


John William White (1937–2023)

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ABSTRACT

John William White FRACI FAIP FRS FAA CMG AO (1937–2023) was a pioneer in the application of neutron scattering to chemistry, one of the most influential advocates for neutron facilities globally, particularly in Australia, and was a friend and mentor to a great many neutron-scattering scientists working worldwide. This biographical memoir will demonstrate the enormous legacy that he leaves through his service to science by following his career from the University of Sydney to Oxford University—initially as a DPhil student, but subsequently as a fellow at St John's College—through to Director of the Institut Laue Langevin (ILL) neutron facility in Grenoble, France, before returning to Australia as Professor at the Australian National University in Canberra.

Keywords: Australian National University, inelastic, Institut Laue-Langevin, neutron scattering, Oxford University, quasielastic, reflectometry, small-angle scattering, synchrotron.

Introduction

John William White was born in Newcastle, Australia in 1937. After education to Master's level at the University of Sydney, he moved in 1959 to the Chemistry Department at Oxford University for his doctoral studies, followed by a University lectureship and Tutorial fellowship in St John's College, which he held until 1985. From 1975 to 1980 he was based in Grenoble, France, first as Associate Director, and then British Director, of the Institut Laue Langevin (ILL) neutron facility. In 1985 he returned to Australia as Professor of Physical and Theoretical Chemistry at the Australian National University (ANU) in Canberra, where he remained until his death in 2023 (having become Professor Emeritus in 2013).

In this memoir the authors (former postgraduate students separated in their commencement with John by almost thirty years) will describe how his realisation of the wide-ranging potential of neutron scattering for understanding molecular structure and dynamics influenced his whole academic career, and allowed him to leave an extensive legacy. This comprises the many researchers in academia and industry who as students and collaborators he introduced to the technique; in the innovative use of newly developed instrumentation which opened new areas of research; his extensive publications in the field and his support for building international facilities across the globe, and most particularly, construction of the Australian neutron source, OPAL.

Family and childhood

The son of George Alexander John White and Jean Florence White, John William was the eldest of three siblings. His sisters, Jean Elizabeth and Faith Wendy, became, respectively, a school teacher and a medical practitioner. The family had been early settlers in the Hunter Valley, and John's paternal grandfather and namesake was superintendent of police, in charge of the northeast division of New South Wales. John's father was an engineer, and the family indulged and nourished the boy's curiosity about science from an early age (Fig. 1). John recalled (J. White to the AAS, pers. comm. 1993) that one of his earliest memories was being interested in steam engines, and this would be an enduring passion. Around the age of ten, his father gave him the chemistry textbook *Inorganic and*

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Fig. 1. John White as a young boy in Newcastle, Australia. Photograph courtesy of the White family.

Theoretical Chemistry by F. Sherwood Taylor, which he kept by his bed. At the age of eleven, he set up his own laboratory room with a selection of chemicals and electrical equipment that included war surplus electronics; there are family photographs of John clutching wires and electric lamp bulbs. The chemical collection was added to by his grandmother, Mrs Lillian White, who even purchased dangerous materials at his request from a local chemist, such as yellow phosphorus, sodium, and concentrated acids. By the age of twelve, he knew a great deal about the chemicals mentioned in the book and the processes used to make them. John remembered at one time managing to suck up some mercuric salt into his mouth and having to eat egg yolk to avoid being poisoned. His family seems to have been remarkably tolerant of such accidents, including when John conducted experiments using a ‘furnace’ he built in the garden.

In his personal memoirs (J. White to the AAS, pers. comm. 1993), John recalls that he was greatly influenced by his headmaster in junior school (Cardiff Public School, 1942–1948), Mr J. Petfield, and subsequently in secondary school (Newcastle Boys High School, 1949–53) by his excellent masters in mathematics, physics and chemistry, including Mr J. Simpson and Mr W. Storer, who encouraged a great deal of extra-curricular science. Classes at Newcastle High School were small, the school highly selective, and the teachers enthusiastic and committed. The emphasis was on

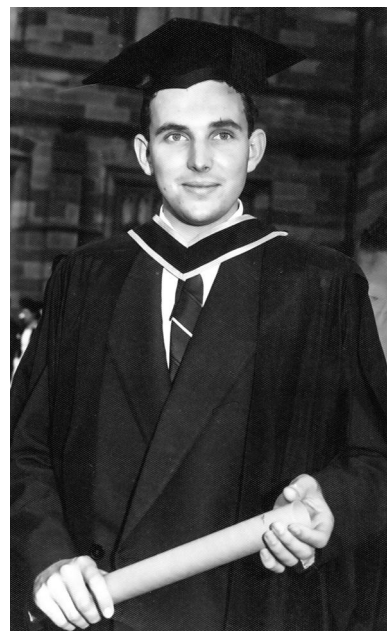


Fig. 2. John graduates from the University of Sydney. Photograph courtesy of the White family.

small group practical physics and chemistry with experiments carried out in pairs, and insistence on carefully prepared notebooks. It is hard to imagine a better education and family background for a future experimental scientist.

‘My aim was to learn about it and put it into action’

Encouraged by his schoolteachers, parents and grandparents, John’s continuing interests in experimental science resulted in his joining the University of Sydney in 1953 at the young age of 16, eventually specialising in chemistry, although geology had also featured strongly (Ailsa White, pers. comm. 2025). His curiosity was further motivated by his tutor and honours research supervisor Lawrie Lyons (FAA 1971; White 2016). His Master’s degree included measurement of photoconductivity on anthracene systems to elucidate its electronic structure (Lyons and White 1960). In his personal memoirs, John remarks that during this time, ‘I was considerably influenced by the fact that people seemed very committed to their science and worked all sorts of hours of the day and night. It was quite common at Sydney in the late 1950s to work until midnight and then go home in group cars. It was pleasant and convivial’ (J. White to the AAS, pers. comm. 1993) (Fig. 2).

Lawrie Lyons encouraged him to go overseas to obtain a doctorate, and John won an 1851 Great Exhibition scholarship to go to the Physical Chemistry Laboratory (PCL) at Oxford in 1959. There he studied for a doctorate with (Sir) Rex Richards (FRS 1959), and built a double resonance spectrometer to exploit the Nuclear Overhauser Effect

(Richards and White 1962a, 1962b, 1963, 1964a, 1964b, 1965); the latter refers to the coupling of electron spins and nuclear spins in a magnetic field such that a nuclear magnetic resonance (nmr) signal is emitted when the electron spin resonance (esr) transitions are stimulated. Two high-field instruments were available with permanent magnets, one with X-band (30 mm) and the other Q-band (7 mm) esr signals. This started a long-term interest in the time-scale of molecular relaxation processes. In an interview (Anonymous 1985), John remarked of nmr: 'My aim was to learn about it and put it into action'. At the University of Sydney John had lived a bachelor existence enabling him to concentrate on his research, and the same happened in Oxford where he was quickly elected to a fellowship at Lincoln College in 1961; the latter provided for all his creature comforts and enabled him to throw himself fully into the work of the Richards group. Indeed, he recalled of the time: 'Everything was provided from a point of food and service and all I had to think about was the science which I was most keen on. I can remember at that time being quite puzzled by the behaviour of some of my colleagues at dinner in Lincoln College—they were extremely subdued, it was the time of the Cuban missile crisis in 1962 and, regrettably in a certain sense, I was so wrapped up in the work I was doing that I was unaware of the great danger that the world was facing at that time.' On completion of his DPhil in 1963, he was appointed to a Fellowship at St John's College, Oxford, due to Harold 'Tommy' Thompson, (FRS 1946), who pioneered the study of molecular vibrations with infra-red spectroscopy after World War 2. When Tommy was given a personal professorial chair in 1965, John took over all his tutorial duties in the College.

While unmarried, residing in St John's, John was also given the duties of Junior Dean, assisting Donald Russell, the Senior Dean, in charge of student life and discipline. The College remained responsible for the many members under the age of 21. Later, he was appointed to be one of the two University Proctors, and served in this role during the student unrest in 1968 (Ron Ghosh, pers. comm. 2025). These positions lasted for two years, and John later commented that since the Proctors were present at most University management meetings, this limit avoided misuse of any privileged information.

The Oxford Chemistry curriculum included a fourth year of research contributing to the first degree, and during his years at St John's College, John White taught physical, organic and inorganic chemistry to the whole cohort of students; many of them undertook their final year research projects with him providing a continual source of research mentees. Topics given to his students included esr studies in non-aqueous solvents (liquid ammonia), and conductivity in organic compounds. In the early part of the Fellowship, John continued collaborative work with Rex Richards, but his interest 'to learn about and put into action' another technique for chemistry, namely neutron scattering, intervened.

An aside on neutron scattering

Soon after the discovery of the neutron by James Chadwick (FRS 1927; Chadwick 1932), interest rose among experimental scientists in using this neutral particle as a probe to investigate crystalline and molecular structure and dynamics. Nuclear reactors were built for this purpose in the USA and in Europe, including in the United Kingdom, and instrumentation developed for them. In 1959 when John White arrived in Oxford, there were two high-flux reactors situated close by at the Atomic Energy Research Establishment (AERE) in Harwell. Named DIDO and PLUTO, these fed neutron beams to a number of instruments as well as being used for isotopic applications. The physics of the neutron-nucleus interaction in a scattering experiment means there are two cross sections for each isotopically distinct species in the sample governing the neutron scattering intensity, one coherent and one incoherent; in the former, the interference in the scattered beam contains information about crystalline or molecular structure, as well as correlated motions, while in the latter such structural information is mostly lost but information on dynamics is retained. Of practical importance for chemistry is the difference in cross sections between the two most common isotopes for hydrogen, protium (more generally referred to simply as hydrogen), and its heavier counterpart, deuterium.

