Theor Chem Acc (2011) 129:271–289
DOI 10.1007/s00214-011-0948-2

EDITORIAL

Editorial

This issue of *Theoretical Chemistry Accounts* is dedicated to Professor Pekka Pyykkö on the occasion of his seventieth birthday. Pekka Pyykkö was born in Hinnerjoki, a small village north of Turku, on October 12, 1941. He studied physics at the University of Turku, where he received his M.Sc. (1964), Ph. Lic. (1965), and Ph.D. (1967) degrees. He completed a dissertation in experimental NMR spectroscopy on as experimental NMR spectroscopist on "Deuteron Magnetic Resonance Absorption in $NaBD_4$, CD_4, and ND_4NO_3" at the Wihuri Physical Laboratory, University of Turku, under the supervision of Väinö Hovi. In 1968–1969, he had a 1-year postdoctoral stay as NORDITA scholar at the University of Aarhus (Denmark), followed by another postdoctoral year at the University of Gothenburg (Sweden). Back in Finland, he worked at the University of Helsinki (1970–1971), the University of Jyväskylä (1972–1974), and the University of Oulu (1973) from 1970 to 1974, except for an eight-month research stay in 1973 at CECAM (*Centre Européen de Calcul Atomique et Moléculaire) CNRS* (*Centre National de la Recherche Scientifique)* in Orsay as "Attaché du CNRS détaché au CECAM". In 1974, he was appointed Associate Professor of Quantum Chemistry at the Åbo Akademi University in Finland. Since 1984, he has held the Swedish Chair of Chemistry at the University of Helsinki. This position was established in 1908 as a parallel chair to the one of Johan Gadolin's former position, founded in 1761. From 1995 to 2000, he was a Research Professor of The Academy of Finland, and from 2006 until his (official) retirement in October 2009, he was the Chairman of the Finnish Center of Excellence in Computational Molecular Science.

Pekka Pyykkö is an internationally highly acclaimed and recognized quantum chemist. He began his scientific career as an NMR spectroscopist and published his first paper on relativistic effects in 1971. In an interview with the Royal Society of Chemistry in Britain in 2007, Pekka explained how he got into relativistic quantum chemistry: *While I was working on the theory of NMR properties, I realized that there were very significant relativistic effects influencing the heavy elements' spin–spin coupling constants, which no one had told me about. I started to try to calculate them and had a few early papers on the relativistic theory of NMR parameters. After we had started to do relativistic molecular calculations, I was comparing certain properties for silver and gold compounds and I realized that the entire difference between them comes from relativity, which was a revelation*. Pekka also pioneered numerical quantum chemistry and published many important articles on heavy-element chemistry, such as on the understanding of the metallophilic interactions. Furthermore, his research interests include the search for and understanding of new chemical species and chemical bonds: *If you push your calculations to the currently available limit, more often than not, you find new science. Half of chemistry is still undiscovered. We do not know what it looks like and that is*

the challenge. He predicted new inorganic species of which several have been synthesized and characterized in the meantime: In salts: Pt^{2-}, BC^{2-}, BN^{3-}, PBP^{3-}, NBC^{4-}, $FCNF^{+}$, N_5^{+} and $OCNCO^{+}$, in mass spectroscopy PS_3^{-}, NUO^{+}, AuC^{+}, $AuXe^{+}$, $XeAuXe^{+}$, the WAu_{12} family, (including $MoAu_{12}$ and MAu_{12}^{-}; M = V, Nb, Ta), $OUIr^{+}$ and also $OCNCO^{+}$, and finally, in matrix spectroscopy the MH_4 models of the 1970s (M = Ti, Zr, Hf, Th), WH_{12}, CdH_2 and the HZn-ZnH, with a zinc-zinc bond, and NBNN in matrices. XeO_2 has just been reported, but it is not clear whether the molecular form is also there. Many further species remain experimentally undiscovered. Pekka also worked on the determination of nuclear quadrupole moments from high-precision quantum chemistry calculations combined with spectroscopic data. Two of his most recent contributions are "*Relativity powers car batteries*" (*Phys. Rev. Lett.* 2011, *106*, 018301) and "*A suggested periodic table up to nuclear charge* 172" (*PCCP* 2011, *13*, 161), both hit the news worldwide. Most recently, he worked on how to incorporate quantum electrodynamic effects (QED), such as the vacuum polarization and electron self-energy, into electronic structure theory, a long-standing problem in relativistic quantum chemistry. He showed that such effects are quite sizable for superheavy elements (trans-actinides) and regards QED studies as *the last train from physics to chemistry*.

