

J. Am. Soc. Mass Spectrom. (2013) 24:1319–1323 DOI: 10.1007/s13361-013-0692-z

ACCOUNT & PERSPECTIVE

Jim Morrison, Friend and Colleague

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Abstract. Our long-time association with Jim Morrison and the work that came from it is the result of a series of fortunate coincidences. We are pleased to be able to share recollections here of our interactions with Jim and how his life and work have influenced us and the field of mass spectrometry.

Key words: Triple quadrupole, MS/MS, Retrospective, Biography

Received: 30 April 2013/Revised: 28 May 2013/Accepted: 28 May 2013/Published online: 23 July 2013

First Contact and Intervening Years (Chris)

y first contact with Jim was in 1964, almost 50 years ago. Jim came to Princeton University as an invited visiting professor. However, his host, physical chemist Donald Hornig, had just left for Washington to be the President's Science Advisor. That left Jim to find things to do on his own. To his amazement and chagrin, there were no mass spectrometers at Princeton at that time, so he turned his attention to using the university's mainframe computer to write programs for mass spectral interpretation and iontrajectory modeling (the beginnings of SIMION). He also befriended George Leroi, an assistant professor in Physical Chemistry. George remembers Jim as being very bright and articulate. He also credits Jim with inspiring him to continue his studies of vacuum photoionization. Jim's suggestion that George use a quadrupole mass analyzer to sort out the ionic products was very helpful and typical of his willingness to share his knowledge. Through my friendship with George Leroi, I met Jim and his wife, Krysia. Jim was then 40 years old and I was 31. We interacted socially throughout that year to my great pleasure. Jim's Scottish accent and dry wit made for delightful conversation. I was fascinated by Jim's and Krysia's stories of their graduate years in Scotland and their subsequent emigration to Australia.

My electrochemical research interests did not overlap with his significantly, but we shared an interest in electronics and instrumentation. One story I remember particularly was about the time he hooked up the detector output signal of a scanning sector instrument to an audio amplifier. Different compounds produced a different timbre to the fundamental frequency of the scan repetition so familiar components could be identified by the *sound* of their mass spectra [1]! Most remarkable to me was the depth of his knowledge in all areas of chemistry and physics. Also, it was his indomitable good nature that enabled him to find productive things to do when his goal of working with Hornig could not be achieved. In fact, in his interview with the Australian Academy of Science, he says that he and his family loved it at Princeton. But at the end of his year's appointment, he returned to Australia.

It was not until 1977 that I saw Jim again. It was at the Washington DC ASMS meeting, which Rick and I were attending. Totally new to the field of mass spectrometry, I scanned the list of attendees in the hotel lobby (You could actually do that in those days!) to see if there was anyone I knew. To my delight, I saw that Jim Morrison was there. We arranged to have a dinner together and Jim brought us up-todate on his life in Australia and his field work on the odors of wet rocks and the dangerous components of honey. If Jim was curious about something, he just jumped in. He was full of spontaneity and fun. By this time, in addition to his professorship at La Trobe University, he had an adjunct professorship at the University of Utah, where he spent most summers for 30 years. With him at this meeting was Austin Wahrhaftig, Professor of Chemistry at the University of Utah. The four of us went back to Jim and Austin's room to continue our talk after dinner.

There, our discussion turned to more serious science. Inquiring what brought us to the meeting, we explained that

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we were looking for an efficient means to fragment ions selected by a quadrupole analyzer so we could identify them with a second quadrupole analyzer. Our goal was a computer-controlled analytical machine in which the two quadrupoles would perform the operations of separation and identification respectively. The difficulty was that it was widely believed (through experience with tandem sector instruments) that ion energies in excess of 1 keV were necessary to achieve collisional dissociation. Ion kinetic energies in the quadrupoles were only in the low 10s of eVs. After puzzling over that for a while with no promising ideas, Jim told of a problem he was having with his studies on photodissociation of ions. He selected ions with one quadrupole, used a second one to contain the ionic products, and a third to determine their quantity and mass; his instrument, in Figure 1, had not yet been published. A collinear pulsed laser beam illuminated the selected ions. The process was so inefficient he had to use synchronous demodulation to detect the photo-induced dissociation products in the presence of the all-too-abundant background ions. I said, "What background ions?" and then we all realized that whatever was producing Jim's noise was the process we were looking for. The next day, I asked Jim if Rick could come to his lab to do some experiments on his apparatus. With characteristic generosity and good will, he readily agreed.