In the 1950s and 1960s, the coherent scattering was most typically exploited by physicists using diffractometers to obtain crystal structure; triple axis spectrometers were also designed to determine phonon (lattice) or magnon (magnetic spin wave) energy dispersion curves in crystalline materials. The incoherent scattering cross section could be exploited to determine neutron energy changes where energy is gained or lost to molecular vibrations in analogy to infra red and Raman spectroscopy, but was little used.

A chance meeting and a practical chemical application of neutron scattering

Roger Elliott [FRS 1976], the physics tutor at St John's, invited the Harwell scientist Peter Egelstaff to dine at the College High Table. Peter was head of the group working on reactor moderators, measuring diffusive motions in water and liquid metals using neutron scattering; the Chudley-Elliott model of jump diffusion could be applied to these moderators (Chudley and Elliott 1961). Peter had already built a time of flight (TOF) spectrometer on the DIDO reactor using two high-speed phased disc-choppers on the 4H5 beam tube. In a TOF spectrometer, the energy of the beam is selected using mechanical choppers to allow passage of neutrons with a chosen velocity and then the energy of the scattered neutrons is measured by their flight times from the sample to detectors (hence the name). While the inelastic spectrum carries spectroscopic information on molecular vibrations

and rotations, the so-called quasi-elastic spectrum—seen as broadening of the incident energy spectrum—arises from diffusive or Brownian molecular motion. Peter was very keen to establish links with the academic community outside physics to expand the use of the instrument; joining the conversation, and with his background in nmr and relaxation phenomena, John quickly realised that the difference in the incoherent scattering cross section of hydrogen and deuterium opened up the possibility of molecular labelling to study problems in chemistry.

John proceeded to recruit one of the authors (JSH)—a recent physics graduate in Oxford—as his first DPhil student in 1964 to work on neutron scattering from clathrate inclusion compounds. The idea was to deuterate the clathrate cages and thereby highlight the vibrations of the caged hydrogenous molecules. In his personal records, John notes how ‘we set to work to produce highly deuterated quinol (hydroquinone) using the hydrogenation bombs in the Dyson Perrins laboratory next door to the PCL. To her credit, Julia was able to produce 10 g of the material and initial proof of principle neutron scattering results were obtained shortly after’ (Downes and others 1966). Experiments also started on another type of inclusion compound (zeolites) (Egelstaff and others 1968) and thus another important line of John’s research began. Although focused initially on using neutron scattering from the available TOF spectrometers to examine chemical spectroscopy and diffusive motions of molecules, it will be shown that John later expanded his interests to high resolution quasi-elastic scattering, small angle scattering, and reflectometry as these techniques became available in subsequent years, mainly at the Institut Laue Langevin in Grenoble (from 1973), the Intense Pulsed Neutron Source at Argonne National Laboratory in the United States, as well as the ISIS pulsed neutron source in Rutherford Appleton Laboratory (RAL), adjacent to Harwell (from 1985).

Marriage and family

As a fellow of St John’s, John was able to continue a privileged existence; however, this was about to change. Ailsa Vise obtained her BSc (Hons) and her MSc at the University of Queensland in microbiology before going to Oxford on a Walter and Eliza Hall Travelling Scholarship, where she obtained a second Master’s—an Oxford BPhil. Her research career was, however, curtailed by meeting John. Ailsa relates that soon after she arrived in Oxford in 1964, she was introduced through a mutual friend to (Sir) John Houghton (a Fellow in Physics at Jesus College, who went on to chair the Intergovernmental Panel on Climate Change and head the United Kingdom Met Office); he suggested that she should meet another Australian. John Houghton facilitated the introduction at the annual Research Scientists Christian Fellowship conference in London shortly afterwards, where John gave one of the research papers. John (apparently intentionally) stood



Fig. 3. The marriage of John White and Ailsa Vise in 1966. Photograph courtesy of the White family.

in the lunch queue behind Ailsa and they chatted. Followed up by occasional dates, and regularly meeting at St Ebbe’s church in Oxford on Sundays, ‘the rest is history’ she says. John Houghton, who continued to be a firm friend of John’s, some years later became the godfather of Sarah, their eldest daughter.

In 1966 John had arranged to spend a sabbatical term at the University of Queensland, and after two years in Oxford, Ailsa’s parents facilitated her return trip to Brisbane where they were married, before returning to Oxford later that year (Fig. 3). John left his college rooms and, after some brief stays in student housing, the couple moved into a house in Benson Place north of the University Parks. Over the next few years the White family grew to six members. Sarah was born in 1968, Catherine in 1970, David in 1973, and Rachel in 1974. Ailsa’s time was much occupied by her young family and she was only able to return to a career much later when the family moved to Canberra; there she worked with the Science Group under various guises in the Industry and Education Departments of the Australian Government, but also found time to co-author a paper with John on the discovery of the neutron as a legacy of the Curie family’s work (White and White 2011).

The Oxford years—exploiting neutron scattering and influencing the community

Following the first exploratory neutron scattering experiments, John began recruiting a group of research students focused on using inelastic scattering and diffraction to solve problems in the dynamics and structure of molecular crystals, liquids, polymers and the adsorbed state. At the outset, the importance of isotopic contrast was demonstrated and used to show how simplification and analysis of the scattering law from molecular liquids could be achieved experimentally (Aldred and others 1967; Longster and White 1968,

1969; White 1969, 1971a; Aldred and others 1972). While much of the work exploited the difference in neutron scattering cross sections between hydrogen and deuterium, differences with other nuclei, for example fluorine, were employed. Where possible, experiments were supported by model calculations, or by molecular dynamics simulations. An underlying aim was often to test model intermolecular potentials and so provide the basis for calculating macroscopic properties. At the same time as building his research group, John himself became a frequent visitor at neutron sources wherever there was a chance of exploring the applications of neutron scattering; indeed, throughout his career, instrumentation was as important to him as experimental design. For example, he recruited George Stirling as a post-doctoral fellow in the PCL, who quickly became involved in building a second time of flight apparatus (6H) on the DIDO reactor at Harwell (Bunce and others 1970). 6H became a workhorse spectrometer for British chemists in the 1960s and early 1970s until the ILL spectrometers IN5 and IN10 came on line. While in Oxford, John was also a regular visitor to the Herald reactor at Aldermaston with its own instrumentation and, when he joined the staff at the ILL in 1975, he became involved in the design of the second time of flight spectrometer IN6 (Carlile and others 1976).

In a seminar presented at his 75th birthday symposium (White 2012) John described how, from 1964 onwards, his group of young chemists explored the many possibilities to exploit neutron scattering and differences in scattering cross section to investigate structure and dynamics in molecular materials. His initial forays into the field had been prompted by the opportunities offered by the absence of the selection rules in neutron scattering that govern infra-red and Raman spectroscopy; by the replacement of specific hydrogenous groups or whole molecules for their deuterated analogues, new information could be achieved (Aldred and others 1967). Beside the use of isotopic substitution, many opportunities arose simply from the difference in neutron cross sections across the periodic table which are not related to atomic number as in optical or X-ray spectroscopy, useful examples being the differences between chlorine and fluorine atomic cross sections (Reynolds and others 1974). Another way of identifying vibrational modes in the often complex spectra of molecules was also developed based not on chemical labelling, but on comparisons of the infra-red spectra and neutron inelastic scattering. The relative intensity of the neutron scattering peaks is related to those in the optical spectra via the amplitude of the hydrogen vibrations using extensive force field and normal co-ordinate calculations (Reynolds and White 1969). These included molecular (Reynolds and others 1974) and polymeric crystals (Twisleton and others 1982), where the experimental data were compared to force-field calculations.

While physicists attempted to improve instrument resolution, at the expense of reduced intensity and longer measurement times, chemists adapted their materials for study

through the use of atomic substitution. Through contacts made during a visit to the PCL in Oxford in the late 1960s, the Imperial Chemical Industries (ICI) Runcorn (Plastics and Polymers) research manager Duncan Davies and John initiated a decades-long collaboration between the company and the White group, and John became an ICI consultant; coincidentally John had held an ICI Fellowship at Oxford University during his DPhil. A very early study using the TOF spectrometers at Harwell reported on the atomic motions in acetic acid and methanol (Aldred and others 1967). By making selective substitution of deuterium and fluorine, for the hydrogens in the CH₃ and OH groups of these molecules, the separate contributions to the quantised and diffusive motions of each were analysed. Vibrational assignments were made and, in the quasi-elastic region, broadening was analysed by determining an effective molecular diffusion coefficient, and by comparing this with values from bulk-phase studies. Particular attention was devoted to the question of the extent to which intramolecular hindered rotation contributed to the quasi-elastic scattering. Frank Longster, a staff member at Runcorn, was eventually seconded to the PCL, later followed by Huw Thomas. With the donation of crystalline material from ICI and oriented fibres from DuPont, the phonon dispersion curve for longitudinal lattice vibrations perpendicular to the chain axes in hexagonal polytetrafluoroethylene was determined and the crystalline elastic constant perpendicular to the chains calculated (Twisleton and White 1972a, 1972b). Despite this promising debut, after his 1972 publication John Twisleton's name does not appear again among the White publications until 1982 (Twisleton and others 1982); in this publication, the dispersion curves for a large fully deuterated polyethylene sample with single crystal texture from John King (North-Western University) are reported with data having been obtained on the triple axis spectrometer TAS II at AEK Risø.

It would be fair to say that John's group was a major contributor to the modern understanding of the dynamics of crystalline polymers. In a series of papers, John was the first to show how deuterium substitution, and the 'contrast' arising in inelastic scattering from very different vibrational amplitudes in a molecule, could be used to assign the spectra of polymers (Longster and White 1968, 1969; Twisleton and White 1972a, 1972b; White 1972a) and molecular crystals (Reynolds and White 1969, 1971b; Pawley and others 1971), in addition to adsorbed species (White 1972b) and organometallic complexes (White and Wright 1970a, 1970b, 1971). For the latter, the addition of a beryllium filter analyser to the PLUTO TAS extended the range of inelastic scattering measurements into the mid infrared range, allowing studies of torsional modes and weak optical modes involving hydrogen invisible to optical spectra. These studies, supported by calculations of the neutron scattering cross-sections (for example Reynolds and White 1969), allowed the incoherent scattering to be calculated and made possible much of the subsequent work in 'chemical' molecular spectroscopy with neutrons.

