Optical detection of electron spin resonance by coherent Raman spectroscopy: application to metallo-enzymes

S. J. Bingham[1], D. Wolverson[1], J. J. Davies[1], T. Rasmussen[2], and A. J. Thomson[2]

[1] *Department of Physics, University of Bath, Bath BA2 7AY, U.K.*

[2] *Centre for Metalloprotein Spectroscopy and Biology, School of Chemical Sciences, University of East Anglia, Norwich NR4 7TJ, U.K.*

Optically detected ESR provides more information about electronic structure than can be obtained by the separate application of magnetic resonance and optical spectroscopy:

- ***Enhanced chemical selectivity*** allows overlapping ESR and optical spectra due to multiple chemical species to be deconvoluted.

- ***Enhanced orientational selectivity*** allows the relative orientation of the optical and magnetic anisotropies of paramagnetic centres to be deduced, even when these centres are randomly orientated in the sample.

Coherent Raman detected ESR is superior to previous optically detected ESR methods because the spectra can, like conventional ESR spectra, be simulated and interpreted without detailed knowledge of the magnetic relaxation processes. Accurate lineshape simulation provides detailed quantitative information about the species concerned.

These features of coherent Raman detected ESR will be illustrated by data from the copper enzyme *nitrous oxide reductase*.