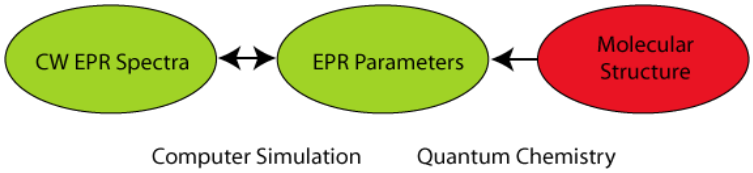
The Evolution of Spectral Interpretation – From Spin Systems to Molecular Structure and Beyond.

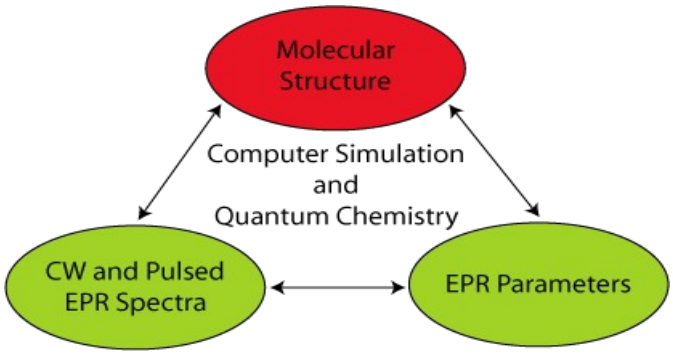
Christopher Noble,[1] Simon Benson,[1] Graeme R. Hanson[1]

[1]*Centre for Magnetic Resonance, The University of Queensland, St. Lucia, Queensland, 4072, Australia.*

Determination of the geometric and electronic structure of paramagnetic species from continuous wave and pulsed EPR spectra relies heavily on computer simulation techniques. Computer simuation of continuous wave EPR spectra has, over the last four decades, developed from the use of pertubation theory for specific spin systems to matrix diagonalisation for a general spin systems (XSophe-Sophe-XeprView).[1] Once the spin Hamiltonian parameters have been obtained, scientists have employed the 'traditional approach' to determine the molecular structure of the species (Figure 1). This has involved either a comparison of these parameters with those of known structures or the application of quantum chemistry calculations (crystal field theory, ligand field theory, *ab initio* methods and density functional theory) to reproduce the spin Hamiltonian parameters from an initial structure.



Over the last five years we have developed an integrated approach 'Molecular Sophe' [2] for the computer simulation of continuous wave and pulsed EPR and ENDOR spectra, energy level diagrams, transition roadmaps and transition surfaces. This approach, based on molecular structure, will revolutionise the 3-dimensional molecular characterisation of paramagnetic materials using EPR spectroscopy as until now the analysis of complex CW and pulsed EPR spectra has been based on spin systems rather than molecular structure.



Insights into the future application of computer simulation to the analysis of CW and pulsed EPR, ENDOR and ELDOR spectra will be discussed in relation to Resonanz.[3]

1. Mitchell, A.; Noble, C.J.; Benson, S.; Gates, K.E.; Hanson, G.R. "XSophe: An Integrated Molecular Approach to the Analysis of Continuous Wave and Pulsed EPR Spectroscopy from Metalloproeteins", *J. Inorg. Biochem.*, **2003**, *96*, 191.
2. Hanson, G.R.; Noble, C.J.; Benson, S. "Molecular Sophe: An Integrated Approach to the Structural Characterization of Paramagnetic Species. The Next Generation of Computer Simulation Software", Biol. Magn. Res. **2007**, *28*, In Press.
3. Benson, S.; Noble, C.J.; Hanson, G.R "Resonanz", **2007**, Unpublished Results.