The annual Winter School in Theoretical Chemistry founded by Pekka in 1985 has had (and still has) a huge impact on the education of a new generation of theoretical chemists. The bright idea that the theme of the school can vary from year to year implies that knowledge transfer is maintained in almost all areas of theoretical and computational chemistry, which finds a large and enthusiastic audience every year. As a result, the Winter School has brought new and important know-how to Finland while at the same time has helped to create fruitful research contacts between young participating Ph.D. students and postdoctoral fellows with well-established scientists from all over the world who deliver the lectures.

His work has been recognized by many awards and honors including the *Harry Elving Prize* in 1978, the *A. I. Virtanen Prize* in 1997, the *E. J. Nyström Prize* in 1998, and the prestigious *Humboldt Research Prize* in 2002. He was decorated by the president of Finland in 1995 (FVR R I) and received the *Palmes académiques* in France in 2009. He was invited to the *Väisälä Lecture* (Turku) 1991, *Löwdin Lecture* (Uppsala) 2003, and *Glenn Seaborg Lecture* (Berkeley, CA) 2008. He became member of Finska Vetenskaps-Societeten in 1985, Suomalainen Tiedeakatemia in 1989, Royal Academy of Arts and Sciences in Uppsala in 1990, European Academy of Arts, Sciences and Humanities, Paris, in 1991 (Correspondence member since 1981), International Academy of Quantum Molecular Sciences in 1992, Bayerische Akademie der Wissenschaften (Correspondence member) in 2000, and Academia Europea in 2007. Presently, he is the Chairman of Finska Vetenskaps-Societeten (since 2010) and the President of the International Academy of Quantum Molecular Sciences (since 2009).

Pekka Pyykkö has played a central role for the development of the scientific field of relativistic quantum chemistry, in fact he is regarded to be one of the main players and pioneers in this area. He was the Steering-Group Chairman of the Program *Relativistic Effects in Heavy-Element Chemistry and Physics* (REHE) in 1992–1998. The REHE funded by the European Science Foundation (ESF) is still active forming the infrastructure network of relativistic quantum chemists. He has taken a number of responsibilities for scientific journals as member of editorial boards and was a referee for more than 50 manuscripts annually over the last 20 years. In this context, the list of commission of trust includes Member of the Editorial Board of International Journal of Quantum Chemistry (1979–1986), Chemical Physics Letters (1981–1990), Molecular Physics (1983–1990), Finnish Chemical Letters (1983–1989), Advances in Quantum Chemistry (since 1987), Theoretica Chimica Acta/Theoretical Chemistry Accounts (1992–2008), Chemistry—A European Journal (since 1994), Physical Chemistry Chemical Physics (since 2006), and since 2009, he is the Chairman of the Editorial Board of Physical Chemistry Chemical Physics.

The scientific work of Pekka Pyykkö is documented in more than 300 original publications and book chapters (see attached list). Pekka inspired a large number of students in quantum chemistry, of whom several advanced into university careers. His work has been cited more than 12,000 times, and his Hirsch-index currently stands at 53 (for those who adore statistics), a truly outstanding achievement. Pekka is both an inspirational teacher and a dedicated researcher and every now and then likes to give thoughtful comments. In an interview some years ago, an interviewer asked him: "*If you weren't a scientist, what would you be?*" After having reflected upon his eventual success in languages—because he speaks a number of them—Pekka thoughtfully replies: "*Oh, I could have been a plumber*". They had a demanding plumbing problem at his house and, evidently, he solved it satisfactorily (From Henrik Konschin's "*A tribute to Pekka Pyykkö*") (see below).

We all, colleagues and co-workers, wish Pekka many more productive years of continuing exciting research (don't retire Pekka!), and last but not least a very healthy and long life.

