Available online at www.sciencedirect.com
ScienceDirect
Journal of Molecular Structure 834–836 (2007) 2–6
Journal of MOLECULAR STRUCTURE
www.elsevier.com/locate/molstruc

Editorial

Molecular spectroscopy with Gerhard Herzberg

1. Prologue

This opening lecture at the 2006 EUCMOS congress in Istanbul is a tribute to our grandmaster of molecular spectroscopy, Gerhard Herzberg, affectionately known to his friends and colleagues simply as GH. His classic trilogy [1–3] published half a century ago continues to this day to be regarded as the "Bible" of molecular spectroscopy. GH received the 1971 Nobel Prize in chemistry, but at heart he always remained a physicist. And yet, he understood that molecular spectroscopy is not the sole prerogative of physics, but that it also serves other disciplines such as astronomy, chemistry, the life sciences and even the arts. In fact, when at the age of 90 he visited the Institute for Biodiagnostics in Winnipeg, GH marveled at how far we had taken "his" molecular spectroscopy.

To all of us who had the privilege of working with GH at the National Research Council in Ottawa, he was not only a great scientist, but also an inspiration and a genuine role model. Herzberg was not only the brilliant and dedicated scientist whose work defined an entire field of research, but he was also the man who set high standards for both excellence and for humanity. I hope that for those young people who are just embarking on their scientific career, the story of Gerhard Herzberg will nurture the desire to follow a career in molecular science. I have selected only a few, representative highlights from his long and fulfilled life that spanned most of the 20th century. For those interested in more details I strongly recommend the excellent biography from the pen of one of his close collaborators, Boris Stoicheff *Gerhard Herzberg: An Illustrious Life in Science* [4].

2. Gerhard Herzberg, the scientist

Herzberg was an ardent promoter of fundamental science, or as he himself liked to put it, curiosity-oriented research. His definition of curiosity-oriented was meant literally as "let people wonder along the path of curiosity and they will find the right things". Herzberg did not believe in separating basic and applied research. When asked to testify at a parliamentary enquiry on public support for research he said "it is argued again and again whether government should support basic or applied research... I believe this debate is unnecessary... in my opinion there is only good and poor research... and good research always starts out as basic, but inevitably turns into applied research". This point was well elaborated by his friend, Charlie Townes one of the inventors of the laser. At a 1994 meeting in Toronto where twelve Nobel Laureates assembled to celebrate Herzberg's 90s birthday, Charlie Townes recounted the story of his attempt to patent this newly discovered gadget (Fig. 1). He was told "the laser is such an esoteric invention, it will never, ever be of any practical importance". Bell Research Labs refused to patent the invention.

It is only fair to state that molecular spectroscopy in Canada started with the arrival of Herzberg at the National Research Council (the NRC) in Ottawa in 1948. He immediately embarked upon the difficult task of building a world class spectroscopy laboratory and was fortunate to attract a number of talented young scientists. Alex Douglas promptly set about building spectrographs for the visible, ultraviolet and infrared regions; Cec Costain, a former radar officer during the second world war, was responsible for setting up a microwave laboratory; Hin Liu was building an atomic beam laboratory, while Don Ramsay was assigned the task of setting up a flash photolysis apparatus for the study of short-lived species (free radicals). By the early 1950s Herzberg's lab was well equipped for studying the spectra of atoms and molecules in any spectral region. Soon postdoctoral fellows began to arrive from all over the world, along with many visiting scientists. John Polanyi and Dudley Herschbach were among the early arrivals, and later shared the 1986 Nobel Prize in Chemistry. Harry Kroto, a postdoctoral fellow from 1964 to 1966 and Robert Curl, a visiting scientist during this time, also shared a Nobel Prize in 1996. Kroto, whose pursuit of the role of carbon in space led to the discovery of "buckminsterfullerene", stated unequivocally that Herzberg and NRC's program in fundamental science was responsible for the discovery of the C_{60} molecule.

0022-2860/$ - see front matter
doi:10.1016/j.molstruc.2007.01.062

Fig. 1. Herzberg turns 90 – A celebration of minds.Toronto 1994. From left to right: Herzberg, Porter, Watson, Prigogine (front row), and Perutz, Smith, Herschbach, Brockhouse, Polanyi, de Duve, Townes, Kendall (back row).

Many other Nobel Laureates and distinguished spectroscopists visited this bastion of spectroscopy in the Northern city of Ottawa at one time or another during their career. Herzberg's enthusiasm for molecular spectroscopy as a tool to study molecular structures was contagious: his lab in Ottawa became the Mecca for molecular spectroscopy for the second half of the 20th century.

