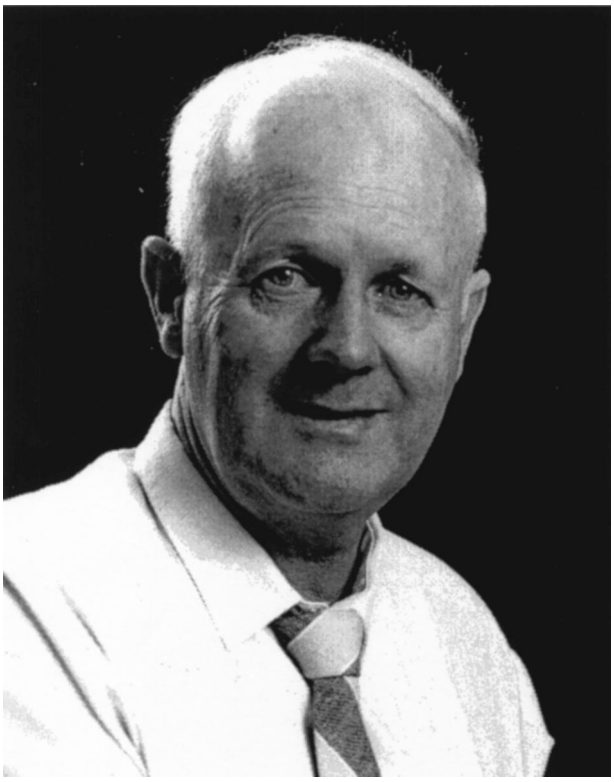
SHORT OBITUARY
John Charles Taylor, 1935–2002



John Charles Taylor, MSc(Syd), PhD(NSW), DSc(NSW) died suddenly while playing tennis in Sydney on 30 September 2002. John had spent the whole of his working life as a crystallographer using both X-ray and neutron diffraction methods. He authored or co-authored 99 fully refereed journal publications, 19 lightly or non-refereed publications, various conference papers and 4 seminar/workshop papers and 8 Internal (Lucas Heights) Divisional Publications. John also co-authored a book, ''A Rietveld Made Easy''.

John's start in crystallographic research was in ''Old Chemistry'' (now the Department of Pharmacy) at the University of Sydney. Under the supervision of H C Freeman, John collected data on the crystal structure of potassium bis-biureto-cuprate (II) tetrahydrate using a Metropolitan-Vickers ''Raymax'' X-ray generator with a demountable tube. The ''Raymax'' had arrived from England as a gift shortly after the appointment of R J W Le Fevre as Professor of Chemistry.

John had collected and visually estimated 929 diffracted intensities (another possible 331 were very weak and were not observed) and had manually corrected them for Lorentz, polarization and Tunell effects but not, at this stage, for absorption. John was determined to locate the hydrogen atoms in the anionic complex. Obviously he felt that his collected and visually estimated data was good. The next step truly displays his stubborn determination, patience and persistence. John disappeared to home for quite a few weeks and graphically calculated absorption factors (method of Joel, Vera and Garaycochea, Acta Cryst., Vol. 6, 1954) for all of his data. Subsequent cycles of Fourier and Least-Squares refinement (thanks to SILLIAC programs written by H C Freeman) led to the placement of all hydrogen atoms in the structure.

It must be stressed that Sydney University has a long history of X-ray analytical work going back to the early 1930s; D P Mellor and F P Dwyer read their paper regarding *The Crystal Structure of Indium* before the Royal Society of New South Wales, 6 July 1932. This was barely 20 years after the world's first X-ray crystal structure analysis. Mellor provided continuity in structure analysis. This short obituary is important for historical reasons as well as reflecting on the life of John Taylor and his early work (at Sydney University) of which not many people have knowledge. John's work at Sydney was commenced in the era *before computers in Australia* and was completed with the aid of the ''SILLIAC'', Australia's second and then best electronic digital computer.

These were the days when John and his co-worker John E W L Smith had mentors such as A McL (''Sandy'') Mathieson, Janis Fridrichsons, Barrie Dawson and A D (Dave) Wadsley. John was a quiet person who didn't seem to worry about membership of organizations such as the International Union of Crystallography and others and hence his pioneering work in crystallography is little known.

After completing his MSc, John transferred to the University of New South Wales using both X-ray and neutron diffraction techniques to determine the structures of ebeline lactone and uranium compounds. In August 1962, John met Mavis McKinnon who was to become his wife and typed his

https://doi.org/10.1154/1.1773072 Published online by Cambridge University Press

PhD thesis. John was awarded his PhD in 1963 for his thesis ''Crystal Structure Analysis by X-ray and Neutron Diffraction Methods''. In 1981, the University of NSW awarded John the Degree of Doctor of Science in recognition of his research excellence.

As a post-doctorate, he spent several years at Argonne National Laboratory co-publishing papers on neutron diffraction studies of uranium and thorium compounds with, among others, Mel Mueller.

John became interested in the Rietveld method after reading Hugo Rietveld's initial papers on quantification of mineral phases from X-ray powder diffraction, adapting the single crystal program (ORFLS) for profile analysis for his research. This work was the early beginnings of the software program SIROQUANT that allowed multi-phase quantitative analysis of a wide range of materials. That John developed the algorithms from first principles allowed him to incorporate some innovative features, such as the use of observed HKL files for analysis of materials that have a poorly crystalline or amorphous nature.

His research was leading edge although to his colleagues the apparent ease with which he succeeded in solving the most complex problems was daunting. This was due largely to his extraordinary high level of intellect. His work on coal minerals was a classic example. To quantify minerals in coal, it was usual to measure the pattern of a low temperature ash to remove organic matter. A problem with this approach is the alteration of some minerals such as pyrite and the reaction of sulfur with calcium-bearing phases. It was suggested to John that a direct analysis of the raw coal would overcome this problem. However a major obstacle was the presence of a high background at low 2-theta angles. John solved this problem ''in a few days'' by modelling the reflections based on an anthracene derivative. This enabled SIROQUANT to be applied directly to raw coals, providing not only a quantitative estimate of all the minerals but also a measure of the total organic matter present which, in turn, gave the total mineral matter content.

SIROQUANT has undergone considerable enhancements since those early days in association with Sietronics Pty Ltd, a Canberra-based scientific instrument company. Both CSIRO and Sietronics have developed the software to a stage where it is now one of the most popular programs for quantitative XRD sold throughout the world.

John was the classic individual researcher, best described as the quiet achiever, who shunned the tedium of budgets and management constraints but always delivered on his research. John was also an accomplished pianist and landscape painter of considerable merit. His painting commenced as a relaxation at the age of 40. He leaves a widow, Mavis, and two children, Phillip and Karen.

A full obituary will be printed in the Newsletter of the International Union of Crystallography.

Chris Kelaart and John E.W. Lambert-Smith

https://doi.org/10.1154/1.1773072 Published online by Cambridge University Press