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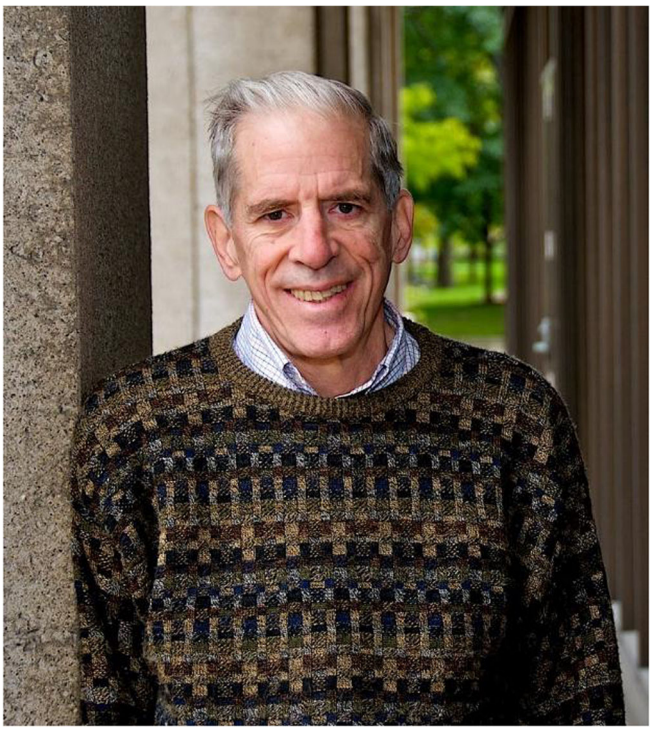
OBITUARY

Robert C. Dunbar (June 26, 1943–October 31, 2017)

Robert Copeland Dunbar, Professor Emeritus of Chemistry at Case Western Reserve University, passed away on October 31, 2017 in the Cleveland Clinic of heart failure at the age of 74. Rob is survived by his wife Mary, sons Geoffrey and William, daughters-in-law Nancy and Ari Sato, granddaughters Sarah and Emma, and sister Anne Walston.

Rob was born on June 26, 1943 in Cambridge, MA, and grew up primarily in Washington, DC. He received a BA degree in Chemistry from Harvard University and a PhD in Chemical Physics from Stanford University. His thesis, titled "Ion Cyclotron Resonance Studies of Ion-Molecule Interactions," was completed under the direction of Professor John D. Baldeschwieler.

About 1970, Baldeschwieler was promoting a new Varian ion cyclotron resonance (ICR) mass spectrometer around the country. George Olah, the future Chemistry Nobel Prize winner and then-chairman of the Chemistry Department at Case Western Reserve University, bought one and hired Rob as an Assistant Professor to make good use of it. And so began Rob's career at CWRU. He had a fruitful collaboration with Olah, publishing six papers together, five of them in *JACS*. [1, for example] The very same Varian ICR spectrometer with a 1.0 T electromagnet was collecting data up until the late nineties when the relocation of Dunbar's lab forced the instrument to be abandoned. During these times of his career, he enjoyed Alfred P. Sloan and J.S. Guggenheim Fellowships and a Sigma Xi Research Award.



Many remember Rob from his contributions to photodissociation of trapped ions [2], a subject on which he published more than a hundred papers. Ion–molecule reactions were always on the top of Rob's list of interests, too. He published many elegant examples of organic and organometallic reactions in the gas phase. Having realized that the low-pressure ICR conditions closely resemble those of interstellar space, he was able to accurately model various aspects of "space" chemistry. This drew interest from the astrochemistry community and led to a number of interesting collaborations [3]. Rob also was able to interrelate radiative association kinetics to binding energy, leading to a novel and accurate technique for ion-neutral binding energy determinations [4]. Over the course of his 47-year career at CWRU, Rob published more than 250 papers.