Experiments at La Trobe (Rick)

Needless to say, I was excited about a visit to "Prof" Morrison's lab in Australia to perform our first experiments on collision-induced dissociation (CID) of ions in a triple quadrupole mass spectrometer (our own triple quad instrument at MSU, funded by the Office of Naval Research, was still under construction). Jim's triple quadrupole system (built simultaneously with a triple quad instrument built by Marvin Vestal in Jean Futrell's lab at Utah, based on an idea conceived by Jim that he shared with Jean during one of Jim's regular visits to Utah in 1971), was designed to measure <u>optical</u> spectra of mass-selected ions, measuring absorbance indirectly, by measuring the intensity of photodissociation product ions.

Although I had an invitation from Jim, we had no travel funds in our ONR grant for such a visit. I contacted our ONR program officer to see if I could hop a ride on a Navy ship heading across the Pacific, but he agreed to add travel funds to cover the visit, and it was a significant expense in 1977 (my airfare was equivalent to 9 months of a graduate student stipend!). We then set to planning for the visit. Since all sector MS/MS researchers had found helium to be the best collision gas, I wrote Jim asking if he had any helium; he responded that helium was a nonrenewable resource, and unavailable in Australia; if I wanted to use helium, I should bring my own! The home-built triple quad in Jim's lab had a gas inlet, an electron ionization (EI) source, and a mass range to m/z 100, so I planned all my samples and experiments around those limitations.

When I first arrived at La Trobe, I asked Jim how to obtain a mass spectrum on the triple quad. He replied, "We've never done that (all our experiments monitored a single photodissociation fragment ion from a single parent ion)". Jim guessed that I should simply "turn this knob" (the one he's turning in Figure 1) at 1/4 rpm for ~20 min. "And if I wanted to scan the first quadrupole?" He pointed to another knob. I turned that knob for 20 min, and obtained the first mass spectrum on that instrument. I then headed to the machine shop, where I scrounged a ¹/₄rpm synchronous motor and a ring stand and lab stool. I connected the motor to the knob with a piece of Tygon tubing, started the motor, and went for a cup of tea! To minimize the collisional background in their photodissociation experiments, they used a liquid nitrogen trap directly above the collision quadrupole to reduce the pressure to $<10^{-7}$ Torr; I simply added a piece of tubing to introduce gas between the rods of the quadrupole up to a pressure of $\sim 2 \times 10^{-4}$ Torr for CID.

Morning and afternoon tea with the other graduate students in Jim's group (including Don McGilvery, Dianne Smith, Russell McLoughlin, and Gary Willett) was an important part of life in the department. On my third day at La Trobe, Jim called me into his office and asked if he could at least tell everyone in his group a little about the experiments I was doing—he had the impression from our discussions at the ASMS conference that our Navy-funded project was top secret! I assured him that there was nothing secret about our experiments, which relieved Jim and made interactions with his group much more relaxed.

One of the major questions we wanted to address was whether we needed high collision energy to fragment ions for MS/MS. The maximum collision energy was 20 eV, far less than the keV ion energies used in sector MS/MS. We wondered whether we could add enough kinetic energy to the ions by increasing the rf amplitude or frequency on the rf-only quadrupole collision cell; unfortunately, increasing the rf amplitude (or frequency) did not increase the CID efficiency. To help understand that observation, Jim suggested that we might use SIMION, a new computer simulation program that he had conceived and Don McGilvery in his group had implemented (on a PDP 11/40 minicomputer with 56 kb of memory!), but had not yet published. The insight we gained from those simulations was invaluable in our research (see Figure 2 for an example simulated ion trajectory of an ion in the rf-only quadrupole), presaging the remarkable role that SIMION has had in design and understanding of mass spectrometers and ion optics for the 35 years since. Since the sector MS/MS community found that lighter gases were more efficient for CID, and I hadn't brought any helium with me, I tried hydrogen gas. Fortunately, more massive gases such as argon led to substantially higher CID efficiencies, up to 65 % because of the strong focusing of the CID product ions in the rf-only quadrupole.

