FOUNDATIONS ADVANCES

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Dieter Schwarzenbach (1936–2024)

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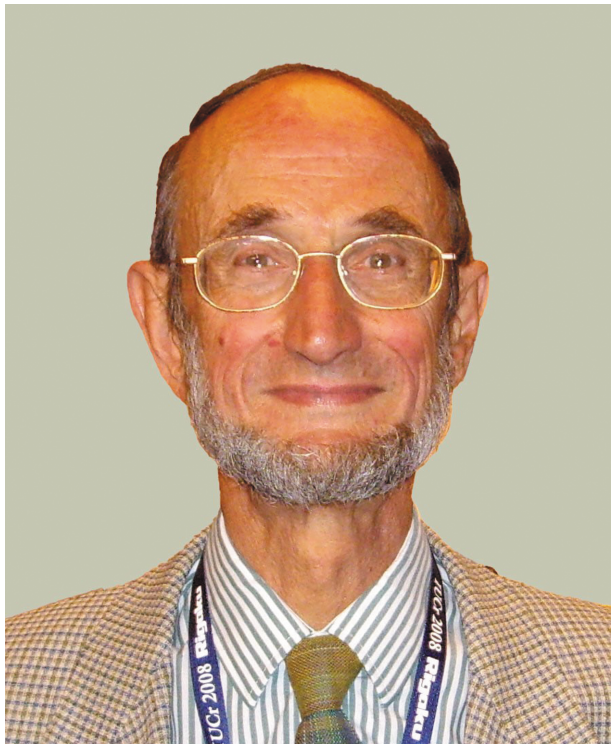
Dieter passed away at the hospital in Lausanne, Switzerland, after a long neurodegenerative decline. He leaves behind his wife, Vera, and his two children, Charlotte and Thomas.



I met Dieter in 1966 when I started my doctoral studies at the Institute of Crystallography at the ETH in Zurich. That was shortly before his departure for a postdoctoral internship in the USA. In 1969 he returned to Zurich, bringing with him the newly developed *X-ray System* of programs for the solution of crystal structures. I was very fortunate to take advantage of it: it allowed me to crack a difficult structure by direct methods and finalize my PhD thesis. Later, it was also Dieter who helped me to find the most suitable place for a postdoctoral position, in David Templeton's group in the Lawrence Berkeley laboratory.

The experience gained by Dieter in America, first in Pittsburgh in Professor George Allen Jeffrey's Department of Crystallography and then at UCLA in Professor Ken Trueblood's Laboratory, in addition to his PhD with Professor Fritz Laves' group at the ETH in Zurich, formed an excellent basis for a successful career in crystallography. Indeed, shortly after his return from the USA, in 1970 he was offered a position as a lecturer in the Science Faculty at the University of Lausanne for a basic course in crystallography. Three years later, he was offered the opportunity to create and lead the Institute of Crystallography at the same institution with the position of Extraordinary Professor, which was later upgraded to full Professor in 1978.

My stay in Berkeley was coming to an end when Dieter visited me in 1973 and invited me to complete his team in Lausanne. Thus, in 1974, I returned to Lausanne to pursue my career in crystallography as a lecturer in Dieter's lab.

Since its creation, the Institute of Crystallography has delivered lectures and practical courses in various fields of crystallography to students of the University of Lausanne (UNIL) and of the Federal School of Technology (EPFL). In particular, students of physics, chemistry, materials and earth sciences have followed the basic and advanced courses. Our common book (Schwarzenbach & Chapuis, 2006) resulted from our experiences in teaching crystallography.

In parallel, the research work of Dieter and his team developed in numerous directions of crystallography. Measuring electron density in crystalline structures using diffraction methods was an important part of Dieter's interests. Would precise electron densities measured by diffraction be able to reproduce certain physical quantities, such as electric field gradients (EFGs)? One of his most cited articles (Lewis *et al.*, 1982) concerned the charge densities and EFGs in corundum, α-Al_2O_3, where the capabilities and limits of diffraction methods were clearly demonstrated. Other important studies followed, including of the charge densities in cuprite, Cu_2O (Restori & Schwarzenbach, 1986), a paper published with his PhD student Renzo Restori in which the influences of the data-reduction processes, anisotropic displacements and the deformation models were explored. Other compounds like Li_3N, TiO_2, CoS_2 and NiS_2 were all part of an important programme of studies on charge densities.

During his career, Dieter developed some very fruitful collaborations with colleagues from nearby institutions. Hans-Beat Bürgi, head of the Laboratory of Crystallography in Bern, and Howard Flack from the University of Geneva were among them. The discovery of C_{60} resulted in many interesting studies, both in Bern and Lausanne. The development of the *Xtal* system of programs by Dieter's PhD student Eric Blanc contributed greatly to obtaining successful results. His *LSLS* ('Lausanne least-squares') program had some new capabilities regarding absorption, extinction corrections and twinning which led to the C_{60} paper by Bürgi *et al.* (1992). This fruitful collaboration on fullerenes resulted in four additional papers on various modifications and phases, improving models and obtaining more precise data on the orientational disorder and C—C bond distances.