There are many highlights in Herzberg's research, clearly however a leitmotif was hydrogen. Hydrogen is not only the most abundant atom in the universe, but also the most fundamental, and so it comes as no surprise that Herzberg worked on hydrogenic species throughout his life. His work was pivotal to the advancement of a number of disciplines. In physics, he blazed a new trail with his work on atomic and molecular hydrogen, of forbidden transitions and of pre-dissociation. In chemistry, the discovery of spectra of free radicals, notably CH_2 and CH_3 (for which he actually received the Nobel Prize), and of the Rydberg molecule H_3 were all outstanding contributions. In astrophysics, his true love, his work furthered the quest to understand the structure of matter in the universe. The search for molecular species in extraterrestrial bodies and in the interstellar medium started with the reproduction of the spectrum of CH^+ in the laboratory and the prove of its presence in the interstellar medium, and progressed to the identification of the spectra of C_3 and H_2O^+ and their detection in comets. Obtaining the quadrupole spectrum of H_2 and the discovery of hydrogen in the atmospheres of the planets also contributed greatly to our understanding of the universe.

Herzberg was consumed by the search for an explanation of the diffuse interstellar bands; he felt that these bands must come from molecular ions or from free radicals because if the spectra were due to neutral molecules they would have long been found in the laboratory. Ions and free radicals should certainly be favoured in the interstellar medium where they would be more stable than under ambient conditions. So after having studied the spectra of atomic and molecular hydrogen for many years, Herzberg subsequently turned his attention to the H_3 molecule and its H_3^+ ion. As the simplest polyatomic molecule (more than 2 atoms) with only three protons and two electrons, it is the starting point for the creation of many other molecules in interstellar space. The H_3^+ ion has been known since 1911 when J.J. Thomson discovered it in an electrical discharge however its spectrum was to remain unknown for a long time. The search for H_3^+ afforded GH a life-long challenge. There was no question in his mind that for H_3^+ to be found in the interstellar medium, its spectrum had to be identified in the laboratory first. Quantum theory predicted that H_3^+ would have the structure of an equivalent triangle, with the three hydrogen atoms separated by 0.88 Angstrom. Thus the infrared spectrum was calculated to be around 2522 cm^{-1}. In the hunt for this elusive species Herzberg searched the absorption spectrum from the far ultraviolet to the infrared, but initially without success. Only when in his laboratory Takeshi Oka started using laser techniques, was the spectrum of H_3^+ finally observed in 1980. Albeit the fact that Herzberg did not directly participate in theses experiments, he was delighted that the first observation of the long sought H_3^+ spectrum had been made in his laboratory. Eight years later another disciple of GH, Jim Watson found H_3^+ in Jupiter. Images of Jupiter, taken using H_3^+ emission spectra, would reveal that the brightening at the polar regions is due to H_3^+ in its ionosphere. Meanwhile emission spectra of H_3^+ were also observed in Uranus and in Saturn. Eventually H_3^+ was also found in interstellar space, as predicted by Herzberg 30 years earlier. It is now well accepted that H_3^+ plays a pivotal role in interstellar chemistry and its spectrum has become a tool for astronomers and geophysicists to study the morphology and the temporary variations of planetary plasmas. Herzberg never once claimed that his ideas and perhaps his enthusiasm for H_3^+, actually started these breath-taking developments, nevertheless he followed them with great interest right to his last breath.

3. Gerhard Herzberg, the man

Herzberg preferred to talk about his good luck, and not about difficulties though life forced him to overcome many. It all began when he was born on Christmas Day in 1904, though he later complained that because of this he missed out on extra gifts. In high school in Hamburg he was lucky to have a superb physics teacher who aroused the interest of his students by giving extra classes on the new ideas in physics, thus exposing the young Herzberg early to the atomic theories of Niels Bohr. He was further lucky with his PhD supervisor at the Technical University in Darmstadt, who encouraged his students to think and work independently. Herzberg certainly was lucky to start his scientific work just as the new quantum theory was developing with new applications to atomic and molecular problems. In Göttingen he was to work under the direction of Max Born and James Frank who were applying quantum mechanics to molecular structures. During that period he

met Werner Heisenberg, Peter Debey, Friedrich Hund and rubbed shoulders with the younger group of Max Delbrück, Walter Heitler, Eugene Wigner, Hertha Sponer, Victor Weisskopf, Edmund Teller and also collaborated with some of them. An amusing anecdote from this time is his joint publication with Teller on the vibrational structure of electronic transitions in polyatomic molecules [5]. Teller was a young assistant in Göttingen, having just completed his PhD with Heisenberg. Herzberg enjoyed telling everybody about his so-called "collaboration" with Teller. Teller had the ideas which he shared freely with others, but he did not care much about putting them on paper. So Herzberg had to play the role of a "midwife", literally extracting them from Teller. When it came to the publication, though Teller's contribution was clearly the more important one, the latter insisted that the names be in alphabetical order, listing Herzberg's first. GH was so impressed that he followed the alphabetical order of names in all his later publications. Herzberg had great respect for Teller as a scientist, but he disapproved of his role in the building of the hydrogen bomb and later in supporting Reagan's ideas of a laser-based missile shield.

