Obituary

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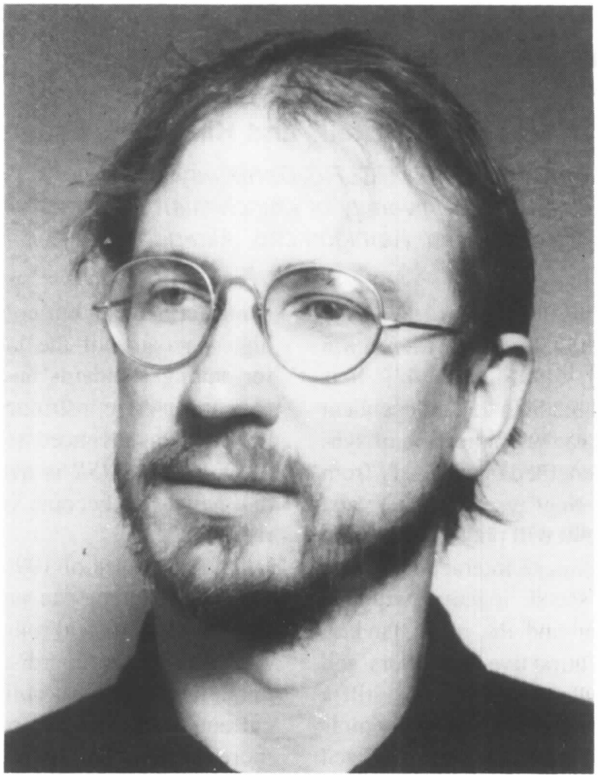

Theo Thole, 1950–1996

Theo died in hospital on 4 July 1996, after a fatal fall down the stairs the previous day. He devoted his life to science, in particular to the theory of core-level spectroscopy, and made major contributions to the understanding of the fundamental aspects of polarized synchrotron radiation studies. Theo will be remembered for his theoretical talent and for his successful efforts in stimulating experiments in magnetism, but most of all he will be remembered as a friend who was always ready to help.

Theo, born 1 April 1950 in Emmer-Compascuum in the Dutch province of Drenthe, was the third son in a family of five children. He studied chemistry at the University of Groningen, where, during his specialization in Physical Chemistry under Jan Kommandeur, he developed a computer program to predict global climate changes, a subject which has nowadays grown into a major research area. Theo and I were fellow students and he stood out because he was more proud of his ability to solve almost any integral equation than of his abilities in ice skating, which is the national sport in the northern part of the Netherlands. He never mastered the laws of physics which are so terribly vital in this sport, but I must admit he did much better in billiards. His knowledge in mathematics and programming must have impressed his supervisor, because after his study he was offered an appointment as mathematical advisor. This was exceptional, because when we started our study they promised us mountains of gold, but the economic recession of the 1970's changed all that and by the time we graduated it was practically impossible to find a decent job. One fellow victim from the 'lost generation' even kept a folder which contained over 100 rejection letters from job applications. Theo always refused to apply for jobs. He found such an act degrading, although he admitted that it would be acceptable to express an interest in a particular job on the back of a picture postcard, like Einstein apparently did. Piet van Duijnen from Theoretical Chemistry finally made him an offer that he could not resist and his passion for quantum mechanics made Theo decide to do a PhD on reaction-field Hamiltonians.

After the successful defence of his thesis in 1982, Theo spent half a year at the University of Amsterdam. When I mentioned to him that the Solid State group of George Sawatzky at Groningen could use a theorist to explain the absorption measurements on rare-earth metals that I had carried out at the ACO storage ring in Paris, Theo did not need much persuasion. The first reaction of George was: 'Do you really think that it is possible to get him. That guy is extremely clever!'. Fortunately we could get him, and since Theo always refused to apply for other jobs he stayed on as a postdoc at Groningen. For Theo, who was not at all interested in wealth, standing or management, this basic position with few responsibilities and commitments offered the ideal opportunity to devote his efforts to scientific

research. In this way he was able to put all his energy into his theoretical work.

