

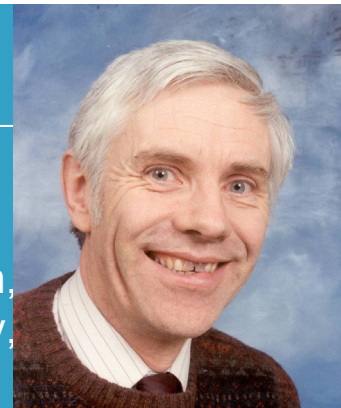
Prof David W H Rankin

Professor of Structural Chemistry

e-mail: d.w.h.rankin@ed.ac.uk

tel: 0131 650 4728

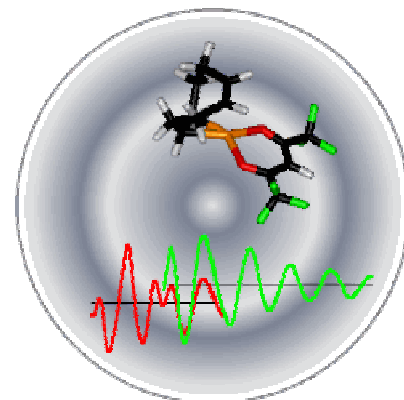
Research Interests: molecular structure, electron diffraction, combining computational and experimental chemistry, metals in plants and soils, chemical taxonomy of plants



Structural Chemistry

Knowledge of [molecular structure](#) is essential for understanding of properties. We concentrate on structures in the gas phase, where freedom from inter-molecular interactions allows molecules to adopt their most stable arrangements. We use a uniquely wide range of structural methods, this broad approach allowing study of structures that could otherwise not be determined and achieving exceptional accuracy for simpler molecules. But most importantly, we develop new methods to extend the range of compounds that can be studied.

[Electron diffraction](#) is the central technique. We collaborate with many synthetic chemistry groups, both within the UK and around the world, so we study many interesting and unusual compounds, including polyhedral boranes and carbaboranes, sterically crowded silicon compounds, precursors to solid-state materials, aromatic heterocycles and organometallic compounds.



When diffraction data alone are insufficient to allow full, accurate determination of a structure, additional spectroscopic data can allow much more complete structures to be obtained. But even that may not be enough. So we recently developed the [SARACEN](#) method, in which we perform [ab initio](#) (i.e., quantum mechanical) calculations, and then use the results to restrain structural refinements. The outcome is a structure that uses all available information, both theoretical and experimental, and is the best that can be obtained at the present state of knowledge. This method has revolutionised small-molecule structural chemistry.

Plants and Soils

Rhododendrons on limestone soils

Rhododendrons and related plants (Ericaceae) are normally regarded as impossible to cultivate on limestone soils - but this appears to happen quite happily in the wild. We are investigating growth of wild (Chinese) Rhododendrons and cultivate plants, to find out what factors allow successful growth in the wild. We then hope to develop methods for successful cultivation of at least some of these plants on limestone soils.

Chemical taxonomy

Identification of plant species is important, but morphology (or appearance) is sometimes not sufficient to allow confident naming of specimens. There are particular problems with some Rhododendrons, where species seem to merge with one another, and cultivated plants may not always be truly representative of wild populations. The waxes on leaves of Rhododendrons (and some other genera) provide crucial information. We are studying these materials, to resolve questions of distinctions between similar species.

SELECTED RECENT PUBLICATIONS

1. An enormous vibrational motion: the gas-phase structure of dimethyl-bis(methoxyethynyl) germanium. K. B. Borisenko, R. N. Yezhov, S. V. Gruener, H. E. Robertson and D. W. H. Rankin, *Dalton Trans.*, 2004, 3878-3882.
2. SARACEN - molecular structures from theory and experiment: the best of both worlds. N. W. Mitzel and D. W. H. Rankin, *Dalton Trans.*, 2003, 3650-3662.
3. Dramatic structural effects of a single hydrogen atom in HNPBu₃. S. L. Hinchley, M. F. Haddow and D. W. H. Rankin, *Inorg. Chem.*, 2004, **43**, 5522-5528.
4. The structures of higher boron halides B₈X₁₂ (X = F, Cl, Br and I) by gas-phase electron diffraction and *ab initio* calculations. P. L. Timms, N. C. Norman, J. A. J. Pardoe, I. D. Mackie, S. L. Hinchley, S. Parsons and D. W. H. Rankin, *Dalton Trans.*, 2005, 607-616.
5. Analysis of leaf waxes as a taxonomic guide to *Rhododendron* subsection *Taliensia*. M. D. Chadwick, D. F. Chamberlain, B. A. Knights, A. J. McAleese, S. Peters, D. W. H. Rankin and F. Sanderson, *Annals of Botany*, 2000, **86**, 371-384.