These studies extended the work on molecular crystals to an extremely anisotropic case and provided the first experimental values for inter-chain elastic constants (in polytetrafluorethylene and polyethylene) (Twisleton and White 1972a, 1972b) allowing a comparison with theoretical and bulk modulus values, and thus an insight into inhomogeneous strain phenomena. Detailed studies of a range of molecular crystals, such as the chlorobenzenes, were among the first to be assigned densities of phonon states (Reynolds and White 1969), including intramolecular vibrations compared with theoretical predictions, and have their phonon dispersion curves recorded (Reynolds and others 1974), much thanks to 4H5. Stuart Pawley from the University of Edinburgh generously made available the programs he developed initially to calculate the dynamics of crystalline naphthalene; the value of Pawley's pairwise additive interatomic potentials as a basis for the intermolecular potential was shown to have wide applicability. Fortunately, a large class of organic crystals that are held together by van der Waals forces crystallise with centrosymmetric unit cells and are compatible with these programs; the program could not be used for systems like simple urea, with interesting directional hydrogen-bonding, but which is non-centrosymmetric with the librational and translational modes having mixed character with complex eigenvectors. Philip Reynolds was a 1969 final year undergraduate student of John's, and later PhD student in Risø Denmark where Jorgen Kjems had constructed an adapted TAS spectrometer with a multi-detector, MARX, that was well adapted to molecular crystals; he and Twisleton evaluated and theoretically simulated some of the much earlier scattering data. By this time, Twisleton had long left chemistry and entered the Anglican ministry, but John and John were glad to meet up again after fifty years in July 2023 in the UK. Philip would rejoin John at the Australian National University twenty four years later, after an extensive detour via inorganic quantum mechanics and polarised neutron diffraction. Contemporaneous papers by others in the White group provided the only extensive phonon dispersion curve measurements made on large polymer single crystals until much later on. In these papers the first transverse acoustic phonons for polymers were observed and comparisons made with calculated dispersion surfaces. This work on phonons in three dimensionally ordered crystalline polyethylene—the sample preparation being achieved by stretching the latter close to the polymer's melting point—and single crystals of deuteropolyoxymethylene, remains the only measurements of their kind, and were possible only by bringing to bear diverse skills including lattice dynamics calculations, chemical synthesis, and neutron spectroscopic expertise to reveal details of the crystalline polymer dynamics (Anderson and others 1982; Twisleton and others 1982). One of the DPhil. students of this work, Robert Anderson, later became an expert on astro-labes and Director of the British Museum.

An associated general theme in John's work was to test the applicability of model intermolecular potentials and

simulation methods for modelling condensed matter, using neutron spectroscopy. As a consequence, studies of the dynamics of molecular crystals were amongst the first to record the full phonon dispersion curves from such single crystals. This work also set limits to the effects of anharmonicity and many body forces in some representative pseudo-harmonic systems (for example Reynolds and others 1972a, 1972b, 1974).

Tests of the atom-atom approximation were pushed further by studies of the crystal dynamics in molecules like 1:4 hexadiyne (Batley and others 1977, 1982; Cockbain and others 1982), where the smeared atomic positions of hydrogens and strong bond-bond interactions strain the validity of this approach; this work represents one of the first reports on neutron tunnelling spectroscopy where they compared the temperature dependence of the splitting with existing theories. The rotational tunnelling excitations observed for this system, their pressure and temperature dependence, along with the very different temperature dependence of tunnelling for adsorbed and intercalated molecules, posed interesting theoretical problems. Subsequent experiments (Batley and others 1982; Cockbain and others 1982) extended insights into the crystal potential and the transition from quantum to stochastic behaviour of a particle in a modulated simple potential. As the higher resolution capabilities of quasi-elastic scattering though greater flux and novel experimental design at the ILL became available, the potential for observing rotational tunnelling transitions began to excite the community. The motion of methyl groups is a classical example of tunnelling; through its threefold symmetry, a methyl group sits in a potential well with three minima. In classical mechanics, in order to rotate between these positions, the molecule needs to obtain enough energy to rotate over the barrier. In quantum mechanics there is a non-zero probability that the wave functions overlap one another, in other words, tunnel through the barrier leading to a splitting of the energy levels associated with the three different positions. At low enough temperatures, when only the lowest levels are occupied, this splitting becomes a series of sharp spectral lines, rather than the continuum of quasielastic broadening seen at higher temperatures.

Starting at Oxford, and extending through his time at ILL and ANU, John developed a longstanding interest in the extent to which adsorption, either at a free surface or through intercalation, modifies molecular dynamics and structure. White's diffraction and inelastic scattering measurements on adsorbed monolayer structure and dynamics were individually either the first or amongst the first to use neutrons in this area (Hunter and others 1971; White 1972c; Marlow and others 1977). Studies of the wetting of graphite by monolayer methane (Bomchil and others 1978, 1980, 1981; Newbery and others 1978) revealed a wealth of two dimensional commensurate-incommensurate phenomena, and led to the first observation of rotational tunnelling spectra (Newbery and others 1978; Smalley and others 1981) from adsorbed

molecules. Accurate tests of adsorption potential models were made using these data. In another set of paradigm experiments, the non-wetting behaviour of ammonia, which is isoelectronic with methane, on graphite was studied. This was the only example where direct measurements of the molecular organisation associated with the Type III BET isotherm had been explored (Bomchil and others 1979a, 1979b, 1979c, 1979d). The studies on both methane and ammonia elicited interest in Europe, the United States, and Canada using Molecular Dynamics methods to simulate physisorbed phases. The general insight, that molecular films at a surface may be quite highly structured, but at the same time very mobile, emerged for both clay-water and graphite systems; this seeming paradox being explained by the presence of a high concentration of defects, in the first few layers, promoting fluidity.

Two series of papers illustrate the way in which physisorption and intercalation modify molecular dynamics. In the series on adsorption of methane and ammonia by basal plane graphite, not only was the first rotational tunnelling for an adsorbed molecule (methane) observed, but the major differences in molecular structure and dynamics (reflected in the adsorption isotherms) were characterised. A similar detailed study defined the situation for intercalated hydrogen and methane, the latter in conjunction with extensive computer simulation, the first of which was conducted on, at that time, the newly available CRAY at Daresbury by his D.Phil. student, Frans Trouw (Trouw and White 1988a, 1988b). This was the first step in attempting to simulate porous structures such as zeolites and clays. Demonstration of the ease with which the molecular motions in a zeolite cage could be observed was the subject of one of John's early papers using neutrons (Egelstaff and others 1968).

John grappled with the effect of surfaces on more complex fluids such as water and ionic solutions; he was the first to show the weak extent of structuring on water diffusion at the silicate-water interface and extended those studies to lamellar liquid crystals, and swollen model membranes where the weak anisotropy of diffusion—on the neutron scattering distance and time scales—was first demonstrated. At the height of the polywater enthusiasm for 'frozen water' at surfaces, it was shown that within 1–2 nm of a silicate surface, water diffusion approached its bulk value (Olejnik and others 1970; Olejnik and White 1972), a result subsequently confirmed at single surfaces. This study gave rise to a line of work on the dynamics of model membranes and biological materials (Hayter and others 1974a, 1974b; White 1975a, 1975b; Hecht and White 1976), which showed how surprisingly isotropic water diffusion is at many interfaces. These experiments also showed the need for a deeper experimental understanding of adsorbed molecules at the gas–solid interface (for example Bomchil and others 1979a, 1979b, 1979c, 1979d), and of the dynamics of diffusion in ionic solutions at molecular resolution (for example Brown and others 1988).

John's work on binary and ternary intercalation compounds followed these ideas, on a quantitative basis, using

both molecular dynamics computer simulation and experimental work with X-rays and neutrons. A high-resolution X-ray diffractometer for variable temperature studies was later constructed for this programme at the Research School of Chemistry (RSC) at the Australian National University (ANU). The group was amongst the first to see the effects of two-dimensional domain incommensurate ordering in intercalates (Beaufils and others 1981; Jackson and White 1987; Naylor and White 1987; White and others 1988). A simple physical model for the alkali metal intercalates and associated molecular dynamics simulations (White and Wielopolski 1987, 1988a, 1988b, 1990) were not only the first of their kind, but also provided new insight into the unusual two dimensional fluid states in these and related systems. Simulation also provided an explanation of the unusual isotherms for gas sorption by intercalates and, in combination with inelastic scattering, allowed model adsorption potentials to be selected (Trouw and White 1988a, 1988b, 1988c, 1988d).

During the ILL years, and the early 1980s back in Oxford, neutron diffraction was used to determine the organisation of surface layers such as from the wetting of graphite by monolayer methane which revealed two dimensional commensurate-incommensurate phenomena and led to the first observation of rotational tunnelling spectra from adsorbed molecules (Newbery and others 1978; Smalley and others 1981). Over subsequent years, studies of a number of both hydrogen, ammonia, and methane intercalates were published, where neutron diffraction provided the organisation of adsorbed molecular layers while high resolution inelastic scattering and rotational tunnelling data tested the models for the adsorption potential (Stead and others 1988; Kellogg and others 1990; Carlile and others 1992). A spectacular example is where, in work with Colin Carlile at ISIS published years later in 1997, the swelling of the lattice of caesium intercalated graphite by hydrogen was shown to have a clear correlation with the changes in the tunnelling lines (Carlile and others 1997). Colin Carlile later recalled in 2023, 'John was an enthusiast who did not allow lesser mortals, bureaucratically-minded people in authority over him, to get in his way. Over all the years that I knew him I never heard him raise his voice once. He had natural authority.'

