

# SAS SPECTRUM eNEWS

## Editor's Note

I'm sitting at the Palm Springs airport typing up this special Newsletter issue, waiting for my first connecting flight to San Francisco (then a red-eye flight to Chicago and then finally to Michigan the next morning). Such connection flights are tiring, but SciX 2019 is totally worth it! So much happened at the meeting that we would like to share with our members, but the deadline for the Newsletter is tomorrow and so all of the SciX content will have to wait till next issue. I also learned that Clara Craver, a beloved pioneering female spectroscopist, passed away the week before SciX. We contacted the Craver family, who shared several memorable anecdotes with us, which we have included in the memorial piece at the end of this Newsletter. I highly encourage everyone to read that to appreciate the challenges facing women scientists in her time, to learn from role models like Clara Craver, and see how she stood up against various discriminations on her career path.

*Contributed by Xiaoyun "Shawn" Chen  
SAS Newsletter Editor*

## Preview: SAS-Organized Symposia at Pittcon 2020

Pittcon 2020 will be in Chicago, Illinois, 1–5 March 2020. The Society for Applied Spectroscopy has traditionally organized two symposia at Pittcon. For 2020, these are "Smartphone Spectroscopy for Analyses and Assays in Low Resource Areas" and "Portable Spectroscopy in 2020".

There is a large research and development effort underway in many university labs to combine the power of smartphones with medical and clinical assays. This is of particular importance in low-resource areas of the world, where sending samples to laboratories may be impractical, expensive, or highly time-consuming. These approaches enable point-of-care decisions, speeding up diagnosis and treatment. The time/date and GPS capabilities of smartphones also enable mapping of infectious disease outbreaks. This symposium brings together some of the principal researchers in this field, from around the world. The invited speakers include Russ Algar (University of British Columbia, Canada), Aldo Roda (University of Bologna, Italy), Brian Cunningham (University of Illinois), and David Erickson (Cornell University). Olivier Burggraaff, from Leiden University in The Netherlands, will set the scene by describing what is required to calibrate smartphones for both wavelength and photometric accuracy. Smartphone cameras are set up to deliver nice pictures, but there is a great deal of hidden processing. Access to the RAW data and understanding any prior processing are critical.

The second symposium provides a state-of-the-art look at portable spectroscopy, both instrumentation and applications, across many different techniques given by experts in each area. Pauline Leary from Federal Resources will discuss portable mass spectrometry and gas chromatography–mass spectrometry. Debbie Schatzlein Griggs (Thermo Fisher Scientific) will describe portable elemental spectroscopy, XRF, and LIBS. Katherine Bakeev from B&W Tek/Metrohm will cover portable Raman and near-infrared, followed by Suzanne Schreyer (Rigaku) on the key issues in turning spectra into actionable results, e.g., databases, calibrations, and algorithms. Finally, Ellen Miseo (TeakOrigin) will describe the applications of portable spectroscopy of food in retail environments. This symposium will be chaired by Mary Kate Donais (Saint Anselm College), who has employed portable spectrometers extensively in archeological artifact analysis. Three of these participants (Katherine, Ellen, and Mary Kate) are former SAS Presidents.

The careful reader will have noticed that all of the invited speakers in the "Smartphone" symposium are male. This is an artifact of who the current principal researchers in this field are. But there is an overall gender balance provided by the all-female panel on portable spectroscopy, and every speaker in both symposia, are experts in their field!

## Isao Noda Visits the University of Utah SAS Student Section

On Friday, 20 September 2019, SAS Fellow and Honorary Member Dr. Isao Noda visited the University