Dieter and Howard Flack published an important series of well cited publications relating to some new theoretical developments in the methodologies of crystal diffraction. Both laboratories were involved in the software developments of the *XRAY* system and its successor, *Xtal*. About a dozen papers covering various topics from the use of least-squares restraints for origin fixing in polar space groups (Flack & Schwarzenbach, 1988) to the evaluation of transmission factors and their first derivatives with respect to crystal-shape parameters (Blanc *et al.*, 1991) were published. Perhaps the most tangible result of their collaboration was the establishment of the Subcommittee on Statistical Descriptors by the International Union of Crystallography (IUCr). A panel of international specialists in statistical methods in physics and crystallography joined efforts to establish a series of recommendations for the proper treatment of statistical errors in crystallographic research. Dieter was the Chair of the panel, which also included Howard as a member. Two reports, *Statistical descriptors in crystallography* parts I and II, resulted (Schwarzenbach *et al.*, 1989, 1995). They listed a series of 13 recommendations, the validities of which form the basis of the current statistical treatment of crystallographic data. It is owing to the second report that the commonly used term 'estimated standard deviations' (e.s.d.'s) was replaced by the more accurate term 'standard uncertainties' (s.u.'s).

While studying the impressive list of Dieter's scientific publications, close to 150, I was struck by the diversity of his interests, which covered a very large number of fields in crystallography. They extended from historical notices to mathematical crystallography, symmetry, diffraction theories and structure modeling, to cite only the most important topics. Dieter had an excellent memory and he always impressed his audience with his vast knowledge of crystallography.

The IUCr also benefited greatly from Dieter's expertise, as he served as a Co-editor for both *Acta Crystallographica* Section A (from 1992 to 2002) and Section B (from 1992 to 1999). He was then appointed as Section Editor for *Acta Crystallographica* Section A in 2002, a position he held to 2011, and as part of this role he was also an *ex officio* member of the Commission on Crystallographic Nomenclature.

Under Dieter's leadership, the Lausanne Institute of Crystallography attracted a large number of international visitors. This was facilitated by two other institutions in Lausanne: the Herbette Foundation from UNIL and the '3^e cycle' of physics (which would now be called a doctoral school) of the French-speaking part of Switzerland. Both institutions were able to support the visit of international lecturers for a few months. During that period, we could greatly benefit from the lectures of a very impressive panel of specialists, including Aloysio Janner, Ted Janssen, David Templeton, Pierre Toledano, Richard Welberry, Terry Willis, Hans Wondratschek and Akiji Yamamoto. The first version of Richard Welberry's book on X-ray diffuse scattering appeared in Lausanne as lecture notes on the same subject! It was also in Lausanne that Howard Flack developed the concept of his famous parameter during the visit of David Templeton and fruitful discussions on Rodger's η parameter.

Under Dieter's direction the Institute of Crystallography led to the creation of the very successful Swiss–Norwegian beamline (SNBL) at the ESRF in Grenoble. In the beginning, the essential problem for Dieter and Hans-Beat Bürgi (who was also interested in this facility) was not the financing of the beamline but rather finding first common objectives between the two participating countries and creating common visions to lead the project. It took a few years to solve all the administrative problems leading to the creation of the SNBL Foundation. Today the SNBL is a flourishing institution for the benefit of Swiss and Norwegian scientists.

Dieter was also admired by members of the Institute for his deep knowledge of the history of Switzerland. He could also cite entire poems from German and English literature, in particular extracts from Goethe's *Faust* and quotes from Shakespeare.

Dieter was a fine musician and very athletic. His career as a musician started as a student in 1957 as a violinist in the Zurich Academic Orchestra. He pursued his musical activities in Lausanne long after his retirement and participated actively in a few amateur orchestras, very often along with Vera, who is a respected violist. Dieter also rode his bicycle to the Institute of Crystallography and back home every day, a distance of about 12 km with a significant hill climb. He liked being accompanied by his son on bike rides and sometimes cycled for more than 170 km to tour around Lake Geneva. He was also a real mountaineer and cross-country skier. I had many opportunities to climb several Swiss summits with him, both in summer and winter. I remember very clearly our party of four starting a ski tour from Rothenboden over Zermatt for the ascent of the Pointe Dufour, the highest point in Switzerland (4634 m). By the end of the ascent, only the two crystallographers had managed to reach the summit.

Dieter also joined from the outset a basketball team called OURRS that brought together professors from UNIL and EPFL. Every Tuesday during term time we would meet for an hour of physical exercise and a basketball game. Dieter participated actively in the team activities until his physical abilities started to diminish. Unfortunately, Dieter passed away just a few days before the celebration of the 50th anniversary of the team.

Dieter was not only my mentor but also a dear friend, whom I will miss.

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