

INTRODUCTION

A special issue in honor of the late Professor Alex D. Bain (1948-2016)

The NMR community lost one of its most brilliant and original thinkers when Alex Bain died in late 2016. Many of his friends and former colleagues felt that Alex deserved some form of special recognition in view of his many contributions to NMR, both in Canada and elsewhere. Since Alex had published a number of important articles in *Concepts in Magnetic Resonance* and also served on the Editorial Board of *Concepts*, it was decided that a special issue of this journal in his honor would be an appropriate form of recognition of Alex's accomplishments, and three of us agreed to be Guest Editors for the issue.

Alex Bain graduated with a double Honors B.Sc. in Mathematics and Chemistry from the University of Toronto in 1970. He then received a National Research Council of Canada Fellowship for M.Sc. studies at the University of British Columbia where he carried out research on photoelectron spectroscopy. Next, he received a Shell Canada Fellowship for Ph.D. studies at Cambridge University. There he began his NMR career, working with Dr. Ruth Lynden-Bell. Returning to Canada in 1974, a time when full-time academic positions in Chemistry were few and far between, he first had an NRC Postdoctoral Fellowship with Professor John Martin at the University Alberta, followed by a series of limited term appointments at McMaster University and the Scarborough Campus of the University of Toronto. Finally, in 1980, Bruker Canada hired him as research scientist with particular responsibility for NMR programming, including for 2D NMR. He remained there until 1987 when McMaster attracted him back as an Associate Professor and later he became a Full Professor. In 2008, due to health concerns, he opted for early retirement to become an Emeritus Professor. However, he still kept very active in research, both at McMaster and as an unpaid research associate in Lewis Kay's group at Toronto. His contributions there are described in the article by Lewis.

Alex's research combined a strong desire to fully understand complex NMR phenomena with a knowledge and depth of understanding of advanced mathematical methods relevant to NMR that very few in the NMR community could match. Thus, use of Liouvillian operators, Floquet theory and sparse matrices featured prominently in his research. His Ph.D. research included elucidation of alternative relaxation pathways in heteronuclear AX_2 and AX_3

spin systems, knowledge that is still used today by Lewis Kay and others in designing 3D and 4D pulse sequences for protein NMR research. His Postdoctoral research included the use of Liouvillian operators to calculate NMR transitions. During his first spell at McMaster, he pioneered the use of Superspin to simulate 2D spectra. He also programmed a borrowed computer from a Nicolet FT-IR spectrometer to acquire and process 2D data on a Bruker spectrometer. This is what likely led to his job offer from Bruker. While at Bruker, he published a very useful paper describing a straightforward procedure for designing phase cycling for multi-pulse sequences. The continuing importance of this paper is well-described in the article by Lewis Kay.

After his return to McMaster, Alex focused on methods for highly accurate measurements of kinetic processes by NMR. This included development of a program, called MEXICO, which went beyond earlier programs by allowing analysis of multi-site exchange processes involving singlet peaks and two-site exchange between coupled spin systems. He also published a series of articles that provided a detailed understanding of the NMR and NQR spectra of quadrupolar nuclei. Finally, he also was fascinated by NMR exotica, such as the use of spin noise to generate an NMR spectrum without RF pulses. In addition to his own research, Alex was also very generous in sharing his expertise in NMR with McMaster colleagues, leading to many joint publications. This is well-described in the article by Giuseppe Mancini and co-authors from McMaster, along with a description of the many other ways that he contributed to life at McMaster. Alex was equally generous in providing help and advice to the broader NMR community, particularly on mathematical aspects of NMR.

Alex was a modest and very personable individual who particularly went out of his way to encourage younger scientists early in their careers. His modesty likely worked to his disadvantage in terms of wider recognition of his important work since he never boasted about or promoted his contributions to NMR. Nevertheless, those of us who were fortunate to know Alex well had tremendous respect for both him and his research. He is sorely missed.

IN REMEMBRANCE OF ALEX: BILL REYNOLDS

My first interaction with Alex was in the spring term of 1966-67. Alex was enrolled in the first year of the Maths, Physics and Chemistry program at Toronto.

