FOUNDATIONS ADVANCES

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Philip Coppens (1930–2017)

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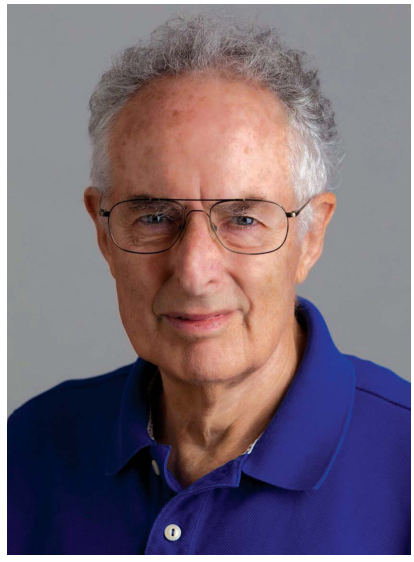
Professor Philip Coppens, born in 1930 in the Netherlands, died suddenly on 21 June 2017 while he was leaving his office at Buffalo University. This was a tremendous shock (both in scientific and personal terms) for the international scientific community, particularly materials science and crystallography. Since his first publications, which were focused on the potential impact of crystallography on the study of the quantum behavior of matter, he attracted young scientists from the whole world. He always emphasized the complementary capacities of his co-workers and helped them to develop their own successful careers. He was undoubtedly the 'father' of global developments in the study of the electronic behavior of matter (from simple systems to biological systems) using X-ray/neutron (X–N) scattering. Many young researchers who had recently enjoyed fascinating cooperations with Professor Coppens in the field of time-resolved crystallography, a prime area for future studies, were deeply dismayed to hear the sad news.



Philip Coppens started his research with Caroline MacGillavry in the area of crystal structures and photochemistry. His PhD (Amsterdam, 1960) was mainly carried out at the Weizmann Institute in Israel. He approached the study of the electronic behavior of condensed matter (at or out of equilibrium) through intense cooperation with Fred Hirshfeld and Gerhard Schmidt. One main result concerned the differentiation of the photo-induced behavior of two polymorphs of *p*-nitrophenol (at a time where lasers did not yet exist).

Just after his PhD, he was recruited by Walter Hamilton at Brookhaven National Laboratory (including stays at the Weizmann Institute and various places in Europe). His innovative work on X–N diffraction complementarity aided the study of the electronic behavior of solids. His paper in *Science* in 1967 [Coppens, P. (1967). *Science*, **158**, 1577–1579] showed the electron deformation density of *s*-triazine and created a worldwide research axis. He focused on the importance of mastering 'real' aspects of X-ray and neutron diffraction (such as absorption, extinction and thermal effects) for obtaining trustworthy electron density. The quality of his research led to his appointment as a

professor at Buffalo University, where he stayed thereafter with his family. Philip and Robert Stewart were the source of every group that developed research on charge, spin and momentum density across whole continents. In cooperation with Richard Weiss and Vedene Smith, he also brought about important triennial conferences such as the Gordon Reseach and Sagamore conferences.

His paper in *Science* attracted me, as it gave a concrete sense to molecular wavefunctions, and I joined his group with my family for my PhD at the end of 1972. Amazingly, I was asked to work on extinction (both for X-rays and neutrons) and to propose a workable model; he also asked me to optimize step-scanned signal *versus* noise data. This was very hard, but all members of the lab used to exchange ideas, in particular through weekly meetings. It was said that Philip first experienced time-resolved research, since he came to us every 15 minutes asking how we had been improving! The experience was unforgettable and the final gift was the determination of the deformation density in tetracyanoethylene (with F. K. Ross), revealing simple, double and triple bonds plus lone pairs: at that time, quantum computations were not possible for such a molecule.

Philip had a fantastic chemical intuition and always put emphasis on finding the potential complementary talents of his co-workers. His priority was to further our international scientific recognition – he never said 'I did', but always emphasized our work. This was extremely positive and opened up long-term international collaborations for us. Each of us could create personal groups and suggest young scientists who could interact with Philip. Another fundamental quality of Philip struck me concerning extinction: when the theoretical strategy was validated by referees, he proposed a simple scheme that would be easily transferable in refinement processes.

A fundamental scheme was proposed by Niels Hansen and Philip: the multipolar development of charge density, which has been used by all groups for nearly 40 years. With Guru Row, we proposed a complementary approach concerning the extension of radial functions, the application of which fits the Slater model for atomic orbitals. It also led to a first joint charge–spin density study with Tibor Koritzansky. The joint refinement of charge, spin and momentum densities is now a key issue in advanced crystallography (for the groups of Beatrice Gillon, Jean Michel Gillet and Claude Lecomte, and at Spring8, among others) and is leading to a promising project towards 'quantum crystallography'.

Another important approach was developed by Claude Lecomte's group, in parallel with Philip's group, and concerned the electronic behavior of proteins. A substantial database built on charge partitioning of molecular groups present in proteins was developed. Crystallography thus allowed this fundamental domain to be approached.

Philip also worked on structural evolution in phase transitions (*e.g.* the metal–insulator transition for TTF–TCNQ with Vaclav Petricek, involving incommensurate modeling) and charge-density evolution under an applied electric field. He also interacted strongly with Anatoly Volkov (from Siberia) and Tibor Koritzansky.

In 1997, Philip thought it was time to move to his 'childhood dream': photocrystallography. As usual, his intuition about which chemical compounds to study was correct. The first we tried was sodium nitroprusside (showing long-lived excited states), which was studied in the lab using laser flashes at low temperature. Then he used synchrotron sources, including at Brookhaven National Laboratory, with picosecond pulses, then the Argonne Advanced Photon Source. He welcomed many motivated young scientists from both Krystok Woszniak's and Claude Lecomte's groups, who became involved in fascinating new studies, such as those leading to the observation of the 0.28 Å contraction of Pt—Pt bonds in $Pt_2(P_2O_5H_2)_4^{4-}$ at 16 K for which the duration of the excited state was 50 µs. Then with Jason Benedict he developed studies of the time-dependent behavior of nanoparticles, again starting a new boundless area of solid-state science.

On 22 October 2016 Jason Benedict organized a retirement ceremony for Philip. It was an unforgettable day, where many collaborators came and enjoyed the strong long-term friendships that had started from their work with Philip.

Owing to his unique influence on developments in crystallography, Philip received many prizes, including the Aminoff Prize in 1996 and the Ewald Prize in 2005. He was President of the International Union of Crystallography (IUCr) from 1993 to 1996, a member of the IUCr Executive Committee from 1987 to 1999, and a member of the IUCr Commission on Charge, Spin and Momentum Densities from 1972 to 1981, the Commission on Neutron Diffraction from 1975 to 1978 and the Commission on Journals from 2002 to 2015. His book *X-ray Charge Densities and Chemical Bonding* (IUCr/Oxford University Press, 1997) summarized in a highly pedagogical way the key aspects of his contribution to crystallography.

Philip remains an eternal guide for us, and his spirit will continue to guide international scientists.