Herzberg emphatically believed in the creativity of the individual. He was always ready to encourage people, but never dictate to others what to do. He also held strong views on how to exercise leadership and often shocked visitors by telling them that as the director of the Division of Physics he was actually not directing. This is how he formulated it "I am not here to tell people what to do, I see my director role mainly as finding the best scientists available and then providing them with the best facilities for their work". In this connection he liked to refer to the much quoted Einstein adage "imagination is more important than knowledge".

Herzberg's belief in the freedom of the individual was not confined to the scientists at NRC, but extended to the freedom for all. He was active in such humanitarian organizations as the Academy of Peace, Science for Peace, the Committee of Concerned Scientists and the Congress of Noble Laureates for World Peace. When asked to support humanitarian actions his characteristic answer was "I am all for it". He also lent his name to petitions, movements or projects for the liberation of detained scientists, and did not hesitate to write letters to Heads of State from behind the iron curtain to plead for the cause of persecuted scientists. Perhaps the best known case is that of Academician Sakharov who in 1980 was banished by Brezhnev to the closed city of Gorki for daring to criticize the Soviet authorities. Herzberg personally participated in demonstrations in front of the Soviet Embassy in Ottawa to appeal for Sakharov's release. After Gorbachev asked him "to return to his patriotic duties", Sakharov travelled to Canada to personally thank Herzberg. When they finally met at NRC in Ottawa, he proclaimed "a dream come true" (Fig. 2).

Fig. 2. Herzberg meets Sakharov: A dream come true. Ottawa 1989.

While Herzberg was admired the world over for speaking authoritatively on scientific subjects, he was somewhat reticent to speak publicly on topics other than his field. And yet, should scientists come under attack from bureaucrats or politicians, he stepped forward and resoundingly expressed his personal views. In one of his public speeches, "The Dangers of Science Policy", he warned of the adverse effects a civil service mentality would have on the scientists at NRC. He argued "science policy makers would like to believe that if only their committees apply the right strategy and the right bureaucratic mix, we would be fine. Yes, the right strategy may win a war or an election, but the use of any strategy is very difficult when one is dealing with discovery and creativity, and strategic planning certainly requires the participation and buy-in of the scientists themselves".

He also spoke out on reorganization and to lend more credence to his point, GH quoted a respected Canadian politician, the former Prime Minister Pierre Trudeau, who in turn cited a Roman officer, Petronius Arbiter from the time of Emperor Nero "we tend to meet any new situation by reorganizing, what a wonderful method it can be for creating the illusion of progress while producing confusion and demoralization".

In 1969, when Herzberg reached the age of 65 the NRC invented the title of "Distinguished Research Scientist" in order to keep him on staff. Two years later he was awarded the Nobel Prize. Upon his return from Stockholm, and while attending a reception held in his honour at Government House in Ottawa, he could not resist taking a shot at the many bureaucrats and politicians present in the room. He compared the situation in science with that in the Army quipping: "recent reports indicate that for every private in the Army there are four of higher rank, now it appears to me that for every working scientist there are four persons spending their time deciding how and where and when he or she should work". GH then added: "I was warned that after receiving the Nobel Prize I would now belong to this higher rank; may I say I have every intention of returning to the rank of private in the army of Canadian scientists, once the first flurry connected with the prize is over". And so he did.

After receiving "The Prize", this is how GH always referred to the Nobel Prize, he was swamped with requests and petitions of all sorts, but he always seemed to find time to help his fellow scientists, young and old, writing letters of recommendation or nominating deserving candidates for awards.

Herzberg always wore a white lab coat. In the Division of Physics lab coats were not used, so when visitors kept asking for GH, the commissioner at the front desk would give them the following directions: "just look for a short man in a white coat" (Fig. 3).

During his time in England Herzberg had become accustomed to afternoon tea as a venue for meeting with colleagues and friends and for carrying on discussions of science or of world affairs. The tradition of afternoon tea with GH, be it at 100 Sussex Drive, at his home in Ottawa (Fig. 4), or at his cottage in the Gatineau Hills (Fig. 5), was observed until his final days. While some considered this to be a waste of time, it was really more like a free trade in ideas.

Herzberg had a great sense of humour and a resounding laugh, and he enjoyed a good joke, even when this was on him (Fig. 6).