A notable achievement in the 1990s was his work with Terry McMahon on the first explanation of the phenomenon of thermal radiation-induced ion dissociation. The method led directly to the development of the so-called blackbody infrared dissociation (BIRD) technique. Terry McMahon recalls: "In the early 1990s after successfully mating our high-pressure ion source to our FT-ICR spectrometer, we were able to trap cluster ions in the ICR cell under conditions of very low pressure. We immediately found that many of the cluster ions that we would trap in the cell would undergo unimolecular dissociation, which was completely independent of the pressure of any unreactive gas leaked in the cell. We quickly became convinced that what we were observing was unimolecular dissociation induced by ambient blackbody radiation in the cell and this conclusion was supported by temperature-dependent and deuterium substitution experiments. During seminar visit to Waterloo in ~1994, I was telling Rob that while we were convinced that we were observing blackbody dissociation, referees refused to believe it and we had been reduced to calling this "spontaneous unimolecular dissociation" in our publications. Rob immediately responded "I believe it". At that time, he had been working closely with Steve Klippenstein on master

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Table 1. People in Rob Dunbar's lab

Graduate students	Some undergraduates	Post-docs and visitors
Jacob Shen		
Paul P. Dymerski	John J. Ennever	Jerry. M. Kramer
Emil Fu	Robert Klein	Bennett B. Hutchinson
Robert Orth	Phillip H. Hemberger	Michael T. Riggin
Robert C. Benz	Jerome Lang	Harry H. Teng
John D. Hays	Peter B. Armentrout	Myung Soo Kim
Jeffrey P. Honovich	Donald Kormos	Yoshiya Takenoshita
Naomi B. Lev	Jeffrey Segall	Thomas Lehman
Jyh-Horung Chen	Joseph T. Snodgrass	Gary H. Weddle
Bruce Asamoto	George B. Fitzgerald	Chava Lifshitz
Hun Young So	Paul Klich	
M. Saber Ahmed	Nathan Diachun	
James D. Faulk	Joseph Ferrara	
Fu-Shiuan Huang	Donald Solooki	
Guy T. Uechi	Rebecca C. Zaniewski	
Yu Wei (Tim) Cheng	Ronald Grimm	
Boguslav P. Pozniak	Jason R. Green	
Chuan Yuan (Eric) Lin		
Yen-Peng Ho		
Victor Ryzhov		
Alexei Gapeev		
John (Brad) Mangrum		

equation modeling to simulate results obtained on laser dissociation of ions in Rob's ICR experiments. This then gave us the ultimate theoretical proof that was needed and that led finally to our joint Science article in 1997 [5]."

Rob trained many graduate and undergraduate students in his research group who went on to doctorates in chemistry and careers in academia, both in the United States and overseas, as well as in industry (Table 1).

In the lab, Rob was the best research advisor any student could possibly wish for. Rob focused his doctoral students on developing independence, while providing constant encouragement. If there was a problem or just a question about anything in the lab, he was available to help 24 hours a day, 7 days a week. He knew every part of his instruments (many of them built by his own hands) down to the last tiny transistor. He could troubleshoot and fix anything in the lab, from machining an ICR part to charging a superconducting ICR magnet. According to Bob Orth, a former doctoral student who was later at Monsanto for many years, "Rob changed my life for the better just by being himself. This has allowed me to have the career and life that I dreamed of. I will miss his physical presence but his lessons will be with me and others as I tried to pass them along. The lessons of life I learned from him will fill my heart."

Rob's contributions, however, go beyond his scientific achievements. The Chair of the Chemistry Department at CWRU Professor John Protasiewicz writes: "As I started my own career at Case, I was greatly impressed by Rob's unique ability to quietly and patiently listen to his Chemistry colleagues at faculty meetings argue over some pressing matter. Rob could then speak a few well-reasoned and logical words that could magically diffuse or resolve the argument. Rob's mind was exceptionally skilled at critical analysis and he was always very kind, thoughtful, unassuming, and willing to give you his time." Jack Beauchamp wrote: "Rob had a kind word and a smile for everyone he interacted with; a true gentleman in all respects. He gave a lot to his family and to his many students, who he also treated as family. We'll all miss his contagious grin and infectious laugh."

Having been used to zapping ions with laser beams, Rob became interested in developments around the turn of the millennium involving the use of widely tunable radiation from free electron lasers for IR spectroscopy of mass-selected ions. At the Free Electron Lasers for Infrared eXperiments (FELIX) center in The Netherlands, an optically accessible FTICR-MS instrument had just been installed in an NSF-funded project awarded to John R. Eyler and Alan G. Marshall from Florida. In 2003, Rob was one of the first US pioneers visiting the Dutch NSF-outpost, in the days when an ESI source was not yet available on the instrument. Rob suggested implementing a simple laser-ablation metal ion source to generate metal–ligand complexes and to investigate their coordination geometries via IR spectroscopy. The first study on the coordination of the Cr^+

ion to aniline was an instant success; the IR spectrum provided crystal-clear evidence for a π–bound complex, where computed thermochemistry was indecisive between π- and *n*-coordination [6]. Since that first visit, Rob never abandoned FELIX and applied for beam time in every call-for-proposals, until his last visit in September 2017.