John White and the ILL years

Reading John's early papers from the 1960s and 1970s, the excitement about the potential of neutron scattering to reveal information on molecular dynamics is evident, as well as the variety of systems that could be studied; superposed was frustration arising from the existing limitations of neutron intensity, and therefore energy and angular resolution. In the UK these problems, combined with the limitations of available beam time arising from the increasing size of the neutron user community, were creating pressure for construction of a dedicated high flux beam reactor. By 1972

these plans were well advanced, but France and Germany were already building the high flux reactor at Institut Laue Langevin in Grenoble. In 1973, when the UK formally joined the European Economic Community, the rational decision was made for the UK to buy into these efforts and become the third partner at the ILL. During this time John was increasingly filling a leadership role in the UK's neutron scattering community, including serving as neutron beam co-ordinator at AERE Harwell between 1973 and 1974. To help him with this work and his post as Vice-President of St John's, Harwell recruited Janet Wallace as his secretary. She followed John to the ILL where she remained as the British Director's secretary for the next twenty seven years.

The original structure of the bipartite French-German ILL was for a German Director with a French Associate Director, thus compensating the Germans for the considerable advantages of ILL being built on French soil and subject to French law. When the UK joined, this structure had to change and the agreement was made for British and German scientists to alternate as Director and Associate Director, with the French providing a second Associate Director. The first British Director, Mick Lomer was seconded from Harwell, serving from 1973 to 1974.

Along with the whole UK neutron scattering community, John quickly became a regular visitor to ILL, exploring the

opportunities opening up as a steady stream of instruments came on line from 1973 onwards. The high neutron flux was being exploited along with innovative experimental design to optimise resolution in both space and in energy. John recounted at his 75th birthday symposium (White 2012) that he was involved in the first neutron spin echo measurement with Feri Mezei at the ILL in March 1974. Experiments were conducted on a sample of Teflon, which was expected to show a transition in dynamics at sub-ambient temperature. Regrettably, the experiment was unsuccessful, but John was able to display the copious laboratory notes nonetheless that he had generated of the attempt to the audience.

It was a surprisingly young John White who was appointed British Associate Director in April 1975 until 1977, and then Director until March 1980 (Jacrot 2006). John transported his young family to Grenoble where they set up home in La Tronche, a small village adjoining the city (Fig. 4). This house remained in the possession of the Whites after they returned to Oxford, and became a pied-à-terre for subsequent visiting neutron scatterers, some of the British Directors at ILL punctuated with occasional family visits (largely spent rescuing the garden, according to Ailsa). John appointed Bob Thomas to run his research team in absentia in Oxford, and also set up an independent surface science group in the CEA-Grenoble research centre laboratory

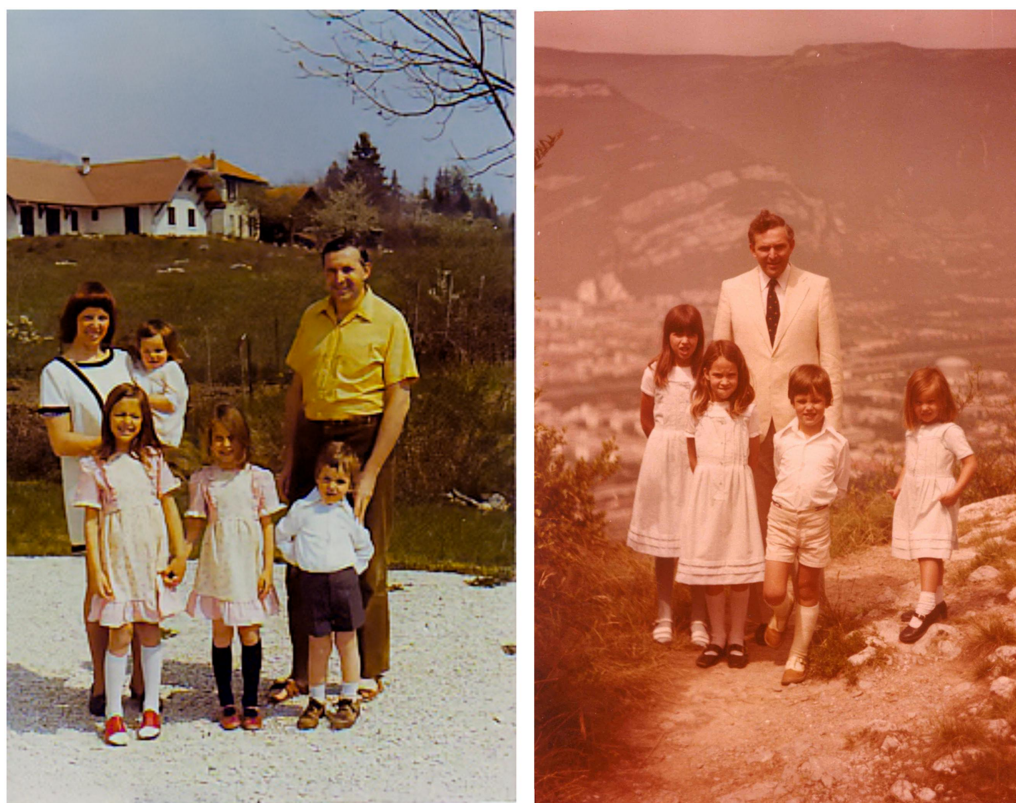


Fig. 4. The White family (left) at home in Montbonnot and (right) at the Bastille. Photographs courtesy of the White family.

adjacent to ILL, mostly to avoid setting up competition with other ILL groups.

The mix of neutron scatterers from the three member countries offered an opportunity to observe the different scientific cultures in practice. John recorded an anecdote about this in conversation with the previous French Director of the ILL, Bernard Jacrot. John and Andrew Miller had obtained some very nice small angle diffraction patterns from the D11 instrument from a biological molecule, collagen, which possesses a large-scale crystalline structure (White and others 1976). Bernard greatly admired the data, but asked whether John or his colleagues had calculated what the pattern would look like prior to experimenting. After John admitted that they had not done so, Bernard indicated that this approach was quite typical—the British never do, the Germans always do and, we, the French believe we should but do not.

The plans drawn up originally by the first two partners for the ILL included many new features compared to existing reactors (Jacrot 2006). It was one of the first reactors designed exclusively to produce neutron beams (not mainly isotopes). The reactor has a swimming pool design with a highly enriched small uranium core surrounded by heavy water. This acts as both a coolant for the 57 MW energy produced, and as a reflector to help maintain the chain reaction. The whole assembly is immersed in the light water swimming pool.

When John took up his post as Associate Director in 1975, the reactor had been running since August 1971 and the first batch of instruments were beginning to make their mark in the published literature (Fig. 5). In 1976 some thirty ILL scientists attended a scattering meeting in Gatlinburg, presenting results from the unique new ILL instruments;

this led to a wave of instruments being constructed, especially in the United States. Pressure on available beam time was building up in response to this success; however, it was already becoming clear that some of the first batch of instruments were suboptimal, and that there were exciting opportunities for new instruments. The reactor itself would need updates, there was potential for adding another cold source, thus increasing the availability of long wavelength neutron experiments, while increased computing power, both for running instruments and for data analysis, was required.

It would be fair to say that John's involvement was a major stimulus to novel instrument design and their application to biological areas during his Directorship. At the inception of the ILL, John Kendrew had foreseen the potential for crystallography of biological systems using neutrons, and pushed for Grenoble as a location of the laboratory. In 1975 the European Molecular Biology Organisation set up an outstation at the ILL, with Andrew Miller as its first director. New methods of structure analysis with neutron polarisation analysis and high resolution spectroscopy were developed. In the former, John and his group, especially John Hayter, developed a technique relying on the polarisation of neutron spins employing magnetic resonance, where they observed the spin-dependent diffraction of slow neutrons by differentially polarised nuclei in single crystals of lanthanum magnesium nitrate (Hayter and others 1974c; Leslie and others 1980). The power of proton spin polarisation contrast—first demonstrated by Hayter and White in 1974—necessitated simultaneous high magnetic fields, ultra-low temperature and microwave radiation; consequently, this labelling technique was only to be realised for



Fig. 5. The ILL triumvirate: John as British Associate director with Rudolf Mössbauer, German director (centre) and French Associate director, Bernard Dreyfus (right) circa 1976. Photograph courtesy of ILL.

biological structure determination more than twenty years later (Stuhrmann 2023).

The initial contract between the three countries lasted up until 1982 and the most urgent question was whether this could be extended. Discussions were already underway on other improvements and innovations described as a ‘deuxième souffle’ or ‘second wind’. John was quickly plunged into these discussions and, while he was Director from 1977 to 1980, he was the main contact between the ILL scientists and engineers, the users, and the funding agencies of the three governments. The programme became a reality in 1979, with approximately 110 million French francs for a programme of new instruments including dedicated computers, reactor renewal, and a staff increase of between 10 and 15% all negotiated between the Institut’s three member countries of France, West Germany, and the United Kingdom. The agreement to fund the ‘deuxième souffle’ was approved by the three associates in April 1979, and was implemented over the next seven years; however, John was back in Oxford and then in Canberra watching from the sidelines. There is no doubt that the deuxième souffle and subsequent renewal programmes kept the ILL at the cutting edge of neutron scattering science, and allowed funding for the reactor to be renewed over a much longer lifetime than was originally envisaged. The inter-governmental agreement on the life of the institute was successfully extended in 1981 with no other changes, and in 2023 the 50th anniversary of the ILL was celebrated.