This was an extremely rigorous program that each year attracted about 300 of the top Science and Maths students from all over Ontario. The courses were far more advanced than typical first year University courses. At the start of that year, the Chemistry and Physics Departments had come up with an unusual arrangement for splitting teaching responsibilities, one that Physics later regretted. The agreement was that Physics would teach a course in Classical Mechanics while Chemistry taught a course in Quantum Mechanics. John Polanyi taught the first half of the Chemistry course, covering fairly hard-core quantum mechanics. I was surprised, as a very junior staff member, to be asked to give the second term lectures. I covered the approximation methods that chemists used at that time to describe structure and bonding for molecules. At the start of 1967-68, we were pleased to discover that more students than usual had opted for one of the Chemistry options in second year, likely because of the impression from first year that Chemistry was more modern than Physics. A number opted for a combined Physics/Chemistry program but only Alex opted for the Maths/Chemistry program. Few before him had attempted that combination and even fewer had succeeded. Nevertheless, Alex not only succeeded but also had an incredibly strong academic record. However, since his Chemistry courses beyond first year were mostly Physical Chemistry, I later used to tease him, with a small element of truth, that I taught him the only real Chemistry course that he had at Toronto.

After Alex left Toronto after his B.Sc., I only reconnected with him in the late 1970s when he returned to Ontario. The first strong recollection that I have occurred at the June 1980 meeting of the Canadian Chemical Society in Ottawa. Although Alex wasn't due to start with Bruker until July, Martin Smith, the President of Bruker Canada, had invited him to come to meet Bruker customers. One evening, several of us decided to go over the Ottawa River to Hull in Quebec for dinner at a French restaurant called "Oncle Tom's" (French Canadian soul food?). The meal was superb and the bill was about \$300, a huge sum for that time. Since I was short of cash, I paid the bill with a credit card and the rest gave me their shares in cash. On the way back, someone (probably me) suggested that Alex should play a joke on Martin Smith, who was known to be tight-fisted when buying meals for customers, by handing him the bill and

saying 'I hope that you don't mind, I took some of your customers out for dinner'. When Alex, naively, did as suggested, Martin first looked surprised and then stunned when he saw the size of the bill. He shoved in under the counter, muttered in an angry tone "You haven't heard the last of this" and disappeared into the bathroom before anyone could say anything. Sensing that the joke had gone bad, we all waited outside the bathroom door and, as soon as he came out, assured Martin that it was a joke and that we had all paid for our own dinners. Thus, Alex avoided being fired before he even started at Bruker.

Two of the papers that Alex published at Bruker were particularly useful for me in using 2D NMR. One was the already-mentioned paper on designing phase cycles. The second was with Tim Allman (JMR, 1986, Vol. 68, pp. 533-539), explaining the impact of digital resolution on COSY cross-peak intensity. That allowed me to understand why I was seeing relatively strong COSY correlations even though the actual long-range couplings were barely resolved in a 1D spectrum. However, it was a conversation with him that first led me to realize how valuable Alex could be in my research. I was puzzled by a ^{13}C spectrum of a fluorobenzene derivative since one of the components of the 1-bond C-F doublet was only half as intense as the other. After very brief thought, Alex's explanation was that it was likely due to cross-relaxation between dipolar relaxation and chemical shift anisotropy, where the two effects were of the same sign for one of the doublet peaks but opposite for the other. Thus, Alex had anticipated the TROSY effect, long before it became popular in protein NMR.

When the McMaster Chemistry Department wanted to bring Alex back, they had a problem in that their only approval for a new hire was for an Analytical Chemist. However, they somehow managed to convince higher University levels that Alex was qualified to fill the position. I remember that Alex was quite amused by the thought that he was an Analytical Chemist, although I suppose that his emphasis on accurate measurement of exchange rates and other NMR parameters could vaguely qualify as "analytical".