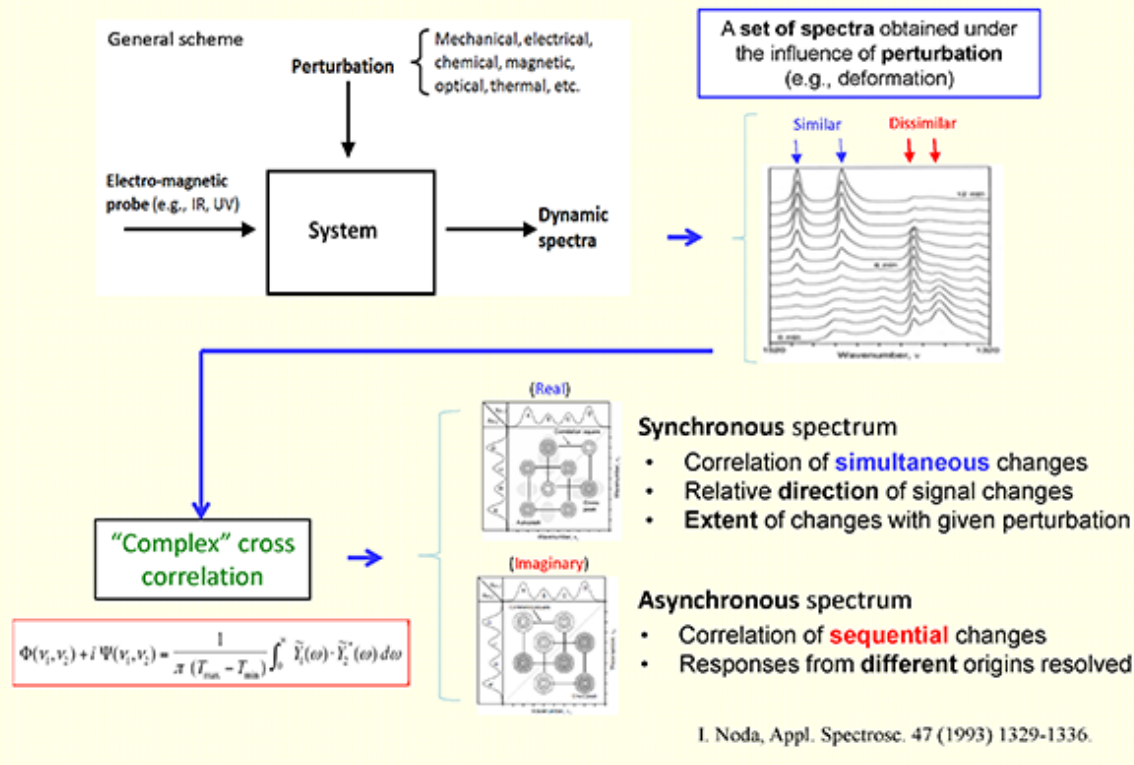
of Utah as a tour speaker hosted by the University of Utah SAS Student Section. It was his first visit to Salt Lake City and our campus. Isao spent the day visiting graduate students in their labs discussing their research and giving a noon seminar attended by 40 students. Isao gave a brilliant lecture describing his development of two-dimensional correlation spectroscopy (2D-COS) and the role this spectroscopic method played in inventing a new class of biodegradable plastics (Nodax) and tuning their properties through an understanding of their structure via 2D-COS (see slide). Isao commented about his visit: "Special thanks to SAS for the travel support through the tour speaker program. It really helps to have a program like this to entice students to consider active use of spectral analysis in their research work. I believe I have accomplished my task for that goal." Following a busy day of appointments and seminar, the graduate students hosted Isao for dinner at an Afghan restaurant (see photo).



Four hungry spectroscopists: Isao Noda, Sasha Moonitz, Grant Myres, and Maryam Zare (SAS University of Utah Student Chapter President).

## Generalized 2D Correlation Spectroscopy

Tool to sort out complex spectral responses to a perturbation



Isao Noda's principles of generalized 2D-correlation spectroscopy as presented.

### Postdoctoral Position Opening

Postdoctoral positions are available in the lab of Dr. Bryan Smith at Michigan State University focusing on the development of nano-immunoimaging and nano-immunotherapy platforms. More information on this position can be found at: <http://careers.msu.edu/cw/en-us/job/501722?|ApplicationSubSourceID=11253>.

### SAS Member Named 2019 Presidential Research Scholars at Ohio University

Peter de B. Harrington is a professor of chemistry and biochemistry in the College of Arts and Sciences at Ohio University. He is an expert in chemometrics, a subdiscipline of analytical chemistry that focuses on maximizing the information gained from chemical experiments. As there is a shortage of this expertise in the United States,

Professor Harrington has focused his research on designing automated, smart methods that can be used by scientists untrained in chemometrics to obtain accurate test results. In 1996, he developed and popularized the Copiosity Principle, which has become an important computational approach in the chemometrics field. Harrington employs his research methods and expertise to characterize botanical medicines, including cannabis. He has a long-standing collaboration with the USDA to develop automated chemometric methods for chemotyping foods and dietary supplements. Harrington won the Eastern Analytical Symposium (EAS) Award for Outstanding Achievement in Chemometrics in 2019.