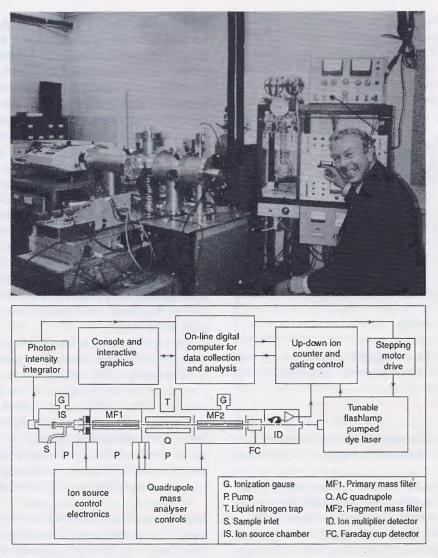


Figure 1. Jim Morrison with the photodissociation triple quadrupole instrument at La Trobe University (courtesy of Michael Grayson). The schematic at the bottom shows the same instrument, but is reversed left to right

Based on the experiments in Australia, we prepared two manuscripts—first, a paper on "Selected ion fragmentation with a tandem quadrupole mass spectrometer" by Chris and me, which appeared in *JACS* in 1978 [2], and a second companion paper on "High efficiency collision-induced dissociation in an rf-only quadrupole" in the *International Journal on Mass Spectrometry and Ion Physics*, including Jim and his graduate students Don McGilvery and Dianne Smith [3]. The ONR also insisted that we file for a patent, and we did so, including Jim as an equal inventor [4].

During my time at La Trobe, Jim served as department head, and as advisor/mentor to a large number of junior faculty, graduate, and undergraduate students. He was also Head of College for Chisholm College, a residential college at La Trobe University that he had designed, supervised the construction, and stayed on as headmaster. He commented that "H. G. Wells had always said that science would save the world, but having to deal with... 360 people in the 18- to 21-y age group gave me a different story of what saving the world was going to be like"[5]. Jim was a deep thinker, consummate advisor, and remarkably practical and down-to-earth researcher.

Subsequent Interactions

(Rick) I had the privilege to interact with Jim (and Krysia) many times over the years after my 1977 research visit to La Trobe. In 1979, Jim visited Michigan State University. I recall that we disassembled our triple quadrupole instrument for him to examine, and he noted (in his typically gentle way) that perhaps I had multiplied by 1.148 rather than divided when I calculated the spacing of the rods in the quadrupole collision cell. I also recall that he didn't have any spare clothes with him, since he had shipped his clothes back to Australia to make room in his suitcase for a fossilized dinosaur femur from the Jurassic period "Morrison formation" in Utah (named not for Jim, but for the nearby town of Morrison, Colorado). Jim was very protective of this

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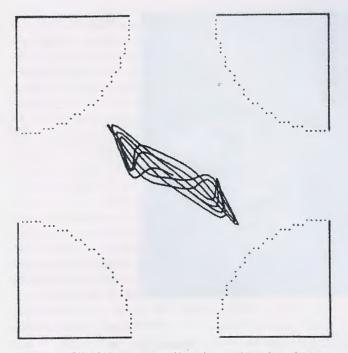


Figure 2. SIMION simulation (40 μ s) of an ion of m/z 36 in an rf-only quadrupole (1.9 cm rod diameter, 25V_p rf @ 350 kHz, 1 eV off-axis energy) [2]

fossil, since it showed red stains that he hypothesized were hemoglobin, and he planned to analyze it by mass spectrometry upon his return to Australia [1]. This was but another sign of Jim's broad interests and inquisitive mind.

