Low Field Optically Detected EPR spectroscopy of transient photo-induced radical pairs

Kevin B. Henbest*, Christopher T. Rodgers*, Philipp Kukura‡, Peter J. Hore* and Christiane R. Timmel

*Physical and Theoretical Chemistry Department, South Parks Road, Oxford, OX1 3QZ, UK.
‡Present Address: Chemistry Department, University of Berkeley, California, 94720, USA.

The effects of simultaneously applied weak static and weak oscillating magnetic fields on the recombination of transient (<100ns) radical pairs are investigated using a low-field detected electron paramagnetic resonance technique. Investigations of the photoinduced electron transfer reaction of perdeuterated pyrene with 1,3-dicyanobenzene are conducted in the presence of simultaneously applied static (0-4mT) and radiofrequency (5-65MHz) magnetic fields. The resulting spectra show a strong dependence not only on the strength of both fields as well as the frequency of the applied RF radiation but more importantly, on the relative orientation of the two fields. The spectra are simulated using a modified form of the \(\gamma\)-COMPUTE algorithm which was originally established for calculating magic angle spinning NMR spectra of polycrystalline samples.

It is shown that the spectra are easily understood in terms of the Radical Pair Mechanism and simulated satisfactorily using parameters whose values are either known or for which estimates are readily available.

The dependence of the obtained data on radical pair parameters such as hyperfine couplings and the pair’s lifetime are examined in detail.

Finally, the significance of the data in the context of the proposal that radical pair processes form the basis of many animals’ ability to use the Earth’s magnetic field for compass information is discussed.