### **In Memoriam: Clara Alberta Craver 1924–2019**

The daughter of Ira and Flora Diddle, Clara Alberta Craver (née Diddle) was born 3 December 1924 in Portsmouth, Ohio. She earned the Bachelor of Science in Chemistry degree from The Ohio State University in 1945, cum laude and Phi Beta Kappa, in an era when not many women chose to enter the chemical field. She worked at Eastern States Standard Oil of New Jersey and the Battelle Institute in Columbus, Ohio, before opening her own analytical laboratory in 1959, Chemir Labs, where she specialized in applied infrared spectroscopy. She was an expert in the analysis of the chemical properties of polymers, plastics, asphalt and oils, coatings, and adhesives, and provided expert testimony in numerous lawsuits. She lectured at chemical conferences across the country on the interpretation of spectra, in which a "fingerprint" is provided to identify chemical compounds and describing much of their structure. She was awarded an honorary doctorate from Fisk University in 1974 for her internationally recognized contributions to the field of vibrational spectroscopy. A member of the Iota Sigma Pi National Honor Society for Women in Chemistry, Dr. Craver was one of the first female chemists admitted to the Chemical Club of New York. Dr. Craver and her husband J. Kenneth Craver, a Monsanto chemist and futurist, were the first husband-and-wife to simultaneously chair separate divisions of the American Chemical Society. A male colleague was heard to remark of her, "[s]he is a towering refutation of the assertion that it is a man's world." In addition to her passion for science, Dr. Craver loved her flower gardens, sailing, the symphony, the Impressionists, and her family.

Dr. Craver is survived by her brother Col. (Ret.) James (Billie Lou) Diddle of Fort Walton Beach, Florida, and sister Patricia (Don) Kegley of Knoxville, Tennessee; four children from her marriage to Ray Smith: Susie Burge and Stephen (Laurie) Smith of St. Louis; Derrin (Mihaela) Smith, currently stationed in Sierra Leone, Africa; and Cheri O'Brien of Plant City, Florida; three daughters of Ken Craver: Mary Ellen Brown, of Carbondale, Illinois; Carole Connet, of Fairfield, Iowa; Iris Craver of Lawrence, Kansas; twenty grandchildren, thirty-two great-grandchildren and one great-great-grandchild; and seven nieces and nephews. Preceding her in death were her husband, her parents, three-year-old sister Gloria, sister Joyce Pinson, and nephew Scot Diddle.

Memorial donations in lieu of flowers may be made in her honor to the Craver Award fund sponsored by the Coblentz Society; the Ira and Flora Diddle Scholarship for the Professions at Shawnee State University, Portsmouth, Ohio; or to the Alzheimer's Association. A private memorial service is planned.

Several memorial moments were held during SciX 2019 in honor of Clara Craver. A moment of silence was held before the Monday morning plenary lecture. The Wednesday's Women in Analytical Chemistry Panel Discussion (chaired by Rina Dukor) was dedicated to Clara Craver. Richard Crocombe (past Chair of the Coblentz Society) and Katherine Bakeev (the inaugural awardee of the Craver award) reviewed Clara Craver's contribution and how she stood up against the many biases against women scientists at the time before the Thursday morning's Craver Award plenary lecture. Below are a few highlights from the slides delivered by Richard and Katherine.



*Clara Craver and Norman Colthrup (attributed) on her arrival in Buenos Aires, Argentina, ca. 1962. Note on the reverse indicated Dr. Craver's quizzical look resulted from her confusion at being photographed. It turned out the photographer was there to document the arrival of the two US scientists. (Image courtesy of Stephen D. Smith.)*



*An early image of Clara Craver, likely taken during her tenure at the Battelle Institute. (Image courtesy of Stephen D. Smith.)*

**Dr. Craver as a "woman in a man's world":**

(i) When she began her first position at ESSO after college, she was asked, "Can you type?" "No," she replied judiciously-realizing she would have spent all her time typing other people's reports.




(ii) When she first opened her consulting laboratory in 1959, her husband had to sign on her business checking account as the bank would not allow her to open an account in her own name as a married woman.

(iii) When she took her husband and fellow chemist Ken Craver to dine at the Chemical Club in New York, the waiter assumed he should be given the menu showing the prices and gave her a menu without prices (although he was not a member, she was). She promptly switched the menus.