After the installation of an external ESI source, the opportunities for generating metal-ion coordination complexes expanded and Rob took full advantage of it. Rob started the investigation of alkali metal ion complexes with amino acids, which were quickly picked up by the ion chemistry community. He revived the question of whether amino acids would adopt their zwitterionic structure upon complexation to alkali or alkaline earth metal ions [7]. His interests gradually turned to peptides of increasing complexity and first-row transition metal ions. He discovered that peptides can undergo a tautomerization of the amide linkage(s) upon coordination to strongly binding transition metal ions [8]. Most recently, Rob addressed several aspects of gas-phase versus solution-phase structures of metal–ion peptide complexes [9].

As his career at Case was winding down, Rob found a new home at FELIX and he became sort of an "unofficial member" of the group. His work at FELIX resulted in more than 30 journal articles, three of which have now received well over 100 citations. Rob seized every opportunity to travel to Holland and combined his research with bicycle trips in Tuscany, family visits in the UK, and concerts at the Concertgebouw in Amsterdam. He was more than an external researcher at the facility; he was a friendly mentor for all at FELIX, as well as for many of the US students traveling to the lab under the NSF-PIRE program. As Nick Polfer, a former FELIX scientist, put it, Rob was "a great role model, both as a scientist and as a human being." In the Spring of 2008, Rob spent a sabbatical at FELIX and he and his wife Mary found shelter in a tiny house in downtown Utrecht, which Rob consistently referred to as "Dunbar Castle" since it was big enough to throw dinner parties.

It was at FELIX where Rob was among the group of scientists who obtained the first IR spectrum of an amino acid radical ion. His Canadian collaborators K.W. Michael Siu and Alan C. Hopkinson recall: "In 2008, Udo Verkerk, a research scientist in our group, was assigned experimental time at FELIX and ran into Rob there; together they performed the IRMPD spectroscopy experiments that were crucial to our study, which identified the captodative alpha-radical ion as the lowest-energy and most-abundant histidine radical cation in the gas phase [10]. Perhaps stimulated by this initial success, Rob then proposed a second collaboration on determining the conformations of gas-phase complexes of histidine and alkaline earth metal ions. Rob told us that he did not consider himself expert in computational methods and would like us to collaborate with him. We readily agreed, and the results were published one year later [11]. Of course, when we were participating in the writing of the manuscript, we finally realized that Rob had already done all the DFT calculations himself, and we were simply invited to participate as Rob's backup and to provide confirmation. This to us showed how rigorous a scientist Rob was, and the extent of devotion and dedication he gave to his art and practice."

With his long and rich experience in laser-induced ion dissociation, Rob was also one of the most prominent practitioners and advocates of (infrared) ion spectroscopy. With Tom Bear, he organized the 25th ASMS Asilomar Conference in 2009, focusing on "Ion Spectroscopy" [12]. Rob successfully lobbied for an "ion spectroscopy" session at the annual ASMS meeting, which was perhaps dominated by work involving the FEL facilities in the early years, but which has now matured and involves many groups in ion chemistry. Each year after the last contribution of the session, Rob would walk up to the microphone and state that this was the best session of the entire ASMS meeting; a true lobbyist for the cause. Rob remained in demand late in his career and even after retiring. He was invited by former graduate student Hun Young So to be the keynote speaker at a conference Hun organized in Korea in 2012. Rob was also a visiting professor at the University of Lyon, France, for a month in the summer of 2016.

Rob's interests extended far beyond science. He was a rare example of a quintessential university professor who knew several languages, took interest in literature, art, and music, and could engage in a conversation on virtually any subject. He was an accomplished pianist, playing daily throughout his life and even taking piano lessons at the Cleveland Institute of Music in the 2000s. Rob loved classical music, enjoying operas, symphonies, and concerts, especially the Cleveland International Piano Competition. He would often drive to ASMS annual conferences listening to Glenn Gould renditions of Bach and "the Beethoven lectures" of Andras Schiff. He also actively participated in the cultural life of the community, e.g., by serving on the Board of Directors of the Lyric Opera of Cleveland. He enjoyed travel around the world, especially family bicycle trips through various countries of Europe.

We will dearly miss Rob's passion for science, his demand to get things right and understandable, and his wry and quiet sense of humor. With Rob's passing, we lost one of our most loyal and most successful gas-phase ion researchers. We lost one of the greatest advocates and promotors of ion spectroscopy. But more than that, we lost our mentor and dearest friend.

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