion; Inorganic and Organometallic Chemistry.

**3:28 152.** C-H activation of toluene by diruthenium nitride: DFT study. **W. Alharbi**, T.R. Cundari

**3:37 153.** Density functional study of methane activation by frustrated Lewis pairs with Group 13 trihalides and Group 15 pentahalides and a machine learning analysis of their barrier heights. **I. Migliaro**, T.R. Cundari

**3:43 154.** Supported palladium catalysts for selective hydrogenation of ethyl phenylpropiolate. **D. Knight**, **B. Santoyo**, J. Whelchel, S. Hussaini, B. Jang

**3:46 155.** Olefin polymerization by zirconium boratabenzene catalysts. **C. Carter**, T.R. Cundari, G. Rodriguez

**3:52 156.** Opening the Co<sup>III,N</sup><sub>2</sub>(m-O)<sub>2</sub> diamond core by Lewis bases leads to enhanced C–H bond cleaving reactivity. Y. Li, **S. Handunneththige**, J. Xiong, Y. Guo, M. Talipov, W. Dong

**3:58** Discussion; Analytical Flash Presentations.

**4:07 157.** Utility of cyanophenylalanine derviates as spectroscopic probes. A.J. Haider, L. Metzroth, A.M. Zerwekh, R.J. Martinez, J.P. Martin CANCELED **4:13 158.** Hybrid additive manufacturing of poly(caprolactone)-modified boneligament composite scaffolds for interface tissue engineering. **O. Sanchez**, L. Mottishaw, C. Salas, C. Buska, M. Rush

**4:16 159.** Indium phosphide quantum dots activated by near-infrared light: A novel treatment for drug-resistant bacterial infection. **C. McCollum**, J. Bertram, P. Nagpal, A. Chatterjee

**4:22 160.** Utilizing multi-angle light scattering to count biological particles. **C. Plavchak**, A.Z. Werner, G. Beckham, K.R. Williams

4:28 Discussion: Analytical Flash Presentations.

**4:34 161.** Effects on membrane oxygen permeability due to lipid changes in breast cancer. **Q. Wang**, S. Pias

**4:40 162.** Design and construction of a Brewster angle microscope. **S. Croslow**, K.G. McLaughlin, A. Goach

**4:43 163.** Effects of pH, conformation, and metal cations on insulin aggregation. **K.G. McLaughlin**, S. Croslow , S.P. Distin, C. VanCleave, D.C. Crans, A. Goach

**4:46 164.** Investigating morphology of mixed monolayers containing shortchain menaquinones with brewster angle microscopy. **C. Van Cleave**, A. Haase, B.J. Peters, J.T. Koehn, D.C. Crick, D.C. Crans

**4:52** Introduction to Session: Career Advancement, Safety and ACS assistance.

4:58 165. Stand up to stand out: Self-advocacy for the reluctant. S. Morris

**5:28 166.** How to convince others (that safety is important and that you're serious about it). **J.A. Kaufman** 

5:40 167. Spotlight on the laboratory safety team workshops. J.A. Martin

**5:52 168.** Chemical business networking with SCHB. **J.E. Sabol**, G.W. Ruger, J. Skinner, A. Kantak, D.J. Deutsch, J.L. Maclachlan

**5:55 169.** South Dakota mines ACS student chapter: Promoting green chemistry concepts through outreach demonstrations and hands-on activities. **K. Ly, L.C. Cutler**, K.D. Barz

5:58 Discussion.

6:00- 8:00 Award Presentation Mixer; Reginal Awards and "Video talk awards". There will be opportunities for mixing and activities (Details TBA).

# Friday Award Banquet 6:00 pm – 8:00 pm

#### Hosts Carlos Olivo-Delgado and Debbie C. Crans

6:00-6:30 pm pre-mixer 6:30 pm Brief presentations by ACS National Board Chair John Adams ACS Regional Board Chair Michael Mosher COACS Margaret Rakowsky,Chair of COACS's Senior Chemist Committee

#### Award Presentation hosts: Connie Gabel and Michael Mosher

George Stanley RMRM2020 Award Chair introducing Presenters of Regional Awards

Bonnie Charpentier, ACS Past President: E. Ann Nalley Award for Volunteer Service

This award was established in 2006 by ACS Past President E. Ann Nalley as part of her presidential initiative to recognize ACS volunteerism.

• Matt Horn, CHED RMR Representative & Connie Gabel, RMR Board Awards Chair Presenting *Regional Award for Excellence in High School Teaching* 

The Division of Chemical Education (DivCHED) established an endowment to support Regional Awards for Excellence in High School Teaching in each of the ACS Regions.

• Connie Gabel & Michael Mosher presenting the award to *Partners for Progress* and *Prosperity (P3) Award* This award recognizes partnerships among industry, academia, government, small businesses and/or other organizations that result in impactful outcomes.

• H. N. Cheng, President-Elect\_ACS Stanley C. Israel Regional Award for Advancing Diversity in Chemical Sciences. The Stanley C. Israel Regional Award recognizes individuals and/or institutions that have advanced diversity in the chemical sciences and significantly stimulated or fostered activities that promote inclusiveness within the ACS Regions.

**George Stanley** presenter of Conference Awards: Flash Presentations 3 ACS Division of Organic Chemistry Awards 1 ACS Award in Sustainability Award

#### **Carlos Olivo-Delgado**

1 Colorado State Chemistry Award

3 ACS awards

#### **Bonnie Charpentier,**

1 Helen Gerhard's LLC Company Award 2 ACS Division of Small Chemical Businesses Awards

#### **Margaret Rakowsky**

1 ACS Senior Chemists Committee Award

H. N. Chen 3 The Royal Society of Chemistry, New J. Chemistry Awards

#### Sandra Bonetti

3 ACS Division of Medicinal Chemistry Awards
1 COACS award in memory of John Conolly
1 COACS award in memory of Kim Pacheco

#### John Adams

3 ACS Division of Inorganic Chemistry Awards 3 Elsevier Coordination Chemistry Awards

Mary Singleton 3 Women Chemists Committee Awards

#### Michael Mosher and/or Connie Gabel

Innovative Project Grant Awards COACS awards

Debbie Crans Chair of COACS's Awards

Michael Mosher will introduction the next team to run the RMRM2021 Closing Comments Debbie Crans or Carlos Olivo-Delgado