Sebastian Riedel (Freiburg), Peter Schwerdtfeger (Auckland), Dage Sundholm (Helsinki)

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Curriculum vitae

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Education: Matriculation 1959 at Turku Latin School (Turun klassillinen lyseo).

M.Sc. 1964, Phil. Lic. 1965, Ph.D. 1967 (University of Turku, Finland).

Current position: Emeritus status since 1.11.2009, Professor of Chemistry, University of Helsinki

Previous position: Associate Professor of Quantum Chemistry, Åbo Akademi, Finland, 1974–1984. Research Professor of The Academy of Finland, August 1995–July 2000.

Extended visits abroad:

- NORDITA scholar, Aarhus, Denmark, 1968–1969 (12 months.)
- 'Nordisk docentstipendiat', Göteborg, Sweden, 1969–1970 (12 months.)
- attaché du CNRS détaché au CECAM, Orsay, France, 1973 (8 months.)
- Universität Erlangen-Nürnberg, Germany, 2003 (5 months.)
- Universität Bonn 2004 (1 month.)
- TU-Berlin 2007 (1 month.)
- Visiting professorships at the Chemistry Departments of: Vrije Universiteit, Amsterdam, 1974 (1 month.)
- École Normale Supérieure de Jeunes Filles, Montrouge, 1981 (2 months.)
- Université Scientifique et Médicale de Grenoble, 1981 (1 month.)
- University of Auckland, 1993 (2 months.)
- Universität Marburg, 1995 (2 weeks)
- Université Louis Pasteur, Strasbourg 2005 (3 weeks)
- École Polytechnique 2008 (1 month.)
- Tsinghua University, Beijing 2010 (1 month.)

Honours:

- The Harry Elving Prize, Åbo Akademi, 1978
- Decorated by the president of Finland (FVR R I, 1995)
- The A.I. Virtanen Prize, 1997
- The E.J. Nyström Prize, 1998
- Humboldt Research Prize (granted 2002)
- Palmes académiques (France) 2009
- Väisälä Lecture (Turku) 1991
- Löwdin Lectures (Uppsala) 2003
- Glenn Seaborg Lectures (Berkeley, CA) 2008

Member of:

- European Academy of Arts, Sciences and Humanities, Paris (corr. 1981, member 1991)
- Finska Vetenskaps-Societeten 1985 (Chairman, April 2010–)
- Suomalainen Tiedeakatemia 1989
- Royal Academy of Arts and Sciences in Uppsala 1990
- International Academy of Quantum Molecular Sciences, Menton 1992 (President, July 2009–)
- Bayerische Akademie der Wissenschaften (corr.) 2000
- Academia Europea 2007

Editorial boards:

- International Journal of Quantum Chemistry 1979–1986
- Chemical Physics Letters 1981–1990
- Molecular Physics 1983–1990
- Finnish Chemical Letters 1983–1989
- Advances in Quantum Chemistry 1987–
- Theoretica Chimica Acta/Theoretical Chemistry Accounts 1992–2008
- Chemistry—A European Journal 1994–
- Physical Chemistry Chemical Physics 2006– (Chairman 2009–)

Some positions of trust:

- National Research Council of Sciences
- The Academy of Finland: Member 1986–1991
- Finnish Center of Excellence in Computational Molecular Science (CMS): Chairman 2006–2008.
- European Union: Chemistry panels for HCM 1992–1994, TMR 1995–1996
- COST: Action D9, Management Committee (MC) 1997–2002, Vice-Chairman 1998–1999, Chairman 1999–2002. Action D26 MC member 2001–2007
- European Science Foundation: Steering Committee Chairman for the programme REHE ('Relativistic Effects in Heavy-Element Chemistry and Physics'), 1992–1998
- Association of Finnish Chemical Societies: Chairman, 1999–2000
- Finska Kemistsamfundet—Suomen Kemistiseura: Chairman, 1988–1989, 1999–2001
- 13th International Congress of Quantum Chemistry, June 22–27, 2009: Chairman of local organization committee.