Australia beckons

In 1980 John returned with his family to Oxford and to his fellowship at St John’s College. The group he had left in Bob Thomas’ care in 1974 had completed their doctorates and moved on to other things, and Bob Thomas himself had been appointed to an Oxford lectureship and was thus setting up his own group. John’s bibliography shows a marked dip in research productivity in the early 1980s. This evidently did not arise from any lack of enthusiasm given his subsequent highly productive years at the Australian National University (ANU), but most likely from a temporary dip in the ready supply of research students. John had not been teaching undergraduates for a number of years and it took some time to rebuild that pipeline. John’s five-year return to the United Kingdom included meeting Queen Elizabeth II when John was awarded the Companion of the Order of St Michael and St George (CMG) in 1981, and his curating of the Royal Society’s 50th anniversary “conversaciones” of Chadwick’s discovery of the neutron in 1982 in London (Fig. 6). In the introduction to the exhibit, John eloquently stated: ‘There is a dark side to the neutron, leading to the bomb and nuclear weapons. There is a neutral side, that associated with neutron beams and pure science aspects and there is a positive side in applications of the neutron to power generation, isotope production and medical treatment.’ (Ailsa White, pers. comm. 2025).

John had received occasional offers to consider moving from Oxford but, as Ailsa reports, such a move required very careful consideration. The invitation in 1985 to apply for the Chair of Physical and Theoretical Chemistry in the Research School of Chemistry within the Institute of Advanced Studies at the ANU in Canberra ticked many boxes. There was \$1 million on offer for research and, with the four children now aged between 10 and 16, there were no serious educational or career issues. Ailsa says the future beckoned in a new and exciting way, and they eventually made the decision to leave. John would succeed Professor David Craig (FRS, FAA) under whom he had previously studied at the University of Sydney in the 1950s (Anonymous, 1985). The School had been founded by Craig and Professor A. J. Birch (FAA) eighteen years earlier and its creation was a bid to attract top Australian chemists to return from overseas to conduct research in their own country. It was perhaps an appropriate new base for John given the motto of the ANU: *Naturam Primum Cognoscere Rerum* or, ‘first to learn the nature of things’. John White’s new Solid state molecular science group sought to apply ‘modern physical methods such as high-resolution neutron and X-ray scattering, magnetic resonance and computer simulation ... to study novel states of matter’ (Fig. 7). All of his research interests would benefit from neutron and X-ray complementarity but, to exploit such opportunities, access to state-of-the-art facilities were required and, if such facilities did not yet exist, this would need to be resolved.

John’s advocacy for Australia’s own neutron and synchrotron beam facilities

Australia’s research reactor, HIFAR, located at the Australian Nuclear Science and Technology Organisation (ANSTO) at Lucas Heights would have been very familiar to John as it was a copy of the DIDO reactor at Harwell. It had been operating for twenty seven years when John returned to Australia and although it had been unquestionably successful in the fields of hard condensed matter, it was an aging facility with no cold source and falling behind internationally including in isotope production. A continual push for improved facilities had led to a series of enquiries, reports and recommendations commencing in 1985, the year of John’s return (Elcombe 2017). That same year John became a fellow of both the Royal Australian Chemical Institute and the Australian Institute of Physics. It would soon become apparent that the experience gained as ILL Director and the international nature of neutron scattering would be well-utilised to shape the future direction of Australian scientific policy. In 1988 he joined the Council of the Federation of Australian Scientific and Technological Societies (now, Science and Technology Australia) and, the following year, became President of the Society of Crystallographers in Australia. In all these roles, he would bring to bear his exceptional knowledge to advocate for

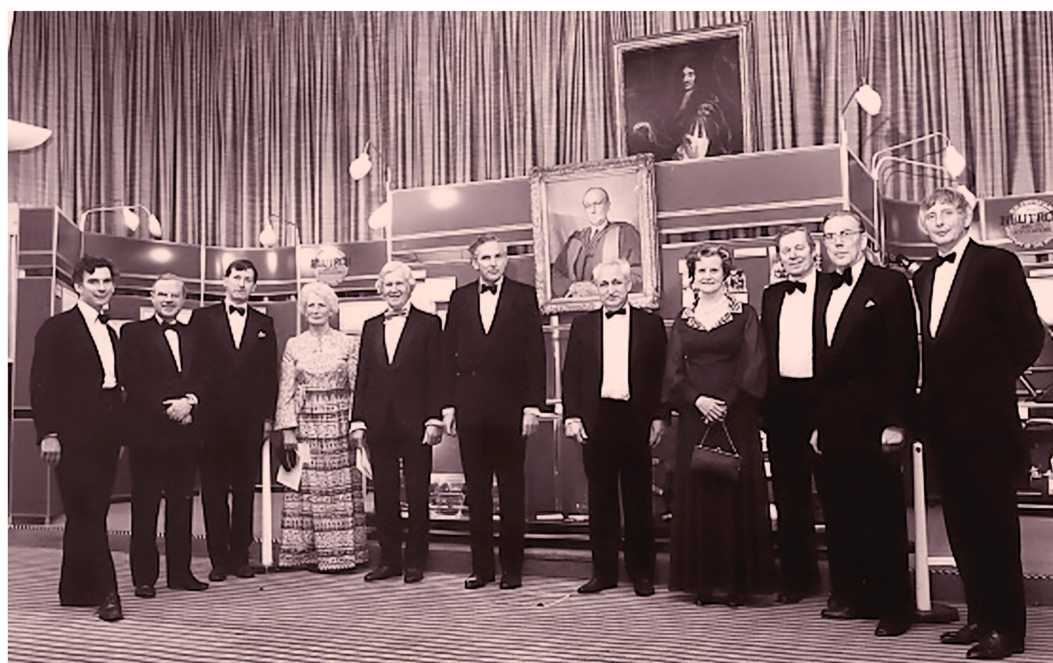


Fig. 6. (Caption on next page)

Fig. 6. Returning to the United Kingdom. (Top) John is awarded the CMG at Buckingham Palace in 1981 and (Bottom) at the Royal Society's 50th anniversary exhibit of Chadwick's discovery of the neutron in 1982 at the Wellcome Hall of the Royal Society, London. John White is pictured to the left of the painting of Chadwick Others included P. Schofield, C. G. Windsor and F. J. Stubbs (Harwell UKAEA), J. R. Askew (AEE Winfrith UKAEA), D. J. Lees (Culham Laboratory UKAEA), B. E. Fender (ILL), H. Wroe and J. B. Forsyth (Rutherford Appleton Laboratory, SERC), Mary Catterall, (MRC Unit, Hammersmith Hospital) and A. Morton (Science Museum London). Photographs courtesy of the White family.

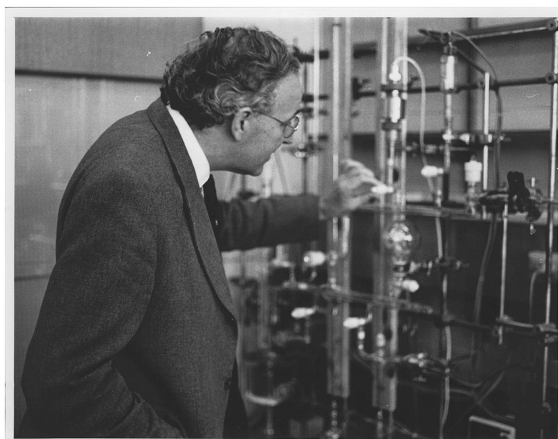
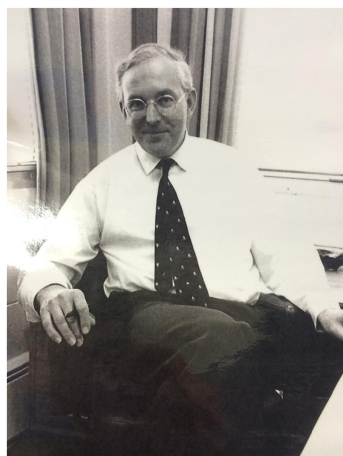


Fig. 7. John in various guises at the Research School of Chemistry. Top left, in his office at the RSC; (top, right) the extended White group surrounding the Phase I 'Bragg Rotor' millisecond reflectometer in 2001 (l. to r.) Sally Jansen, Anna Cunningham, Trevor Dowling, Philip Reynolds, David King, Gordon Lockhart, Mark Henderson, Hana Robson Marsden, John White and Suzy Cunningham. (bottom, left) John manipulating a valve on a vacuum line and (bottom, right) 3 PhD graduations in one day in April 1998 (l. to r.) Wilfred Fullagar, Karen Edler, John White and EPG. Photographs courtesy of (top, left and right) the White family, (bottom left, photographer Warwick Green) the ANU archives and (bottom, right) Wilfred Fullagar.

the potential of large-scale facilities in chemistry, physics, and biology.

In 1989, John along with Peter Colman (FAA 1989; FRS 2014), Ian Grey, Edward (Ted) Maslen (FAA 1995) and Chairman, Hans Freeman (FAA 1984), published *Requirement for Australian Research Access to 'Big Science' Facilities* from the Australian National Committee on Crystallography (NCCr) within the Australian Academy of Science (Colman and others 1989); the report addressed not only access to intense neutron

beams, but also synchrotron radiation sources. It noted that 'the cost of such facilities and the lack of a sufficiently large user base will probably preclude their construction in Australia in the foreseeable future.' Indeed, despite being a resolute optimist, John confessed in 1985 (ANU Reporter, 1985) that the possibility of Australia having a new neutron scattering facility was remote. The Committee concluded that, while there was a strong case for the purchase of a beamline at an overseas synchrotron radiation facility, there was also a strong, though less urgent,

case for substantial Australian involvement in an overseas neutron beam facility due to the obsolescence of HIFAR in the absence of substantial refurbishment and upgrading.

