Memorial Viewpoint for Joop van Lenthe

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Viewpoint

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Photo by Marga van Lenthe

Joop van Lenthe, our dear friend and colleague, passed away on November 15, 2019, after a 23-year-long struggle with multiple sclerosis. Johan Hendrik van Lenthe was born on September 26, 1951, in Velp, The Netherlands. He studied chemistry in Utrecht, where he graduated Cum Laude. A week after graduating he married Marga Bouts. Joop continued his Ph.D. studies in Utrecht under the supervision of Dr. Paul J. A. Ruttink and received his Ph.D. in 1979 on the topic of "MCSCF methods based upon the Generalized Brillouin Theorem − Theory and Applications". As a Dutch Ramsay Memorial Fellow, he worked in the groups of Prof. Gabriel Balint-Kurti in Bristol, U.K., and Vic R. Saunders in Daresbury, U.K.. He continued as a postdoctoral fellow in the Theoretical Chemistry Group in Utrecht, where he was promoted to "Universitair Docent" (Lecturer) and later to "Universitair Hoofddocent" (Senior Lecturer). He was a visiting professor with Prof. Peter Pulay in Arkansas, USA, and a visiting scientist at PNNL (WA, USA) with Dr. Robert J. Harrison. Joop was one of the original developers of GAMESS-UK and remained an active developer of this widely used electronic structure program. Since 2004 he led the Theoretical Chemistry Group in Utrecht until his retirement in June 2019. Joop contributed in various ways to the advancement of science. For example, he was involved in the purchasing of many generations of Dutch national computers for science and faithfully delivered quantum chemistry test jobs for the benchmarking of the candidate computing machines. Joop was a keen sailor and enjoyed vacationing on his boat on the Frisian waters. It was in Friesland as well, in hotel Ie-zicht overlooking the lake "Wijde Ee", that Joop's 60th birthday was celebrated with a Symposium entitled "From He_2 to proteins: Accurate Theoretical Methods in Chemistry".

Joop was a totally dedicated and brilliant scientist. His scientific activities resulted in over 140 well-cited scientific papers (selected publications are provided in refs 1−6), international recognition, and many diverse collaborations with fellow quantum chemists and experimental chemists. He supervised more than 20 Ph.D. students, including Ph.D. students in different fields of chemistry and pharmacology who wanted to use quantum chemistry in their research. Playing bridge with other members of the theoretical chemistry group was a prominent activity at lunch times. As a group leader, Joop was like a father-figure to his students. He was always available for discussions and willing to give advice on academic or personal topics. Dedication, kindness, and generosity were integral parts of his personality. He demonstrated great hospitality and support. R.B. fondly remembers his offer (in 1984) for her to become a guest member in the theoretical chemistry group in Utrecht, allowing her to work in one location instead of having to divide her time between two institutions. H.E. is grateful for introducing him to Joop's former postdoc advisor Gabriel Balint-Kurti, which led H.E. to pursue Ph.D. studies at the University of Bristol. G.C.G. vividly remembers meeting Joop at the 1987 American Conference on Theoretical chemistry. G.C.G. was a Ph.D. student in Eindhoven at that time and in serious need of additional guidance. With no questions asked, Joop took on the role of coadvisor and remained a friend and the go-to person for questions on electronic structure ever since. Joop was always up for collaboration with peers in any field of chemistry, and especially in organic, inorganic, and biochemistry, but also on pharmacology, and even earth sciences!

Joop was not only hospitable, jovial, social, and loyal, but he also had outspoken ideas and could be quite pertinacious. Any colleague who published questionable ideas or results in the field of nonorthogonal methods was contacted and—if feasible—the matter was discussed until agreement. As part of a rather free-spirited generation (he started his studies in the late 1960s) Joop was convinced that existing nondemocratic power structures had to be broken. As a result, he managed to institute that all

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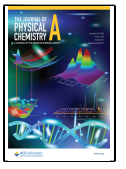

members of the group, including students, secretary, and technician, were also members of the group's Board. Did a new Ph.D. student have to be selected? Every Board member contributed to the decision. The meetings were sometimes quite lively but always ended in consensus. For the students, these meetings were great training opportunities. This system worked well until new national laws prevented the use of such democratic structures.

A major research theme was the development and (smart) implementation of new methods for performing ab initio calculations of molecular electronic structures. Joop's interests included the electron correlation problem, two-component relativity, the use of new computer architectures (parallelism), and the use and optimization of nonorthogonal orbitals in Valence Bond theory. In addition, factors that limit the accuracy and interpretability of first-principles calculations, such as basis set superposition error (BSSE), had his interest. His curiosity in nonorthogonal theories had always been "fun-driven": Joop wanted to have a program that could produce any imaginable wave function. In practice, it meant that Joop could investigate with his program TURTLE whether or not a particular chemical model is tenable. Also mentioned should be his work on the Direct-CI method with Vic Saunders, the continuous development of his Valence Bond program TURTLE with a number of his Ph.D. students, and the massively parallel GAMESS-UK version for performing large-scale ab initio calculations on biochemically relevant systems. Joop's involvement in the latter program started during his time with Vic Saunders; Joop was involved in the early stages of the GAMESS-UK development that led to the code becoming the flagship code of the Collaborative Computational Project 1 (CCP1). Within the theoretical chemistry group in Utrecht, both ATMOL and GAMESS-UK continued to play an important role. For some students, the ATMOL package would serve as a testing platform for new ideas and approaches because of its simpler code structure. Matured ideas would be implemented into GAMESS-UK for distribution to a wider audience.