Ph.D. students, Post-doc, and research visitors of the Pyykkö group at the University of Helsinki

Ph.D. students:

- Dr. Michaela Ekholm
- Dr. Ingegerd Forsskåhl

- Prof. Matti Hotokka
- Doc. Mikael P. Johansson
- Dr. Jonas Jusélius
- Doc. Henrik Konschin
- Doc. Leif Laaksonen
- Dr. Ying-Chan Lin
- Dr. Michael Patzschke
- Dr. Nino Runeberg
- Dr. Michal Straka
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- Dr. Bertel Westermark
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- Prof. Jacek Bieroń
- Dr. Carine Clavaguéra
- Dr. Luiz G. M. de Macedo
- Dr. Jean-Pierre Dognon
- Prof. Kenneth G. Dyall
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- Dr. Igor Goidenko
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- Dr. Peter Hrobárik
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- Prof. Leonti N. Labzowsky
- Prof. Paolo Lazzeretti
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Long-term research partners

- Prof. Jean-Paul Desclaux
- Prof. Laura Gagliardi
- Prof. Bernd A. Hess
- Prof. Björn O. Roos
- Prof. Hubert Schmidbaur

(Prof. Hubert Schmidbaur sent many of his Ph.D. students on short-term computational research visits to Helsinki).

A tribute to Pekka Pyykkö

Introduction

Many of you know Pekka Pyykkö as an eloquent and multilingual speaker at numerous conferences, congresses, and seminars all over the world. Often demonstrating the importance of accounting for relativistic effects in chemical systems, or presenting theoretical evidence for new, exciting, and hitherto unknown chemical species. Sometimes you may find him in a more reflective mood, discussing the intricacies of chemical bonding throughout the periodic system with a definite affection, however, for the heavier elements. Who is the man behind these, so often, elegant and enlightening lectures? As one of the Pekka's former pupils, co-workers, and colleagues, I will try here to convey some impressions from an almost 40-year acquaintance with his teaching, his science, and his person.

A bit of history

Pekka Pyykkö's family can trace their lineage back to old Carelian roots. Two Pyykkö members are mentioned in Gustav Vasa's tax rolls in 1553–1554. The family farm was occupied by Henrik Krstiansson Pyykkö (1678–1754) in the middle of the eighteenth century. The Pyykkö family was, however, forced to move because of WWII, and Pekka Pyykkö was born in Hinnerjoki in the southwest of Finland near Turku. He learned to read so early that his parents found it necessary to put him to school as a 5-year old; he had already read all the books in the home library. He matriculated from the Turku Latin School (Turun klassillinen lyseo) in 1959 and began his studies at the University of Turku where he took his degrees in a rapid succession, M.Sc. 1964, Phil. Lic. 1965, and Ph.D. 1967. Both at school and at the university, the teaching was excellent, and the teachers kept a high standard according to Pekka. He also likes to point out that his second year undergraduate studies in chemistry, physics, and mathematics at the University of Turku (cum laude) remain the foundation for his scientific career.

The beginnings of a scientific career

Although Pekka Pyykkö is known as a quantum chemist and Professor of Chemistry, he in fact did his Ph.D. in

physics, mainly by helping to build an NMR spectrometer and performing measurements on solids. As Pekka himself expresses it: "About two thirds experimental NMR on solids and one third quantum chemistry". A measurement of the deuteron quadrupole coupling constant in a C_6D_6 single crystal together with Ulla Lähteenmäki is still unique, and it later prompted Pekka to observe that one should never publish good work in obscure journals. This work was published in *Ann. Univ. Turkuensis A I*, No. 93, 7 p. (1966), quoted in *Chem. Abstr.* 66, 120609q (1967), and thus failed to get the attention it deserved. Although his work was a very "chemical" kind of physics, quantum chemistry was not a long way off. Pekka's interest in quantum chemistry can probably be traced back to his participation in the famous "Löwdin Summer School" in Uppsala in 1965. At that time, there was no quantum chemistry established in Finland. In fact, with a little hindsight, one could claim that Pekka himself founded Finnish quantum chemistry. The first chair, an Associate Professorship, in this novel discipline was founded at Åbo Akademi, the Swedish-speaking university in Turku, and in 1974, Pekka became Associate Professor of "Quantum Chemistry and Molecular Spectroscopy" there. This was indeed an interesting career move, transferring from being a Finnish-speaking experimental physicist to a Swedish-speaking quantum chemist!

