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John White's contributions to Chemical Spectroscopy

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The physical chemist H.W."Tommy" Thompson became a fellow and chemistry tutor at St John's College, Oxford (SJC) in the 1930s after studying in Germany with Fritz Haber and Max Planck. He pioneered studies with infrared spectroscopy, notably realising that vibrational spectra were useful identifying fingerprints for molecules. His students at SJC continued diversifying these activities. One, Rex Richards, developed nuclear magnetic resonance as a chemical tool. John White obtained a scholarship to study in Oxford, and joined Richard's group. His doctorate project was the measurement of diffusive motions by using the coupling of e.s.r. excitations to stimulate n.m.r. transitions (the Overhauser effect). Two instruments with e.s.r. in the X-band and Q-band frequency ranges allowed observation of relaxation on two different time scales. (One of John's own students, John Collingwood, later built a low magnetic field instrument that offered a third timescale.) In 1963 Tommy was increasingly busy with the Royal Society, and the Football Association (chair 1976-81), and John was appointed to a fellowship at SJC to assist in teaching chemistry to undergraduates, including myself. Tommy engaged Peter Day the following year to teach inorganic chemistry at SJC. Students of John at SJC joined in his research activities. Some who continued with neutron spectroscopy include Andrew Taylor, and Frans Trouw, Philip Reynolds and Andrew Harrison. R.K "Bob" Thomas was initially one of Tommy's students, and took over John's group when he came to the ILL.

In 1963, Roger Elliot, the SJC physics tutor, invited Peter Egelstaff to dine at the college. Peter was head of the Pile Neutron Research Group at Harwell, with strong interests in liquid properties (water, liquid sodium, etc. for moderators). John was invited to use the time of flight (ToF) instruments at Harwell, resulting in the paper with Julia (Stretton Downes) Higgins and Peter on beta-quinol clathrates where the vibrations of the guest molecules could be distinguished from the host by selective deuteration. The success of these measurements led to a wide range of experiments using deuterium substitution to emphasize molecular motions from selected parts of systems. Rotational diffusion in small molecules (e.g. methanol) too was a subject for ToF measurements. Having observed the vibrational spectra of the crystalline hosts in the clathrate experiments, John embarked on projects to measure phonons in molecular crystals, which could lead to a better understanding of intra-molecular forces in solids. Systems studied included urea, and aromatics like naphthalene and p-dichloro-benzene. For the latter two Stuart Pawley offered his phonon calculation program, which was specific to crystal structures of this symmetry. Inelastic neutron measurements followed and prompted improvements to the simple models initially proposed which were originally intended to improve accuracy in crystallographic studies. Both ToF and triple-axis spectrometers were used. Later Philip Reynolds benefited greatly from visits to Risø where Jørgen Kjems took an active interest and generously gave instrument time. Further experiments extended to crystalline polymers (polyethylene, poly-oxy-methylene). Diffusion in restricted environments was examined in experiments with water in Montmorillonite clay layers. The inter platelet spacing can be varied by changing the concentration of ions in the aqueous solution. The gaseous state was not ignored either. The dynamics of adsorbed gases first on fumed silica, then Graphon could be assessed. As with many experiments started at Harwell the later availability of high-resolution measurements at the ILL could be analysed in more detail over greater ranges. Other intercalate experiments looked at hydrogen and methane in caesium/graphite supports. New results from proton tunnelling showed the sensitivity of the technique to examine effects of the local environment on the dynamics.

John's interest in resonance experiments continued with John Hayter and Graham Jenkins using polarised neutrons at Harwell to examine the potential for modifying diffraction patterns by flipping proton spins selectively, as in ENDOR measurements. When John came to the ILL he brought Graham Jenkins to work with Peter Seifert on the dynamic spin polarisation filter IN9.

I will try and present a few topics from these wide ranging experiments.

His later works after returning to the ANU in Australia were mostly in the fields of small-angle scattering and neutron reflectivity using the Opal reactor at Lucas Heights.

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