(iv) Around 1961, Clara and her family lived in Evansville, Indiana. Clara had frequent business travel to New York. Only one flight would allow her to return in time to see her children before bedtime, but American Airlines (AA) had designated that a "Businessmen's Flight" that was for men only. Clara's son stated they have an exchange of letters between AA and Clara, the airline patiently explaining they wanted the men to be able to smoke and take their shoes off without ladies present. (Nevermind that the flight attendants were all "stewardesses" at the time.) Her replies include a letter she wrote to the editors of the Wall Street Journal on the subject.

Clara Craver was the driving force behind the Coblenz Society's "Desk Book" collections of infrared spectra. These lay the foundations for today's widespread spectral libraries. The income from sales of these collections continues to greatly benefit the Coblenz Society, and enables it to fulfill its mission. These collections are available today in digital formats from ACD Labs.

The Society for Applied Spectroscopy offers its sincerest condolences and thanks to Dr. Craver's family, specifically Stephen D. Smith, for providing the reminiscences and images for this obituary.

	<b>Why did you join SAS and what do you hope to gain from SAS?</b>	<b>What is your area of research?</b>	<b>What are your hobbies?</b>
	Zhiping He, researcher at Shanghai Institute of Technical Physics (SITP)		
	I joined SAS in order to publish research results more conveniently, and I hope to have more interaction with international spectroscopy professionals.	My area of specialty is space optics and opto-electronics technology, and main interest is the technology for lunar and deep-space spectroscopic observations.	My hobbies are swimming, jogging, and reading.
	Chuck Gardner, director of project management at ChemImage Corporation		
	I am a longtime member of the Spectroscopy Society of Pittsburgh and I finally decided that it is time to support the work of the national SAS. Also, as former President of Pittcon, I hope to work to continue the excellent cooperation between Pittcon and SAS.	My main spectroscopy interest is the application of hyperspectral and multispectral imaging to the detection and identification of hazardous materials and to improve the visualization of anatomic structures during minimally invasive surgery. My area of specialty is project management which combined with my technical abilities, allows me to lead multi-disciplinary teams at ChemImage to develop and test these novel detection systems.	My wife and I are very active on the Pittcon Organizing Committee as well as the Society for Analytical Chemists of Pittsburgh and the Spectroscopy Society of Pittsburgh. In addition, I enjoy vegetable gardening as well as trap and skeet shooting.
	Corianna Borton, Ashland University graduate student		
	I joined SAS this past summer after attending the conference at John	In undergrad, my research was focused on the root exudates of a plant called Syrian rue. We extracted	Hobbies of mine include reading and spending as much

	<p>Carroll University; my membership was a part of being the recipient of the Yeager Award. I hope that being a part of SAS will help to keep me updated in what new research is going on and also help me to make connections with others.</p>	<p>and quantified these harmful alkaloids using silicone tube microextraction and then HPLC with fluorescence detection. I also began to explore the toxicity of the alkaloids to other plants. I am studying forensic chemistry, so currently I am very interested in the area of microspectrophotometry (specifically Raman and IR). This is because it is becoming more prevalent due to the fact that it is non-destructive to evidence being examined. I just recently learned about this area and some of the neat applications of it.</p>	<p>time as I can with my family and friends! I also really enjoy spending time on the lake, where my parents have a small cottage.</p>
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Kristin Dexter

<p>I joined SAS because I hope to learn from experienced spectroscopy experts and continually improve my work.</p>	<p>My area of expertise is in ICP-AES soil and water sample analysis, but my interests lie in ICP-MS.</p>		<p>My current hobbies include playing violin for a local symphony and playing a lot of Destiny 2 with my partner.</p>
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Changhao Liu, University of Delaware graduate student

<p>I joined SAS because I had been looking for a community to share my expertise and research work with others, as well as learning more about others' research work. In addition, it would be great to expand my connections to facilitate my career development. My joining SAS was also encouraged by my advisors.</p>	<p>I have been focusing on using vibrational spectroscopy (IR+Raman) to characterize polymer thin films to understand how processing parameters, blends, and additives influence polymer chain conformation, crystal structure, crystal orientation in the films. I am particularly interested in using AFM-IR to characterize polymer ultrathin films.</p>		<p>I love playing tennis and running (5k).</p>
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**Do you have something spectroscopy-related you want to discuss in the newsletter?  
Or something that will help our membership such as career tips or application tips?  
Please let us know by emailing [xchen4@dow.com](mailto:xchen4@dow.com).**