The first few years were invested in implementing the atomic multiplet code of Bob Cowan, the group theoretical code of Phil Butler, and the Auger program of Akio Kotani into a general and versatile program capable of calculating core spectra including multiplet structure, hybridization and configuration interaction. The program became highly popular among scientists in the field to underpin their experimental results. For Theo, however, the program was first of all a tool-box to check his unconventional ideas about spectral analysis using angular momentum theory. In an era when both physicists and chemists were losing their grip on the atomic structure and multiplet theory established earlier in the century, Theo developed as a master in this subject by studying the works of Racah, Biedenharn and Judd. Group theory, an infinitely deep subject, was the main source of inspiration for his contributions to spectroscopy. He stood at the origin of magnetic X-ray dichroism, first by predicting a strong effect in the $3d$ absorption edges of rare-earth metals, and later by collaborating on the experimental verification of this effect.

Theo was always very eager to condense general knowledge into simple rules. The postulation of the sum rules for orbital and spin magnetic moments is among his most celebrated results. This has been considered as one of the most important discoveries in magnetism over the last decade, at a time when the separation of spin and orbital contributions was chased as the holy grail of magnetism. The continuous controversy over the sum rules and their applicability was much to Theo's delight; he never became tired of presenting convincing new arguments. After deriving the sum rules Theo took a keen interest in spectral moment analysis. Integrated intensities as supplied by the sum rules correspond to the zeroth moments of the spectral distribution. The spectral shape contains additional information in the form of higher moments that can be related to ground-state properties multiplied by final-state parameters.

Although Theo was a true believer in the power of mathematics, he also liked the intuitive approach. But he never confused the two. Together we made a systematic study on the branching ratio in X-ray absorption. Strong deviations from the statistical value for the spin-orbit split p to d absorption in transition metals and d to f absorption in rare-earth metals were not understood at that time. Using graphical methods Theo could show that the branching ratio was directly proportional to the spin-orbit coupling in the ground state. Hence, a sum rule was born, relating a ground-state property to integrated peak intensities. We had then still a long way to go before we could formulate any sum rules for magnetic X-ray dichroism. However, by studying the influence of the crystal field on the dichroic signal, we found a systematic dependence of integrated intensity on the spin-orbit splitting. Again by using diagrammatic techniques Theo was able to derive a simple relationship between the integrated signal and the orbital magnetic moment. This was soon followed by the derivation of the second sum rule for magnetic dichroism, which related the spin moment and the magnetic dipole term to the weighted difference of the spin-orbit split dichroic signal.

The observation of core-level spin polarization and magnetic dichroism in (angular dependent and resonant) photoemission has been one of the most extraordinary developments of recent years in synchrotron radiation research. These phenomena are due to the interaction between the core level and the polarized valence shell. Theo gave teeth to the theoretical analysis that was presented in a series of papers.

In his final years Theo also had a part-time appointment in the theory group of the ESRF and collaborated intensively with Massimo Altarelli, Paolo Carra and Michel van Veenendaal on a wide range of subjects, such as X-ray resonant Raman scattering, magnetic X-ray Compton scattering and anisotropic X-ray anomalous diffraction. Theo was further a frequent visitor to many other synchrotron radiation sites around the globe. Twice a year he came to Daresbury Laboratory for several weeks to offer his craftsmanship in the analysis of X-ray absorption and photoemission. He spent productive spells at Orsay, Brookhaven, Düsseldorf, Ames, Tokyo and Hiroshima, where many students benefited greatly from his didactic gifts.

Theo took great pleasure in cycling, such that his visits to relatives at distances within 100 km were made on bicycle. He enjoyed listening to Frank Zappa and watching Monty Python, with whom he shared a touch of witticism. He also liked to read novels by Nabokov, with whom he shared the sharpness of description. However, his greatest passion was always mathematics. His sharp analytical mind could solve almost any problem, as long as it was formulated in the right way. In order to come up with a possible answer, he often took a long walk for a few hours to think about the problem. Since he was a nightbird, these walks were usually after midnight and therefore often drew the attention of the local constable. Also renowned were his birthday parties; the amount of food and drinks that he provided could easily feed and quench a small army and lasted for a whole week. It was out of the question to discuss physics during his 'birthweek'.

In his short life span Theo did an impressive amount of work. He became an authority in magnetic X-ray dichroism. His wanderlust in the last ten years made him the exchange particle that brought together many groups in the field. He made physics fun and will be remembered not only for his scientific contributions but also for his enthusiasm, modesty and friendship. One of his friends, Johan, has made some memorial pages that can be found on the web at http://theochem.chem.rug.nl/~theo.

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