After Alex explained my C-F mystery, he became my go-to person for help in resolving other NMR mysteries. We also co-authored three papers, two on artifacts in 2D NMR and one giving a full explanation of BIRD pulses in place of the simple vector explanations I had used in 2D pulse sequence development. We would also often meet socially. For a number of years, his wife, Janet Rossant, was carrying out research in Toronto, first at Mount Sinai Hospital and later as director of Research at Sick Children's Hospital, so they lived in west end Toronto. Particularly after Alex retired from McMaster, the two of us

would get together for a pub lunch several times per year. The last time was in October 2016, when I, along with a mutual Mexican friend, Raul Enriquez, met with Alex for lunch. While Alex was his usual cheerful, outgoing, self, both Raul and I were shocked by how much weaker he appeared than the last time that we had seen him. Thus, while saddened, I was not really surprised when, a month later, I got an email from Alex, saying that he had, at most, a few more months to live. Immediately on hearing the bad news, Lewis Kay and several of Alex's McMaster colleagues set out to organize a symposium in his honor. This was held on Dec. 13, 2016 in Toronto and was extremely well attended by many of his friends and several of us gave speeches in his honor. Alex clearly enjoyed seeing so many old friends and managed to give a short speech. However, for the rest of us, it was a bittersweet occasion, knowing that it was very likely the last time that we would ever see him. This was unfortunately confirmed when we heard from Janet that Alex died just after Christmas, 2016.

My final memory of Alex concerns the hat that he is wearing in his photo. This was a Tilley Endurable hat that he always wore in public. It made him very easy to pick out in crowds at NMR conferences. Tilley Endurables is a Toronto company that manufactures rugged travel clothes. They are so confident in the durability of the Tilley Endurable hat that they guarantee a free replacement if one ever wears out. However, they obviously underestimated Alex's devotion to his hat. At the memorial service for Alex, his brother mentioned that Alex had worn out a number of his Tilley hats over many years (he suggested ten), each time getting his free replacement.

IN REMEMBRANCE OF ALEX: GENE MAZZOLA

I don't remember when I first met Alex, but it could have been in 1988 when I took a mini-sabbatical with Bill Reynolds at the University of Toronto. I met many Canadian NMR spectroscopists during that 4-month stay, and occasionally Alex dropped by for lunch. It was obvious to me, very early on, that Alex was a very bright individual and possessed a substantial breadth of NMR Knowledge.

I had developed a considerable interest in the nuclear Overhauser effect and was intrigued by the maximum magnitude that NOEs might attain in a 2-spin system that was devoid of additional protons that could provide competing relaxation. In 1997, I was given a sample of 1,5-dimethoxy-2,4-dichlorobenzene by a colleague in our Industrial Chemicals Branch. Having an isolated proton that was relaxed solely by six equivalent protons, this molecule appeared to be an excellent candidate for maximum-NOE studies.

I determined some quick NOEs by irradiating the two equivalent methoxyl groups and observing their combined effect on H-6, which was situated between them. The NOEs were greater than 40% without degassing, and subsequent, more carefully determined NOEs in degassed solutions were close to the theoretical maximum of 50%. At that point, I was concerned with cross-correlation relaxation, which usually has very small, if any, detectable effects on measured NOEs. However, if one is pursuing a maximum NOE, even small effects, like cross correlation, could be a problem. I subsequently discussed this matter with Alex, probably at an ENC, and he was very much interested in this chase for a maximum NOE. We had many other discussions at the meeting and then later when we got home. We ultimately decided that, with the sensitivity of our instruments, a maximum 49% NOE seemed reasonable (*Magn. Reson. Chem.*, 1998, **36**, 403).

What impressed me so much on both the above deliberations and in listening to Alex discuss NMR in general with students and colleagues, was what an exceedingly decent person and scholar he was. Every question that was posed, and some were considerably better than others, was answered in a kindly and respectable manner. I don't believe that I ever heard Alex say anything remotely unkind about anyone, although he did find one particular former administrator at McMaster University somewhat amusing.