Early recollections

My own first—very faint—memory of Pekka goes back to the beginning of the 1970s, when I think he lectured about something connected to hyperfine coupling (or perhaps it was spin–spin coupling) at a seminar in the Research Institute for Theoretical Physics, University of Helsinki, Finland. I did not understand a word of the lecture, but the lecturer was impressive. Just to give you an idea of how Pekka could get your attention. In another lecture later, the audience and I saw Pekka dash to the blackboard, write down a lengthy expression for the Hamiltonian, then turn to the audience and with a big smile announce that "This Hamiltonian is like ancient Gallia—divided into two parts!" Thus, later when I found that I needed insight into quantum chemical methods while working at the University of Helsinki, I decided to become a "long-distance" pupil of Pekka, that is, traveling to Turku for his lectures and to perform the laboratory work attached in order to qualify for a second M.Sc. An organic chemistry professor at the University of Helsinki then scornfully made his opinion clear: "You don't need quantum chemistry or computational chemistry to do real chemistry!" I wonder what that professor thinks today, when Pekka's contributions also have reached classic organic texts, such as Jerry March's "Advanced Organic Chemistry"?

The time at Åbo Akademi

When I started my M.Sc. studies for Pekka at Åbo Akademi, the times were really exciting. Jean-Paul Desclaux and Pekka had finally got their program for relativistic molecular calculations working, and the air was full of phrases like "relativistic contraction", "infinite speed of light", "heavy element chemistry" and so forth. Pekka's group was rather small. I remember Matti Hotokka and Johan Sjöblom, both now with a professor's chair of their own. In fact, Matti Hotokka became Pekka's successor when Pekka moved to Helsinki. Also at this same time, the difference between silver and gold was shown by Pekka and Jean-Paul Desclaux to be of relativistic origin, a discovery which in Pekka's own words was a "revelation". This discovery, the use of quantum chemistry and relativity to explain why gold is yellow and silver is not, even made the daily papers in Finland at that time. Similarly, the explanation of why mercury is a liquid at standard conditions, or why lead has a face-centered cubic crystal structure instead of being diamond-like, could be attributed to relativistic effects. Quite recently Pekka also explained why lead batteries in cars work; yes, you guessed it, again relativity! Then, at the end of the 1970s, the article, which probably really made other chemists aware of the importance of relativity in chemistry, appeared in Accounts of Chemical Research, written by Pekka and Desclaux. That Pekka has made such an outstanding contribution toward the understanding of chemical systems where relativity is important perhaps follows from his thorough background in NMR spectroscopy. He realized early on that relativity had a very significant influence on the spin–spin coupling constants of heavy elements. The moral here of course is a talented chemist should never forget what she/he learned early in her/his career.

Pekka Pyykkö's lectures in Quantum Chemistry and Molecular Spectroscopy were intensive, but very good, and somewhere in between he had managed to write very useful Lecture Notes for his courses. As his pupil, you were also supposed to participate in all other courses and lectures delivered by a number of "special guest stars," who had been invited to Åbo Akademi by Pekka. Thus, one could follow lectures given by Jean-Paul Desclaux, of course, Herman Jansen, Ian Grant, A.D. Buckingham, Larry Lohr, Björn Roos, Arlen Viste, Roald Hoffman, John Pople, and many others. To say that these lectures were inspiring is an understatement. There were not many chemistry departments in Finland at that time, which could show such an impressive list of internationally highly acclaimed lecturers. Pekka even persuaded Björn Roos to become a Docent at Åbo Akademi. This was the only place outside Sweden where Björn could—in fact, was required to—lecture in Swedish! The present "Winter School" tradition in Helsinki really started at Åbo Akademi with many of these guests

giving series of talks over a longer period. Today one would call these sessions "Schools" according the season, because they occurred whenever Pekka had a sufficiently prominent speaker and persuaded him or her to give lectures.

At the time when I had put the finishing touches to my M.Sc. in quantum chemistry for Pekka, his research group had acquired some new members. Leif Laaksonen and Dage Sundholm had already been working with the two-dimensional (2-D) numerical methods for solving Schrödinger and Hartree–Fock equations and presented two-dimensional fully numerical MC SCF calculations on H_2 and LiH with a calculated dipole moment of LiH. The 2-D method was also later very effective in the calculation of nuclear quadrupole moments, and the values of these calculated moments still retain their usefulness. The method was first presented at the International Congress of Quantum Chemistry in Uppsala 1982. In the satellite symposium "Relativistic Effects in Quantum Chemistry" at Åbo Akademi after the International Conference in Quantum Chemistry (ICQC), current relativistic research in chemistry was presented. Perhaps this symposium could be seen as Pekka's farewell to Åbo Akademi.