This position was strengthened the following year in the 1990 *Small Country—Big Science* report to the Prime Minister of Australia from the Australian Science and Technology Council (ASTEC) based on the working party convened by Don Nicklin that again included John, along with Colman, Freeman, and joined by ASTEC Secretary and Chairman respectively William John McGregor Tegart and Raymond Leslie Martin (FAA 1971; Nicklin and others 1990). It was concluded that the HIFAR facilities were no longer suitable for many types of neutron beam research and limited by the relatively low neutron flux. Furthermore, with an increasing number of scientists having to do research overseas, this need would soon become acute. The report concluded that an upgrade or replacement of HIFAR was needed before 2000.

The report recommended the taking of associate scientific membership of the ILL contributing 1.5% towards its annual operating budget, establishing an Australian beamline at the Photon Factory in Tsukuba in Japan, as well as Australia's participation in high energy physics at CERN. All funding would be provided to the Minister for Industry, Technology and Commerce, and coordinated by an advisory committee to take responsibility for policy, proposal review and funding decisions; ANSTO would take administrative responsibility and \$350,000 would be provided for travel and living expenses for Australian scientists through the Australian Research Council.

John, Dudley Creagh, Steven Wilkins (CSIRO), Hans Freeman (University of Sydney), and John Boldeman (ANSTO) worked on the development of the Australian National Beamline Facility at the Photon Factory at KEK in Tsukuba. The instrument, known as The BigDiff, commenced construction in 1991 and represented Australia's first formal foray into the exciting world of synchrotron science (Barnea and others 1989, 1992). The monochromator and incident beamline optics were designed and built by Dudley Creagh and Fred Johnson at the Australian Defence Force Academy (ADFA) in Canberra, while the diffractometer section of the instrument was designed and built at the CSIRO Division of Materials Science and Technology, under engineer, Sandy Janky, before being transported to Japan and installed on Beamline 20B. John not only chaired the programme committee for beamline access, but also, in his role as Chair of the National Committee for Crystallography, advocated for greater utilisation of synchrotron facilities for Australia. With its official opening in 1993, the beamline enabled X-ray diffraction, reflectometry, X-ray absorption fine structure and phase contrast imaging to be performed (Anonymous 2013) with resident beamline scientists, David Cookson and Garry Foran. With the establishment of the Australian Synchrotron Research Programme (ASRP), access would subsequently expand from the Photon Factory to beamlines at the Advanced Photon Source at Argonne National Laboratory and the Taiwan Photon Source

at the National Synchrotron Radiation Research Center; in addition, funding was also made available for a feasibility study for a domestic facility. The knowledge and expertise gained provided an important training ground for Australian synchrotron science and formed the basis for the case to build the Australian Synchrotron, which subsequently commenced operation in 2007 (Anonymous, 2025).

The availability of travel funding not only greatly benefited the new generation of 'suitcase scientists', but also provided critical opportunities to stay abreast of international developments in source and instrumentation design that would later be so essential for their subsequent construction at the OPAL facility. In parallel, John led the charge to build the AUSANS SANS instrument at HIFAR which ultimately had to be built outside the reactor containment building, and also pushed strongly for the development of a neutron reflectometer, to complement the X-ray facilities at the ANU. However, both techniques suffered from the lack of cold source at HIFAR. John's contribution to strongly advocate for large scale facilities, and Australian access to them, would continue following his election as fellow to the Australian Academy of Science (AAS) in 1991, and as Chairman of the Australian National Committee on Crystallography in 1992. The 1992 ASTEC report 'Major National Research Facilities' recommended that a program of continual review and investment in major national research facilities be undertaken immediately; in turn, the Government commissioned an independent Research Reactor Review (RRR) in the latter half of 1992.

John's further contributions would be apparent through both the AAS Submission to the 1993 McKinnon Review *Future Activity* on the Lifetime and Replacement of the Lucas Heights Reactor, HIFAR (Anonymous 1993) and within the 1994 NCCr Working Party on Australia's Future Needs for Synchrotron Radiation (Anonymous 1994). The resulting McKinnon Report, published in August 1993, recommended that HIFAR continue to operate, \$2 million per year be provided for scientists to access overseas facilities and the decision on the construction of a new reactor to be based primarily on the benefits to the national interest and science; however, the decision was to be delayed for five years (until 1998) (McKinnon and others 1993). In the meantime, to make matters more pressing, the Nuclear Safety Bureau advised that it would subject HIFAR to a safety assessment against contemporary research reactor standards which would require upgrading of safety systems by 2003, unless the reactor was to be permanently shut down within an acceptably short period from that date.

In 1992 an agreement was reached with the Rutherford Appleton Laboratory (RAL) in the United Kingdom that would allow Australians to apply for beam time at the ISIS neutron spallation source; ANSTO paid the fee for six years with a further extension obtained through a five-year grant (Elcombe, 2017). On top of this were further travel funds, not only for neutron, but also synchrotron, from the Access to Major Research Facilities Program. As part of the

agreement a scientist would be temporarily based at the RAL as in-kind support and to learn reflectometry; this scientist is now Director of the Australian Synchrotron, Michael James. Through John's advocacy, not only was access to ISIS organised, but so was planning and partial funding from Australia of the SURF neutron reflectometer based there.

While the success of Australia's neutron scattering programme through international access and demonstrated utilisation, only partly determined the outcome, finally, in September 1997, a decision was made by the Australian Government to fund ANSTO for the construction of a replacement research reactor on the existing Lucas Heights site. Initially known as the Replacement Research Reactor, it would be a state-of-the-art pool-type design, have a maximum power of 20 MW, would use low enriched uranium fuel, and once commissioned, the existing 10 MW HIFAR research reactor would be shut down. While the journey was not yet complete, Australia would emerge with a robust neutron scattering programme championed in no small measure by John White. John was a member of the Beam Instruments Advisory Group (2000–4), as well as first a member of (2004–11) and subsequently chair (2008–11) of ANSTO's Bragg Institute (later the Australian Centre for Neutron Scattering) Advisory Committee. The OPAL research reactor would commence operations in 2006, and it would be here that one of the authors (EPG) would build the SANS instrument known as QUOKKA. John had already initiated the Australian small-angle scattering meeting series in 1999 which would subsequently later be organised by ANSTO and AINSE. But, as AINSE president between 2005 and 2006, John proposed that research fellowships be reintroduced to seed new neutron-scattering groups in universities and enhance long-term, excellent, research output from the new instruments at OPAL with a clear intention that, at the end of their fellowship, they would be in a strong position to be employed at their university. John also played a key role in gaining funding for the National Deuterium Facility at ANSTO, which would provide so many opportunities for neutron scattering in the subsequent years.

Developing a domestic X-ray scattering infrastructure

Centred on an GX-13 rotating anode X-ray generator from Marconi-Elliott and a linear detector, machined at the RSC to the drawings of André Gabriel at the European Molecular Biology Laboratory in Grenoble, John immediately proceeded to develop small-angle X-ray scattering facilities. Much of the credit for this goes to Thomas Zemb, who came to ANU on sabbatical from CEA in Saclay. Coaxed to Canberra with a generous research budget and the help of two technicians, he was given the formidable task of building from scratch a Huxley-Holmes-based SAXS instrument as well as a reflectometer in eighteen months. If that were not enough, he would also participate in similar activities at the Photon Factory in Japan. John advised Thomas that he should not

be concerned about his frequent absences to the ILL or Argonne National Laboratory, as the RSC would soon have a fax machine. While Thomas ordered and assembled the detector electronics, Dean Gilkes built the detector positional control system, Stephen Henderson programmed the instrument based on software from John Hayter, but the fact that the instrument worked as reliably as it did over the following years owes much to the excellent technical skills of Trevor Dowling and later, David King (Fig. 8).

John noted in the RSC Annual Report of 1986 that 'since the rotating anode and the ordered detector are the best now available on the market, improvements have been introduced in the optics and the collimation achieving what is actually the most intense and smallest-angular-aperture beam produced with a laboratory-size anode.' Rat tail collagen, with its associated scattering peaks, is a common calibrant for SAXS instruments; however, since this was an Australian instrument, and with a larger source too, collagen from kangaroo tail was deemed more appropriate! Studies of clays, microemulsions and polymers were successfully conducted in the last days of 1986 and, while there were undoubtedly challenges with reliability early on, the instrument proved to be a workhorse for much research (and many PhD theses) over the following years, both at the RSC and a steady stream of external researchers, many of whom would have their first taste of SAXS. In just a few years, John would team up with Dudley Creagh at the Australian Defence Force Academy (ADFA) at the University of New South Wales to commence design for an X-ray reflectometer; this involved the conversion of the GX-13 to a GX-18 by putting a spare, air-cooled, electron gun in the unused port on the anode housing and enabling a downward beam trajectory unlike the SAXS camera's horizontal beam requirement (T. Dowling, pers. comm.). While growing capability locally, John would also be simultaneously championing the case for neutron and synchrotron science at the national level.



Fig. 8. John pictured with the SAXS instrument on the GX-13 in 2008. Photograph courtesy of the White family.

Maintaining research activities in parallel with management at the RSC

John's interest in intercalation continued on his arrival at ANU, but he also expanded into other areas, including the structure of buckminsterfullerene and intercalates thereof, clays (Tsvetkov and White 1988, 1989), superconductivity (Fullagar and others 1993), as well as soluble conducting polymers (Armes and others 1986; Aldissi and others 1988). A particularly advantageous synthetic route to soluble polyacetylene was perfected with Dai (John's first ANU PhD student) (Dai and White 1991) and, in John's first foray into reflectometry, the first experiments of their kind on conducting copolymers, a significant 'surface excess' was detected using critical external reflection of neutrons from polyacetylene 3:4 polyisoprene block copolymers at an air liquid interface (Dai and others 1989); later work was focussed on polystyrene (Saville and others 1994). Notably this technique had largely developed through the work of John Hayter at ILL and a pre-PhD Jeff Penfold who moved from the Rutherford Appleton Laboratory at Harwell to the ILL during the period that John White was Director (Penfold 2016). John was apparently highly supportive of the new technique, although it took some time to convince others at ILL of its potential; John also made an important and crucial contribution in introducing Hayter and Penfold to Bob Thomas, who later became renowned in the field of neutron reflectometry, producing the first comprehensive study of surfactant adsorption at air-water interfaces.