(Chris) Two later meetings with Jim stand out from the normal connections at ASMS. One was his visit to Michigan State University. His talk to the department impressed everyone as did his personal discussions with the faculty and students. He was equally at home with people in all the divisions of chemistry. A physical chemist by interest, his broad background enabled him to follow wherever his curiosity took him, whether to support his interest in rocks or the energetics of ion formation and fragmentation. My group felt honored to have him with us. We were just a few years into work with the triple-quad and still struggling with getting a heated source and improved ion transmission. I think he thought we should be doing more with applications and, in hindsight, I am sure he was right. The second was the 1988 San Francisco ASMS meeting at which he gave the plenary lecture, "Forty Years of Mass Spectrometry in Australia." His characteristic low-key but awe-inspiring presentation brought everyone to their feet applauding in appreciation of him and his work.

(Rick) I once again had an opportunity to visit Jim at La Trobe in 1988 en route to the ANZMS conference in Brisbane. My wife, Katie, and our 9-mo-old daughter accompanied me. In classic Jim style, he and Krysia moved into the guest house so we could stay in the main house (which he and Krysia had built brick-by-brick 30 years before). We also visited their "cabin" (still under construction by Jim and his sons) on the Great Southern Ocean. Jim toured us around, climbing up and down the hills and canyons, showing us wallables and pademelons, we in our jeans and hiking boots, Jim in a tweed coat and tie, as always.

Also on his way to the ANZMS meeting in Sydney, a famous US mass spectrometrist dropped by La Trobe for tea with Jim. The visitor offered his opinion that all the great advances in mass spectrometry had been made, and that there was little left to be discovered in mass spectrometry. After he left, Jim observed to me that our visitor was "too young to have given up on our discipline." He pointed out that as he had gotten older (he was then 64, just a year away from forced retirement at La Trobe), he had fewer new ideas, and that indeed he "probably had only one new innovative idea a day" anymore. As the creative mind behind so many innovations (the measurement of ionization potentials, the first use of deconvolution, the triple quad, SIMION, development of an Aboriginal Pharmacopeia based on GC/MS analyses), Jim certainly had a lot of innovative ideas left to share.

Jim was scheduled to present a lecture on "Forty Years of Mass Spectrometry in Australia" at both the ANZMS meeting in Brisbane in May 1988 and then again at the ASMS Conference in San Francisco 3 wk later. While Jim was confident that the audience in Brisbane would appreciate his reminiscences, he was fearful that the ASMS audience would find the talk uninteresting, since they would know none of the players from Australia. Nevertheless, Jim gave a wonderful talk, from the heart, full of personal insights and anecdotes, and earned a standing ovation, as Chris mentioned above.

My last visit to Melbourne was in 2011, with the goal of interviewing Jim for a book that I will someday write; we spent several days discussing his reflections on 65 y of mass spectrometry in Australia, as well as visiting old haunts (including the now-completed cabin on the Great Southern Ocean). Amongst the fascinating memories Jim shared with me was how he came to Australia in 1948. After receiving his Ph.D. in Chemistry at Glasgow University in Scotland, Jim and Krysia decided to set sail for the "sunny beaches of Australia." Jim's first assignment as a new Ph.D. scientist at CSIRO in Australia was "to see whether a mass spectrometer could be of any use in chemistry" [1]. Getting that mass spectrometer, the first commercial mass spectrometer in Australia (a CEC 21-102), was a challenge, however, since the US government had embargoed the export of mass spectrometers and anything else having to do with isotopes and atomic weapons. It took the intervention of Australian Prime Minister Chifley with US President Truman to get an exception for shipment of an instrument to Australia "in light of our nations' successful collaboration in the recent war" [1].