Time to "jump ship" (in Pekka's own words)

Pekka had started to feel that he should perhaps try for a full professorship, but no such positions were available in Turku. In Helsinki, however, the situation was different. From 1982 to 1984, Pekka had worked as an Acting Professor at the University of Helsinki, and in 1984, he was appointed Full Professor of Chemistry at the Chemistry Department, Laboratory for Swedish-speaking Students, at the University of Helsinki. At the time, this was the only professor's chair in Finland without a closer specification of the branch of chemistry involved. Consequently even a quantum chemist could apply, an impossibility if, for example, a Professorship in Analytical Chemistry would be involved. This also meant that the competition for the chair was intense, but Pekka emerged as the winner after the usual academic struggles. Thus, suddenly, Pekka was "my" professor, i.e., leader of the laboratory where I was working, and would continue to work together with Pekka for another 22 years. Evidently, Pekka had also "found" his place and was granted Emeritus status from this position starting from November 1, 2009.

The scientific highlights in Helsinki

In Helsinki, Pekka Pyykkö's interests started to turn toward the prediction of novel chemical species, although together with Desclaux, he had much earlier already predicted the existence of heavy metal hydrides like MH_4 and MH_6. Pekka had to wait about 15 years though, before examples of these hydrides were synthesized in Lester Andrew's group in Virginia. Better late than never! During the 1990s and the early second millennium then followed a number of very exciting discoveries. A totally new nitrogen species appeared in connection with studies of multiply bonded (mainly chain) species AB to ABCDE and turned out to be N_5^+. The wonderfully symmetric WAu_{12} molecule was predicted by Pekka and Nino Runeberg in 2002 and later also synthesized. Similarly, numerous other new heavy metal species were predicted, and many of them have already been synthesized.

Pekka also became very interested in closed-shell interactions due to a discussion with Professor Hubert Schmidbauer (TU Munich) in 1986 or 1987, who told Pekka about the very strong attraction between two closed-shell cations, an interaction that had no plausible explanation. Pekka was able, together with Yongfang Zhao, to show that such an interaction really was a manifestation of a very strong dispersion effect. In other words, Pekka had found the strongest Van der Waals bond hitherto. This research eventually led to the much cited (over 1000 times) article: "Strong closed-shell interactions in inorganic chemistry" [*Chem. Rev.* 97, 597–636 (1997)]. And the term aurophilicity also thereby gained acceptance in the chemical community. In Pekka's own words, these investigations turned out to be a real gold mine, and a very intensive cooperation also evolved between the German research group and Helsinki. During this period, 14 doctoral students from TU Munich visited the laboratory. By writing the review article, Pekka illustrated another piece of good advice for his students. The secret of success in science is a) to do some good work and b) to write the first leading review in *Chemical Review*. So, with the first review about relativistic effects and this article, Pekka had already succeeded twice!

The administrator and the organizer

Pekka Pyykkö is not a believer in the so-called "managing" strategy for doing science. That is, he rejects the modern idea that somebody wants to decide and totally control what scientists are doing. Instead, Pekka is a follower of the strategy: "Spontaneous activity in self-organizing groups". In my opinion, his results speak for themselves. Nonetheless, as a professor, Pekka of course could not avoid a fair amount of administrative duties and organizing activities in Helsinki. However, he has followed his strategy of allowing people to do what they think is important. In dealings with bureaucrats and political decision makers, on the other hand, he has been known to use devious methods… The Chemistry Department at the University of Helsinki was for a long time spread all over

town at various facilities, and all chemists wanted their own campus and new buildings. To show the need for new surroundings, Pekka during his period as Director of the Chemistry Department used to take every decision maker to the "horror" room at our laboratory. It was an old laboratory room where the paint flaked from the ceiling and one could trace every qualitative analysis ever made on the benches and tables. As a result, when these "important" people saw all this, they quickly acknowledged that new facilities were needed. And so the Chemistry Department finally moved to the new campus Kumpula in 1994, after almost 50 years of promises and waiting.