While John had initiated work on zeolites some years prior, in Australia, an enduring interest led to a new programme involving the systematic study of the role of template molecules for inducing nucleation of specific zeolites (Iton and others 1992; Edler and Whiteothers 1995; Brown and others 1998). Much of this early work involved Lennox Iton at Argonne National Laboratory and the Intense Pulse Neutron Source (IPNS) there, where John had won a prestigious Argonne Fellowship in 1985 which he saw as an opportunity to build a relationship between the ANU and the University of Chicago (Anonymous 1987). Both IPNS and the RSC agreed to John's twelve-month Argonne Fellowship being spread over four years in six week tranches. Again, by using contrast variation small angle neutron scattering, it was shown for the first time that a solid silicate hydrogel may undergo almost complete transformation at ambient temperatures under the action of 'template' molecules. This programme attracted considerable interest in the United States within the Department of Energy and the company, Amoco, as these porous materials, based on the templating of silica by colloidal precursors can be used in the conversion of gas to petrol. The first to be investigated was ZSM-5 where the colloidal agent was the tetrapropylammonium ion. In the coming years, MCM-41 that was developed by the Mobil company, was the focus of attention. In many ways, such work continued the tradition by White's group in 1975 on

small angle scattering from colloids (Cebula and others 1978, 1980; Harris and others 1983).

During this period, John's management experience was again brought to bear when he became Pro-Vice-Chancellor and Chairman of the Board of the Institute of Advanced Studies (IAS) (1992–3). In the latter role, John chaired a working group tasked with addressing gender balance in the IAS. This led to a series of recommendations being proposed, and policy initiatives being adopted, to address impediments facing women in academic life.

With John's ever increasing workload, Philip Reynolds, John's former DPhil. student, joined the White group in 1993 to provide supervision to John's growing group. John subsequently became Dean of the RSC (1995–8), during which the RSC went through an external review and, naturally, the publication of a glowing report.

John's fascination continued with the mechanisms by which molecular and intermolecular substances acted as 'templates' for the growth of inorganic structures in the laboratory and in nature (such as shell or tooth). The regular purchase of live abalone to explore pearl growth, at a cost of a rather sizeable \$80 per portion, was the subject of some unjustified suspicion at the RSC.

The methods of neutron contrast variation played a key role in dissecting the mechanism of surfactant templating by selectively revealing the structures of the organising organic molecules and the inorganic component at early stages in the growth process at an interface when no film is visible to the eye. Nanometre resolution on the time lapse structures were subsequently obtained; utilising fast X-ray reflectivity apparatus commissioned at the RSC, this degree of spatial resolution could be achieved with the whole measurement being made in seconds. Fast reactions at interfaces could thus be studied enabling expanded interests to the synthesis mechanism of highly crystalline transition metal oxide films at interfaces using molecular templates. Titania-based films produced by template-induced self-assembly from strongly acidic solutions formed highly ordered material (Henderson and others 2003) that were found to be relevant for solar energy capture; this led to a grant to study zirconia-based films. Through other interactions at IPNS, there began a programme of research as to how mixtures of normal alkanes undergo localised phase separation to form superstructures when quenched from the melt into the solid state (Dorset and others 1990; Gilbert and others 1996b, 1999).

Scientific curiosity and 'usefulness'

John encapsulated his attitude to science at his 75th birthday symposium with five key factors: curiosity, hard work, serendipity, joy and usefulness (White 2012). John's inherent curiosity led to a series of ever-related intersections, for example proteins at interfaces led to studies in nanotoxicology, while interest in graphite intercalation led to associated

studies of the effect of graphite on molecular adsorption (Gilbert and others 1996a). John's approach inspired his students to follow their own curiosity.

John maintained his interactions with ICI, including when the company divested its major shareholding in Australia in 1997, and a new world-class independent Australasian company was formed to become Orica (the world's largest explosive manufacturer). John and EPG were successful in being awarded an Australian Research Council grant to understand the structure and stability of emulsions in the context of exploring formulation problems with Orica as the commercial partner. Indeed, EPG fondly recalls going to the RSC at 9 am the day following the submission of his thesis where John and he prepared the grant application. X-ray and neutron small angle scattering and reflectivity were the key methods alongside surface pressure-area isotherms. This work benefited enormously from the group's expertise developed over the previous decade in studying a variety of polymers and surfactants at interfaces. Studies of industrial high internal phase water-in-oil emulsions demonstrated the presence of inverse micelles in the oil phase that provided not only a reservoir of surfactant, but also a depletion stabilisation mechanism for the whole emulsion structure. The work generated also showed how compatibility matching—the basic physical chemistry of solvency—could play an important role (Reynolds and others 2000, 2001). Characterisation at the oil-water interface was complemented by global refinement of X-ray and neutron reflectivity of air-water and later oil-water interfaces. The ability to create 10 nm oil films at the air-water interface, which were stable and extremely sensitive probes of the stability of the oil-surfactant-water interface, was reported (McGillivray and others 2009). The original grant awarded with Orica in 1997 formed the basis for a steady stream of postdoctoral fellows and PhD students to investigate a multitude of formulation and external parameters, including surfactant and oil type, molecular weight, temperature, and shear.

Further industrial activities expanded in 2000 with the establishment of the University Industry linkages in CHEmistry (or UniChe) project. Initially funded for three years, but subsequently extended, UniChe was designed as a model for industry-university interaction, involving approximately thirty second-to-fourth year students and PhD scholarships in the chemistry and chemical engineering departments at the Universities of Newcastle, Melbourne, and later Queensland, in addition to the ANU (Anonymous 2006). The aim was to provide closer alignment between the way research students were trained and what employers sought by extending the links between research training in university and research in industry. The project was jointly funded by the Australian government with matching in-kind contributions from partners, mainly Orica, and facilitated a summer school introducing industrial skills to undergraduates, an exchange programme, a student research programme, field work experiences, and viewing research laboratories, wineries, mines, and Orica's facilities to gain exposure to the broader aspects of the chemical industry

and innovation (Anonymous 2010). The research activities on emulsions and other topics of interest to Orica's science continued in a series of grants, generating publications up to 2013 (Mata and others 2013), although being applied to hydrophobic mineral recovery by flotation as late as 2022 (DeJuliis and others 2022).

Milk is, of course, a naturally occurring emulsion; however, it would not necessarily occur to anyone but John that such a material was worthy of investigation by X-ray reflectivity (Holt and White 1999). In a study with Stephen Holt, they explored molecular structure of milk as a function of fat content and temperature at the air-milk interface. Indeed, one of the reviewers of the manuscript indicated that such a research project would never be allocated beamtime in their experience, but it was good that the authors had been able to carry out the study on their own instrument since the findings concerning the dissociation of the casein micelle at an interface were interesting and potentially important (White 2012); that is that the structure of a protein layer perpendicular to the surface of skim or full fat milk is similar to that of pure β -casein at the air-water interface. This early exploration led to the development, also in 2000, of the first of several subsequent research grants, this time with the Australian dairy industry, to investigate the nanostructure of milk and strategies for preserving the functional properties of dairy proteins during drying, and the interaction of β -casein with κ -casein at the air-water interface.

John is less well known for his work in biophysics, but the origins of this can be traced back to the 1970s where the first neutron experiments on diffraction from single collagen fibres and viruses (Hecht and White 1976; Miller and others 1976; White and others 1976) by exploiting the dominant methodological technique of contrast variation. Further interests developed on protein stability and denaturation more broadly (Holt and others 2002; Henderson and others 2005) and a new method was also developed, known as the 'flow trough' (Lin and White 2009), which allowed replacement of the substrate under protein monolayers, and the study of specific protein-protein and protein-denaturant interactions. Studies were also conducted of direct relevance to nanotoxicology to test the hypothesis for the protein-corona pathway for nanoparticle entry into human cells (White and others 2009). First tests focussed on comparing human serum albumin and beta-casein interaction with silica sols.

75th birthday celebrations and beyond

Despite some of his former students having since retired, and with associated academic celebrations of their own having already been held, John continued to work at the ANU in the 2010s; nonetheless, a symposium to recognise John's contribution was timely and warranted. John's 75th birthday was in 2012 and, as luck would have it, John's former PhD student and postdoctoral fellow, EPG, was chair

of the international small-angle scattering conference in Sydney. This provided an excellent opportunity for a satellite meeting in celebration of John's work, chaired by Stephen Holt and held in the area of his birth, the Hunter Valley (Knobloch 2013; Fig. 9). Speakers included many of his former group members or ILL colleagues with keynotes from Bob Thomas and Frans Trouw. John subsequently retired from the ANU in 2013, but continued to work in his office at the RSC and later, Department of Chemistry at the ANU until 2018, while continuing to Chair the Australian—Oxford Scholarship scheme that he co-founded in the mid-1990s raising funds from Australian Oxford alumni, a cause very close to his heart. He was made, by Oxford University, a Distinguished Friend of Oxford in 2007. A John and Ailsa White Oxford Australia scholarship is currently being set up with family funds to reflect his commitment to this cause.

John's immense intellect enabled him to still be extremely active across many aspects of science towards the end of his life. At the height of the COVID epidemic, he quizzed the immunologist wife of EPG on some of the finer aspects of vaccine development and the virus itself; in his last visit to Europe in June 2023, he expressed his interest to the Science Director on conducting experiments on the FREIA neutron reflectometer under construction at the European Spallation Source and opportunities for artificial intelligence in analysing

neutron data. Across his career, John published in excess of 250 scientific papers—a Scopus search reveals 258, although the authors are aware of some missing entries—with John's final paper being published posthumously based on his presentation at the fiftieth anniversary of the SANS instrument, D11, meeting (White 2023).