(Chris) We maintained a sporadic correspondence between exchanges of Christmas cards (his last, sadly, arriving after his death). Our emails were particularly intense while I was working on the chapter on Tandem Mass Spectrometry for the History of Mass Spectrometry Volume of the *Encyclopedia of Mass Spectrometry* [6]. I wanted to get it

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right. Since there are so many versions of the story extant, I consulted and verified my telling of it with all the major players, including Jim, Rick, Graham Cooks, and Jean Futrell. Jim was very helpful in this regard and his memory of events was sharp and detailed. In this correspondence, I learned of his very early adoption of the rf-only sections at the end of mass-selective quadrupoles. The parts of all current quadrupole instruments we now call "stubbies." Here is what he wrote:

My own interest in quadrupoles started in 1962 when I met Ken Shoulders at Stanford Research Institute and I started building them. Subsequent to this, Wilson Brubaker, whom I had known since 1957, when he was at Consolidated Engineering Corporation, wrote to me commenting on the fact that the mass spectra produced by a quadrupole were significantly different to spectra produced by a magnetic mass analyser, and seemed to discriminate against the ions of higher m/e. He had an idea that this was due to fringing field effects at the exit of the quadrupole. He believed this could be cured if one added an RF-only quadrupole at the exit, to condition the ion trajectories. He was now retired and didn't have access to a workshop, would I try it out for him. I did, and it worked remarkably well, producing much better and consistent spectra as compared with the magnetic machines. He was delighted and I never heard whether he did any more about it, but I certainly added a short, 1-cm long RF quad section on our machines.

After helping me set the record straight, Jim concluded with the thought, "I have only happy memories, which I want to keep of the wonderful people who were my friends in the early days of mass spectrometry and of how helpful they always were to me and each other. There was never any thought of bickering over priorities or patents." This was a true testament to the size of his heart.

Final Thoughts

(Chris) For Rick and me, the development of the analytical triple-quadrupole mass spectrometer was a key point in our professional lives. It brought me into the field of mass spectrometry, which has been the focal point of my research ever since. It certainly helped launch Rick on his very successful academic career. But for Jim, it was just one of many major contributions to mass spectrometry in particular and science in general. His other contributions include the development of SIMION, the principal workhorse in ion trajectory modeling. Just imagine how many hundreds of person-years of trial and error have been saved in instrument development by being able to predict ion behavior. He recognized very early on the power that digital computing could bring to the field of mass spectrometry, writing programs for spectral identification and peak deconvolution

as well as implementing computer control of instruments. He was also in the advanced group working on the difficult problem of interfacing gas and then liquid chromatographic effluents to mass spectrometer ion sources. This was not just to do it, but so that he could demonstrate the power of this combination in the analysis of complex mixtures. He made many critical contributions and I can't think of anyone who had more fun doing it.

(Rick) It has been an amazing experience to be involved in the conceptualization and development of the triple quadrupole for MS/MS. Reminiscing with Jim during a week of interviews and visits in Melbourne in 2011 brought back many memories over four decades- passing around a quadrupole mass filter in Bonner Denton's undergraduate instrumental analysis course at Arizona in 1974, joining Chris Enke's research group at MSU in January 1975 with the plan to do "something" with computerizing a new instrument incorporating that quadrupole, writing an NSF proposal under Chris' tutelage that failed to convince reviewers that such a tandem quadrupole mass spectrometer would ever work, let alone be amenable to computer control, then a serendipitous meeting with Jim at the 1977 ASMS Conference, two months in his lab in Australia, the successful commercial introduction of the triple quad, and an academic career at UF following in the footsteps of great mentors such as Chris and Jim.

We could all take lessons from Jim on how to be a scientist and mentor. As Jim commented in a 2010 interview [5]:

The great discoveries in the future are going to come just from somebody seeing something odd and being curious about it. It helps, of course, if you're good with your hands, if you know how to use a soldering iron and you're a good scrounger... The only other piece of advice I would give is: don't pay too much attention to the theoreticians who tell you that you can't do it.

That's remarkable advice for any young mass spectrometrist today!

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