Pekka's talents as an organizer and coordinator of scientific activities are manifold, but one program has been particularly fruitful. This is the REHE ("Relativistic Effects in Heavy-Element Chemistry and Physics") program of the European Science Foundation. In this REHE program, Pekka as Chairman, together with Vice-Chairman Professor Bernd Hess (University of Erlangen), succeeded in creating a collaboration between different scientists across European borders and with links even to other continents, all under the title of the program.

The well-known "Winter Schools" every autumn at the Chemistry Department in Helsinki again illustrate the value Pekka places on spontaneous activity without unduly bureaucracy. The Winter Schools started in 1985 and have continued since, gathering young scientists from all over the world for a very informal, but intensively scientific week just before Christmas. Pekka finds it very important for young people to be able to show their work as soon as possible in an international atmosphere, also together with more experienced scientists. Discussions are vivid and the gloomy December evenings do not seem dull at all.

If Pekka's "farewell" gesture at Åbo Akademi was the satellite symposium to the 1982 International Congress of Quantum Chemistry, then being one of the organizers of the 13th International Congress of Quantum Chemistry in Helsinki 2009 perhaps may be seen as his farewell gesture to the University and Chemistry Department in Helsinki where he attained Emeritus Status from November 1, 2009, onward. The congress was a huge success with over 600 participants, many of which would not have traveled to Finland as tourists otherwise. But, who now may well return both for scientific and other reasons.

Current interests

As long as I remember, Pekka has been very fond of Linus Pauling's book "The Nature of the Chemical Bond". If I borrowed it for some reason from his book shelf, he almost always asked me to return the loan soon. Perhaps this mirrors Pekka's almost infinite interest in chemical bonding. If you look at his latest publications—by now over 300 titles—you will find that he, for example, has been compiling a list of single-, double- and triple-bond covalent radii throughout the Periodic System, in fact much in the spirit of Linus Pauling. No doubt Pekka's background in relativistic quantum chemistry has been a major influence here. And it is sobering to realize that one of the greatest discoveries of the 19th century, Mendeleyev's Periodic Table thus has been coupled to one of the greatest discoveries of the 20th century, Einstein's relativity. If I had the usual wishes one gets, if one happens to open a bottle on the beach with Genie in it, I would wish three times for Pekka to write the new 21st century book of "Chemical Bonding". Pekka has the perspective, and the skill and knowledge, to look deeply into the bonding even for the heaviest of elements, something which Linus Pauling could not have had in his time.

Some final words

I have written this account of Pekka Pyykkö as a long-time student, co-worker and colleague, not as someone expressing admiration in glorious and often not very accurate words. Therefore, I have not mentioned his honors, positions of trust, or memberships of various editorial boards. Neither have I dwelled upon Pekka's Finnish Academy Research Professorship 1995–2000 or his leadership of the Center of Excellence at the Chemical Department 2006–2009. These data can easily be found on Pekka's home page http://www.chem.helsinki.fi/~pyykko/ or in the Editorial for those who are interested. I hope I have been able to give to you a small understanding of a great man and his work. It has always been a privilege to work with Pekka. It was also a privilege to be asked to write this article for the "Pekka Pyykkö Festschrift".

And finally:

In an interview some years ago, the interviewer asked Pekka: "If you weren't a scientist, what would you be?" After having reflected upon his eventual success in languages—because he speaks a number of them—Pekka thoughtfully replies: "Or I could have been a plumber". (They had had a demanding plumbing problem at his house and, evidently, he solved it satisfactorily). I have no doubt that Pekka would have made an excellent plumber, had he so chosen. Please remember: a society that scorns plumbing because it is a low-level, menial task, and elevates science and philosophy, because they are high-level, intellectual tasks, will soon be in trouble. Both its pipes and its theories will leak… I am certain that Pekka's pipes would not have leaked. Nonetheless, I am very glad that Pekka chose quantum chemistry for his career, because I think he has been able to convert and teach more disciples in quantum chemistry than he would have as a plumber.

Henrik Konschin