IN REMEMBRANCE OF ALEX: ROD WASYLISHEN

I was first attracted to Alex's research when I noticed a paper dealing with relaxation in coupled nuclear spin systems. It was a 22-page paper, "The Relaxation Matrices for AX₂ and AX₃ Nuclear Spin Systems" published in *Molecular Physics* by Alex and his Ph.D. supervisor, Ruth Lynden-Bell. This was the first time that I had read about superoperator representations, Liouville space, etc. and must confess that I found it challenging to follow. Nevertheless, there were many practical examples illustrating the results which I could readily appreciate because of experiments that I had done while a Postdoc with Ted Becker, 1972-74. If you read Alex's beautiful paper, you will understand one of his favorite sayings, "Everything is a sum of exponentials".

After his Ph.D. studies at Cambridge, Alex returned to Canada to work with my former colleague, John S. Martin at the University of Alberta. Alex applied his theoretical expertise to tackle several problems in collaboration with John, for example, FT NMR of non-equilibrium states of complex spin systems. It was during that time that I first remember meeting Alex. I had just started my academic career at the University of Winnipeg. In the fall of 1977,

Alex and his wife, Janet Rossant, moved to Ontario where Alex took an appointment at McMaster University and Janet accepted one at Brock University. Being adventurous, they drove from Edmonton to Hamilton, stopping over in Winnipeg to spend a memorable visit with my wife Valerie and me, along with my former Ph.D. supervisor, Ted Schaefer. Both Alex and Ted had been recipients of prestigious Shell Canada Fellowships to study at Cambridge and Oxford, respectively, and Janet had studied at both Oxford and Cambridge, so there was a lot of common ground, including magnetic resonance.

In the summer of 1980, I started a 1-year sabbatical with Colin Fyfe at the University of Guelph. Alex was in the process of moving from McMaster to Bruker Spectrospin (Canada) in Milton where he worked as an applications scientist (1980-1987). During my time in Colin's lab, Alex helped to organize regular meetings of the NMR groups working in the Toronto, Hamilton, Guelph and Kitchener-Waterloo region. At one of these get-togethers, I remember trying to convince Alex that it was worth working out how to interpret NMR spectra of spin $\frac{1}{2}$ nuclei that were spin-spin coupled to quadrupolar nuclei in solids. I had several examples. eg ^{31}P coupled to $^{63/65}\text{Cu}$ that had complex line shapes that I did not know how to deal with at the time. Toward the end of his career, Alex became a world expert on dealing with quadrupolar nuclei in solids. However, in the 1980s, he was busy making major contributions in two-dimensional NMR, the design of phase cycling procedures, etc. It was these first discussion groups that we held in 1980-81 that led to the Annual MOOT Conference (MONTreal-Ottawa-Toronto, a name apparently coined by Mike Bernstein). That began in Montreal in October 1981. The first meeting was largely organized by Alex and Charlie Rodgers from Bruker and was modeled on the long-established NMR Discussion Group in Britain. The meeting has been held annually for the last 30+ years now! It was always great to meet Alex at MOOT, when I could attend, or at the Chemical Society of Canada annual

meeting, which both of us attended on a regular basis. Alex was a sounding board, interested in discussing any research problem(s) that one had. We always made a point of getting together in a quiet corner to chat about what we doing, problems that we were having, etc.

After Alex retired from McMaster, he often came to Edmonton to visit his brother so this provided an opportunity for us to get together. Alex spent many hours in my lab, chatting with students, giving us informal seminars, etc. The last talk that he gave at Alberta was last March 8, "Theory is Easy." The audience enjoyed his interesting sense of humor, "Life is an eigenvalue problem," "Programs can be mostly boilerplate—don't write it if you can steal it," etc.

Alex will always be remembered as an outstanding scholar and independent thinker. His manuscripts were well written pedagogically and generally addressed fundamental questions or problems, eg "What is a transition." "From NMR to NQR: The complete range of quadrupolar interactions," "Liouvillians in NMR, the direct method revisited," "Origins of spin noise," "Introduction to Floquet theory," etc. His family, friends, and the NMR community at large greatly miss Alex.

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