Reviewing Joop's role in developments of both electronic structure codes, it is perhaps worth pausing to consider the origin of the GAMESS-UK code and just why it followed a quite different path to ATMOL. While the latter had played a leading role in CCP1, the absence of integral derivatives limited its application to many areas of chemistry, and there was no sign of that functionality being developed in ATMOL with Vic Saunders now focused on periodic systems and the development of the CRYSTAL code. The move to the GAMESS code stemmed from a visit in 1980 by Martyn Guest to visit Michel Dupuis, then a key player in the now defunct NRCC (National Resource for Computational Chemistry). With Michel's blessing, the UK version of GAMESS was born, with developments over time taking a quite different route to the US version of the code still under active development by Mark Gordon at Iowa State University. A period of intense development activity followed, with many of the optimizations undertaken in ATMOL—direct access data sets, free format directive-driven input, DIIS wave function convergence—introduced in short order. Joop rapidly bought into the major benefits afforded by access to analytic energy gradients. Many of the initial developments centered on enriching the range of available post-Hartree−Fock capabilities, with functionality originally developed within the ATMOL suite of programmes integrated in short order. Joop led in the provision of large-scale CI calculations of both ground and first few excited states through integration of the Direct-CI module, while the Daresbury Team focused on conventional CI treatments using the table-driven selection algorithms within the framework of MR-DCI calculations, allowing for the treatment of electronic spectra and related phenomena. Numerous developments followed thereafter with the Utrecht Group under Joop and the Daresbury Team collaborating throughout. We refer the reader to the extended account of these developments in the 2005 Molecular Physics paper, "*The GAMESS-UK electronic structure package: algorithms, developments and applications*".

A key feature of GAMESS-UK lay in the development of the parallel capabilities of the software. Prior to the introduction of the Global Array (GA) tools, Joop had been pivotal in the development of the first replicated data parallel version of the code, undertaken on the Intel iPSC/2 and iPSC-860 hypercubes at Daresbury. While many in the U.K. focused on the OCCAM-based Transputer initiative, the availability of a FORTRAN compiler with associated message passing software on the iPSC hypercubes enabled an initial parallel implementation of GAMESS-UK that rapidly led to an order of magnitude performance enhancement in traditional SCF geometry optimizations. This was a major achievement that heralded the arrival of parallel computing in molecular electronic structure calculations, with Joop featuring at the forefront of these and subsequent developments.

Joop remained focused throughout his collaborations with MG and the Daresbury Team on his perceived role of GAMESS-UK, namely, that it should provide a reliable, supported, and optimized framework for both the methods development and the productions activities of the Utrecht group. He had little or no interest in attempts to commercialize the code, even though these activities were primarily intended to develop funding to support the software.

As indicated above, Joop was an expert in using computers, as the following anecdote illustrates. Joop visited the University of Bristol in 1980 where a new mainframe computer had been installed. The staff of the computer center were puzzled as to why he logged in every night just after midnight. It turned out that he had programmed his job to restart every night at that time, something the staff had no idea as to how this could be done.

He was generous in freely distributing his computer codes. Joop was also a gifted and inspiring teacher. If a student could not grasp a concept, Joop would approach the point from a different and more easily understandable perspective. He had the ability to present challenging topics clearly, making them seem (deceptively) simple. An example of his unique style was a recurring exam question about the physical interpretation of the wave function. Joop was determined that this question would feature in every exam until such a time that all students would answer it correctly. Interestingly, the question was never removed as this bar was never met, even though he announced this question in his lectures and provided the answer (the wave function itself does not have a physical interpretation but the square of the wave function is a probability density).

Joop suffered from Multiple Sclerosis and other health-related issues for many years. His optimism and bravery in the face of his illness were awe-inspiring. With the unfailing and dedicated support of Marga, he found ways to continue to work and sail, refusing to let his illness get the better of him. He fought many battles to obtain the workplace adaptations he needed and in the process became an advocate for equal opportunities for people with disabilities. He continued throughout to come to work to

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give his lectures and mentor his students. Even when struggling to type he still tried to improve code, sometimes asking a Ph.D. student to correct the typos that he made. He would then offer the student a cup of (Gutenburg's) coffee or lunch as a gesture of appreciation. In 2014, he made an improvement in TURTLE, but somehow, the whole code stopped working. Z.R., who was back in Pakistan after completion of his Ph.D., was asked for help. After fixing the issue, as a joke, Z.R. asked Joop to send a cup of coffee (intercontinental). The next month, Joop arranged for Z.R. to attend a conference in Belgium and afterward visit Utrecht to have a cup of coffee with Joop. Such a kind person Joop was!!! Joop continued to travel by plane to scientific conferences and international collaborations. One particular incident stands out: he was staying at a hostel in Daresbury, U.K., and had arranged for the hire of a motorized wheelchair. The wheelchair broke down on the steep hill from the hostel to the laboratory and Joop was thrown into a ditch at the side of the road. He was helped up by passers-by and managed to use his cell phone to call for a replacement wheelchair. Typical for Joop, he was not fazed by such incidents and always insisted that improvements can be found.

Joop will always be remembered as a great scientist and an expert in the field of quantum chemistry and electronic structure method development, in particular in Valence Bond methods. Moreover, we will not forget his outspoken personality and especially his friendship.

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Notes

The authors declare no competing financial interest.

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