

The Bruker logo is displayed in a bold, black, sans-serif font. The background of the entire top section is a vibrant blue and green gradient, overlaid with various chemical structures and molecular diagrams in glowing blue and green lines. A central image shows a white Bruker Magnettech ESR5000 spectrometer with a glass flask containing a blue liquid on top of it. The spectrometer has a control knob on the front and a vented side panel. The flask is a standard Erlenmeyer flask.

EPR

Reaction Kinetics Studied

With Magnetech ESR5000

Innovation with Integrity

Introduction

The world is a very dynamic place, never in equilibrium. Much of these dynamics are chemical reactions involving the transfer of one electron. Each electron transfer results in an unpaired electron creating paramagnetic free radicals. EPR (Electron Paramagnetic Resonance) is the ideal spectroscopic technique to measure these species as well as to monitor the time behavior of their creation and disappearance. The Magnetech ESR5000 has the ability to detect free radicals unambiguously.

Challenge

Transient species are short-lived which makes their detection challenging. Spectral overlap between different radical signals is frequently a major problem.

Solution

Two methods of monitoring and quantifying short-lived radical species are directly recording the EPR spectrum with fast field sweeps or indirectly detecting the species through their reactions with an added spin trap/spin probe. For both methods of detection, simulation and fitting of the EPR spectrum aids in the identification and quantification of the radical species.

Equipment

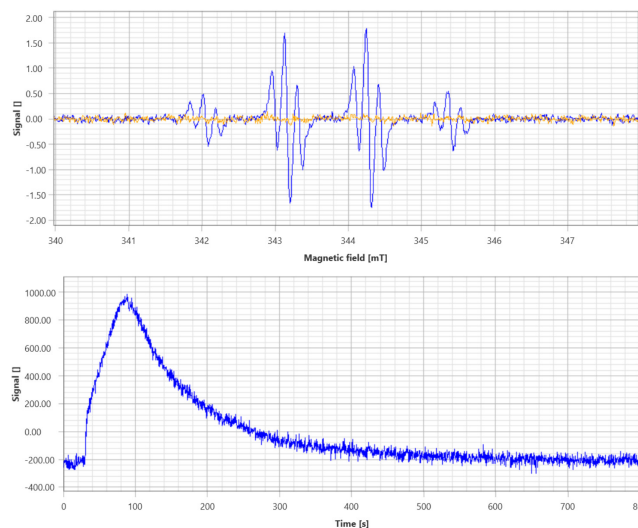
The Magnetech ESR5000 spectrometer ensures high precision results with superior sensitivity thus enabling researchers and students with limited EPR experience to use the power of EPR spectroscopy to identify and monitor reactions rates of free radical reactions in many fields of study.

Key Features include:

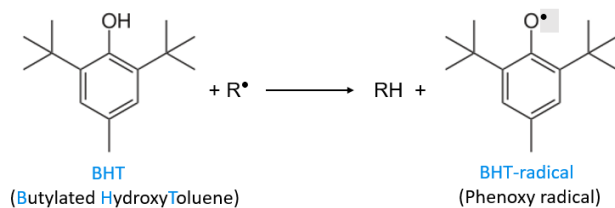
- Easy-to-use software
- Transient mode experiment to monitor the kinetics of a single species
- 2D full spectrum mode to monitor kinetics of multiple species
- Fitting routines to analyze kinetics
- SpinFit Liquids module to simulate and identify multiple radicals in the sample
- SpinCount module to quantify the total number of spins and to determine the radical concentration

1D kinetics experiment

Figure 1 Experimental data of edible oil oxidation containing BHT upon UV-light exposure



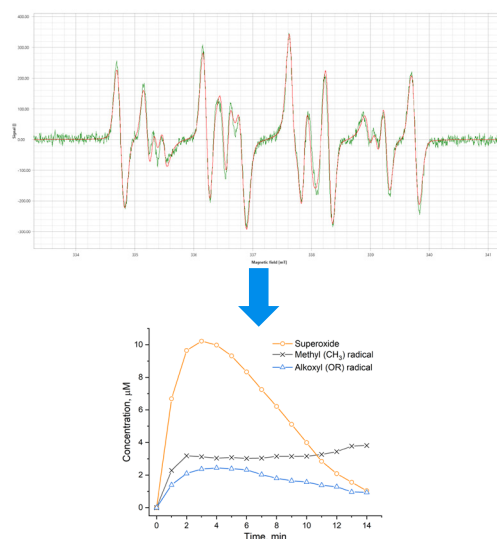
- Three species (superoxide, methyl, and alkoxy radical) can be monitored simultaneously as a function of time and their concentration can be individually determined
- Simulate the multiple DMPO radical adducts using SpinFit Liquids and the spin trap database
- SpinCount provides a report of the fit species concentrations during the time course of the experiment
- The report can be saved as an ASCII file for further evaluation



- Butylated hydroxy toluene (BHT), a potent radical scavenger is used as a common stabilizer and food preservative
- It reacts preferentially with damaging free radicals in foods to form a new, less reactive phenoxy BHT-radical
- Upon UV-exposure the BHT-radical decays via first order kinetics

2D kinetics experiment

Figure 2 Experimental data from UV-irradiation of TiO₂ nanoparticles in DMSO



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