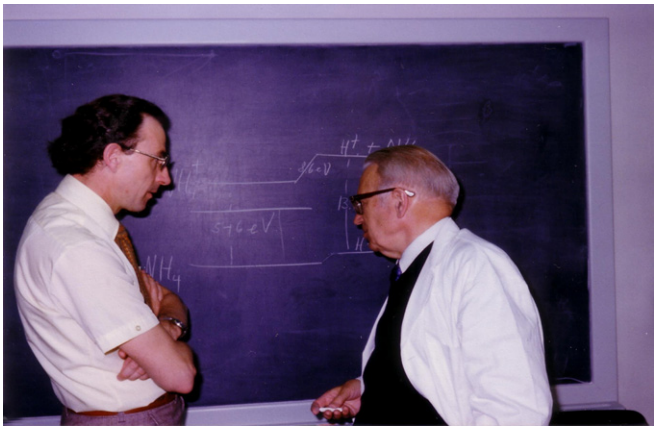

Fig. 3. A Herzberg tradition: whether in the lab, in his office or in front of the blackboard, GH always wore a lab coat.

Fig. 4. Talking spectroscopy at the home of GH. From left to right: Andy Cole (from down under), Norman, Jones, GH the host, and the author Henry Mantsch.

Fig. 5. Enjoying tea with guests on a Sunday afternoon at his cottage in the Gatineau Hills.

Fig. 6. Herzberg and his wife Monika enjoying a joke (this one on him) at his 90s birthday celebration in the Herzberg auditorium at 100 Sussex Drive.

4. Epilogue

People might wonder why Herzberg, a physicist by training, even better known as an astrophysicist, ended up with the Nobel Prize in chemistry. Perhaps, the best explanation is the one given by the Nobel Committee itself: "Around 1950 molecular spectroscopy had progressed so far that one could begin to study even complicated systems of great chemical interest. This is brilliantly demonstrated by Herzberg's pioneering investigations of free radicals. Knowledge of their properties is of fundamental importance to our understanding of how chemical reactions proceed."

It is well known that the dream of young Herzberg to pursue a career in astronomy was shattered by a letter he received from the Hamburg Observatory where he had inquired saying that "there is no point in thinking of a career in astronomy unless one has private means of support", something he certainly did not have at the time. Five decades later he saw the fulfillment of his dream, when in 1975 the NRC created the Herzberg Institute of

Astrophysics as a tribute to his contribution in this field and to Canadian science.

Herzberg was incredibly well organized, dedicated, and impassionate spending every hour, from early morning to late evening, on his beloved subject – molecular spectroscopy. He was a brilliant experimentalist, vastly patient and ingenious, and as a person, gentle and generous. At a memorial tribute held for him in May 1999 in Ottawa, Arthur Carty the encumbent president of NRC at the time, accorded the ultimate accolade to GH "he was a gentlemen of science".

Herzberg's classic volumes on molecular spectra and molecular structures will remain as the encyclopaedic cornerstone of molecular knowledge for all time. As one of his former students put it "they are the expression of his joy (and hard work) in teaching others what he had learned". This sentiment also radiated from Herzberg's plenary lecture at the 1989 EUCMOS meeting in Dresden on "the history of the discovery of the spectra of CH_2 and CH_3" [6].

Perhaps the best way to honour Herzberg's passion for molecular science is to pass it on to the next generation(s) of scientists around the world. The search for yet unknown molecular species, be it in the vast macro-cosmos of the universe or the tiny micro-cosmos of sub-cellular structures, remains a supreme challenge to this day.

References

[1] G. Herzberg, Molecular Spectra and Molecular Structure: I Diatomic Molecules, Prentice Hall Inc., New York, 1939.
[2] G. Herzberg, Molecular Spectra and Molecular Structure: II Infrared and Raman Specrta of Polyatomic Molecules, D. Van Nostrand Co. Inc., New York, 1945.
[3] G. Herzberg, Molecular Spectra and Molecular Structure: III Electronic Spectra and Electronic Structure of Polyatomic Molecules, D. Van Nostrand Co. Inc., New York, 1966.
[4] B. Stoicheff, Gerhard Herzberg: An Illustrious Life in Science, NRC Press, Ottawa, Ont. Canada, 2002, 468 pp.
[5] G. Herzberg, E. Teller, Z. Phys. Chem. B21 (1933) 410.
[6] G. Herzberg, J. Mol. Struct. 217 (1990) 11.

Henry H. Mantsch
Institute for Biodiagnostics,
National Research Council of Canada,
435 Ellice Avenue, Winnipeg, Man.,
Canada R3B-1Y6
Department of Science and Technology,
Canadian Embassy, Leipziger Platz 17,
10117 Berlin, Germany
E-mail address: henry.mantsch@international.gc.ca

Received 25 January 2007; accepted 25 January 2007
Available online 6 February 2007