A man of faith

John White had a long involvement at the faith–science interface, beginning as coordinator of the Oxford Research Scientists' Christian Fellowship (RSCF) during the early 1960s where he met Ailsa. This group of scientists was committed to produce a yearly scientific paper on apparent conflicts with religion and subject them to rational criticism. It is actually difficult to think of a more appropriate Oxford college for John than St. John's. Founded by another White, Thomas, in 1555, the college crest features the 'Lamb and Flag' of the Paschal Lamb, a symbol of Christ as the Lamb of God, often depicted carrying a banner with a cross, referencing St. John the Baptist. Many of those who met John over the years will recall his preference for wearing his college tie. John's wider Christian commitment was reflected in his 1980–1985 membership of the Council of Wycliffe Hall (Oxford), a major evangelical Anglican theological college.



Fig. 9. At the Hunter Valley symposium in honour of John's 75th year in 2012. Photograph courtesy of the White family.

He was also appointed to the Council of Epsom college in the U.K. during this time. Later, on his return to Australia, he was key in establishing ISCAST (The Australian Institute for the Study of Christianity in the Age of Science and Technology) in 1987, serving as its President from 1992 to 2006. He served on the council of St Mark's Theological Centre in Canberra, was a founding member of the International Society for Science and Religion and, with Ailsa, a parishioner of, coincidentally, St. John's church in Reid, throughout his time in Canberra. It was also his vision to establish the biennial Conference on Science and Christianity series (COSAC), which began in 1997 and continues today.

John's thoughtful and informed debating style enabled him to make some key interventions in a number of debates about the important moral issues of the times. For example, as Policy Secretary of the Australian Academy of Science (AAS), he chaired a Working Group about the scientific and ethical issues raised by human cloning. John's Christian faith was clearly important to him and the basis of his views of society, but he never allowed it to intrude into his relationships with students and colleagues. John told the *Australasian Scientist* in 2008, 'I don't think science and Christianity are in conflict at all. I make no judgments about the virgin birth or miracles, largely because I wasn't there.' John simply did not see any conflict between his scientific and religious concerns. Indeed, and as was so eloquently stated by the Rev. David McLennan at John's funeral, 'they (science and religion) may deal with different orders of reality, but they both deal with 'things unseen' (McLennan 2023)'; this is not dissimilar to the neutron itself.

Hobbies and pastimes

Growing up in the coal mining city of Newcastle in New South Wales, and with his strong interest in geology, John became interested in industrial archaeology after discussions with one of his Oxford doctoral students. This broadened into canal construction in the UK and railway and mining history in both the UK and Australia. He was stimulated by exploring a wide range of ideas in philosophy, including Indigenous Australian languages and history, and he loved the time he was able to spend with his family (that increased with seven grandchildren), unobtrusively helping them develop their own ideas and interests.

John also had wide interests in music, including playing the church-organ, art, and being out walking in nature. He had also been an avid skier and squash player in his younger days.

Global scientific outlook

John was acknowledged as an internationalist and had influence in almost every continent as a passionate promoter of global collaboration alongside national aspects of science policy. Through his initial involvement with teaching chemistry

undergraduates, John attracted many highly motivated research students and research collaborators who themselves developed neutron scattering programmes in academia or industry throughout the world. Over the course of his career, he supervised thirty two PhDs (J. White, pers. comm. 2020). As Director of the ILL, he was at the epicentre of European neutron science. As a fellow of Argonne National Laboratory, he was closely connected to the development of spallation neutron science and performed experiments at the Intense Pulsed Neutron Source and LANSCE at Los Alamos. With Japan, as well as his involvement in the development of the beamline at the Photon Factory, high profile collaborations between the two nations in synchrotron and neutron science followed. He was a major driver in the formation of the Asia-Oceania Neutron Scattering Association with the aim of sharing scientifically the region's extensive newly acquired neutron facilities and became its second President. From 2002 to 2012, John chaired the International Advisory Committee overseeing the development of the J-PARC (Japanese Proton Accelerator Research Complex). His passion to maintain and enhance collaborations while supporting Australian scientists to access the very best international neutron and synchrotron facilities, as well as taking key roles to advocate for and succeed in the case to build a state-of-the-art nuclear research reactor, OPAL, and Australian synchrotron are undeniable. As chair of the steering committee in the evaluation of Australia's Antarctic science programme, John even played a role in ensuring the building of a landing strip for planes from Hobart to Australia's various Antarctic stations to replace boat landings, resulting in a major increase in the efficiency of Australia's research efforts. Apparently, when John was asked by the then Prime Minister John Howard whether he thought the landing strip was a good idea, it took all the energy John could muster to avoid replying, 'Yes, Prime Minister'. As a token of gratitude, John received a framed photo of Antarctica from the Australian Antarctic Division.

Honours, awards and recognition

John White was awarded a Fellowship to the Australian Academy of Science in 1991 and subsequently became a Fellow of the Royal Society in 1993 (Lang, 1993) (see Supplementary File 1). The testimonials received, courtesy of the archives of the Australian Academy of Science for the former, demonstrate the admiration from the community:

Apart from the very real quality of his own scientific work, we should consider the extraordinary enthusiasm which John brings to his work. That is an inspiration to a generation of young scientists.

Let me be brief. Amongst all chemists worldwide, John White is by far the most productive, innovative and well-known. His work is filled with many firsts. He has been

instrumental in teaching many newcomers about neutrons and their potential, in chemistry and materials science. The career of almost every chemist using neutrons has been directly touched by John White's work and his advice.

Your committee will know his style, which is inspirational. He has throughout his career transmitted his enthusiasm to research students, colleagues and, during his Directorship of the ILL, to his staff. During that time when he exhibited superb technical and administrative leadership he was often seen carrying out experiments himself.

But one quote will resonate with many that worked with John:

It was said of him that when you go into his office you had better have some very good ideas of your own, otherwise his ideas will be better and you will end up working for him.

John White received the Order of Australia in 2016 'for distinguished service to science globally in the field of chemistry, as an academic, mentor and researcher, and through leadership of Synchrotron and neutron science projects in Australia and the Asia-Oceania region' (Fig. 10). In 2020, he received the Australian Neutron Beam User Group Career Award; its commendation reads: 'Professor John White has been working in the field of neutron scattering science globally for sixty years. He rapidly undertook leadership roles at major neutron research facilities including acting as the neutron beam coordinator at Harwell (UK) and Director of



Fig. 10. John on the awarding of the Order of Australia in 2016. Photograph courtesy of the White family.

the ILL (France). John continued his involvement in advances in neutron science upon returning to Australia in 1985 as a professor at the ANU. He was instrumental in the development of the reflectometer and AUSANS instruments at HIFAR, which directed the design of their successors at OPAL. John's influence continues to permeate through the Australian neutron scattering community through those he has taught and mentored, many of whom are still active researchers in neutron scattering science throughout the world.' A list of his publications appears as Supplementary material to this paper (Supplementary File S2).

Death and tributes

John White passed away on 16 August 2023 at his home in Canberra, Australia. His funeral was held at the church that Ailsa and he regularly attended since their return to Canberra of St John the Baptist Church, Reid on 22 August 2023, and he was buried in the Hunter region of his childhood. John's passing resulted in a number of obituaries in the *Journal of Applied Crystallography* (Gilbert and others 2023), *Neutron News* (Gilbert and others 2024), *Chemistry in Australia* (Gilbert and Gentle 2024) and in articles published by the *Institute for the Study of Christianity in an Age of Science and Technology* (ISCAST) *News* (Pilbrow 2023), *AINSE* (Anonymous 2023a), the Anglican Church League (Anonymous 2023b), and the *International Union of Crystallography Newsletter* (Welberry 2023).

The Chadwick Auditorium at the ILL was a fitting venue for a symposium organised to celebrate and commemorate John's lasting contributions. The two-day meeting on 18 and 19 July 2024 was attended by John's friends, colleagues and family from around the world, with a highlight being a pictorial presentation by Ailsa of their life together. Numerous anecdotes were recounted. JSH described her drive with John from Oxford to Harwell for an experiment on ammonia trapped in a zeolite sieve with the Dewar hanging out of a car window to avoid the potential for asphyxiation! EPG recalled that in the mid-1990s, John had arranged, as usual, to hire a cheap, but rather rundown car, to transport the team to and from a bed and breakfast in Stevenage to ISIS; however, John had failed to appreciate that EPG had only just passed a test to drive an automatic car. To remedy the situation, and at an opportune moment away from the neutron beam, John proceeded to teach him to drive a manual car in the parking area outside the main gate of ISIS, much to the chagrin of a security guard. As one might expect, with a career spanning more than five decades, the attendees spanned a similar range of ages from early career researchers to retirees and many in between (Edler and others 2025). Several current or former Directors of the ILL, IPNS, the European Spallation Source, and ISIS were in attendance, a clear demonstration of John's impact at an international level to neutron scattering and a field

that owes him a great debt. The ILL meeting was a fitting tribute and celebration of a life well lived.

Conclusions

There are many words to describe John: teacher, friend, mentor, intelligent, humorous, curious, influential, enthusiastic, connector, but perhaps his friend and one of the earliest exponents of spallation neutrons, Jack Carpenter, summed it up in his speech at John's 75th symposium when he referred to John as an 'inspirator' or 'one who inspires'. Unquestionably John's greatest contribution is the legacy that he leaves in the numerous students, postdoctoral fellows, and collaborators that were given the opportunity to grow, thrive and form the subsequent generation of leaders in their own respective fields. A red rose has been named in John's honour from the Brindabella nursery in Toowoomba in Queensland; it grows in the garden of Ailsa and John's house in Turner, and in the houses of his children located around Australia. He is sadly missed.

Supplementary material

Supplementary material is available online.

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