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Dependency of hyperfine interactions on Magnetic parameters of irradiated polymers

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Abstract

ESR spectra of irradiated polymers possesses complex shapes due to various reasons . Superposition of component ESR spectra of various free radicals, line width broadening effects induced by surrounding polymer matrix are some of the reasons. In this context the authors have used computer simulation techniques to analyze component ESR spectra. As a case study hyperfine interactions of triplet spectra are discussed in the article.

Introduction

Electron spin resonance (ESR) spectroscopy is widely used in polymer research. They are (i) nature of free radicals produced in polymer and their kinetics (ii) polymer morphology and (iii) molecular relaxations etc. It is observed that the ESR spectra of solutions are usually isotropic nature; while in solids the spectra are appeared to be broadened. In order to analyze such complex ESR spectra, various methods are preferred in literature(1,2). Among them the total curve fitting method is successfully applied to analyze the ESR spectra of polymers.

In this context, the authors attempts to apply the total curve fitting method to study hyperfine interactions in some radicals giving component triplet spectra.

Results and Discussion

Computer simulations are an important tool to interpret complicated ESR spectra. Therefore various methods to simulate the ESR spectra of irradiated polymers is reported(1-3). Among these method the total curve fitting method is reported to be very successful (1,2,3). The method involves generation of various component spectra and superpose them to yield a total ESR spectrum, which has to be

matched with the observed ESR spectrum. If the theoretical spectrum exactly matches with that of experimental spectrum, the free radicals causing the component ESR spectra are expected to be present in the given system.

The component spectra are simulated by magnetic parameters such as line width(a_i), line intensity(y_{maxi}), centre of spectrum(X_{oi}), hyperfine splitting constants(A_i, B_i) due to alpha, beta nuclei, number of hyperfine lines arising due to the alpha and beta nuclei. The component spectra are generated by varying the magnetic described above calculation of these magnetic parameters is described by Sanjeeva Rao et al(3).

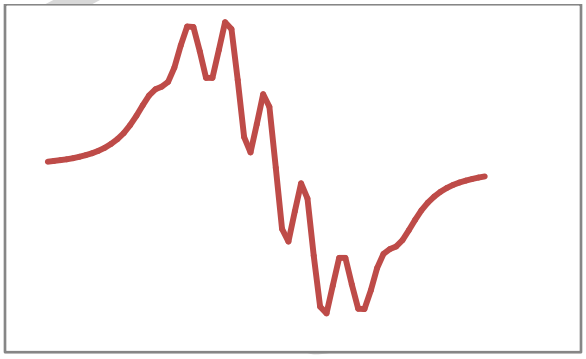
In the present article , the author have described the hyperfines interaction of triplet spectrum. It is observed that the triplet spectrum is reported in many polymeric systems like poly(vinyl alcohol) (4), polyacrylamide(5) and several copolymers(6). The free radical giving component triplet is of the type ~CH_2~ i,e the free radicals will have two interacting alpha or beta proton. The line shape arising due to triplet spectrum depends on the magnetic parameters.

The authors have varied the magnetic parameters are generated component triplet spectrum. The magnetic parameters employed in the present studies are as listed in the table.

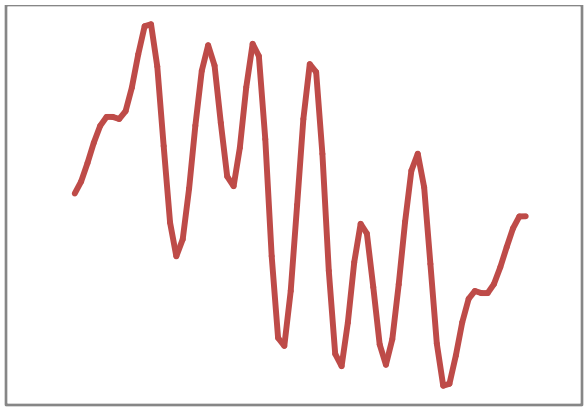
S No	**Line width (a_i) G**	**Relative intensity (y_{maxi})**	**Centre of spectrum (X_{oi}) G**	**Hyperfine splittings (A_i B_i) G**
1	10	40	3232	35 0
2	30	10	3233	34 0
3	15	9	3232	23 12
4	28	8	3233	35 0
5	28	8	3233	35 5
6	28	8	3233	35 10

Table: Magnetic parameters of component Triplet

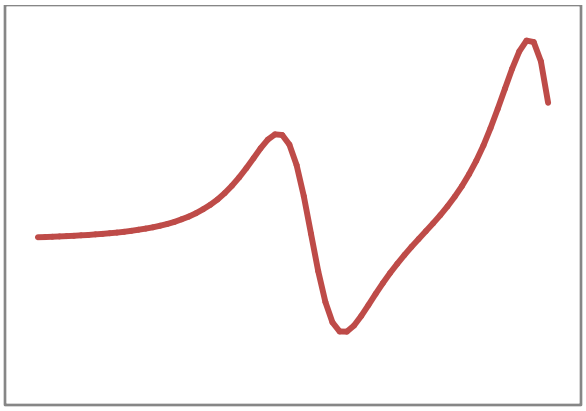
The stimulated spectra are shown as curves 1,2,3,4,5 and 6. Above results suggest that the shape of ESR spectra is strongly dependent on line width and relative intensity. The spectral resolution is found to depend on the (a/y) value. If (a/y) value is less, the spectral resolution is found to be more; whereas the resolution decreased with the increase of (a/y) value.



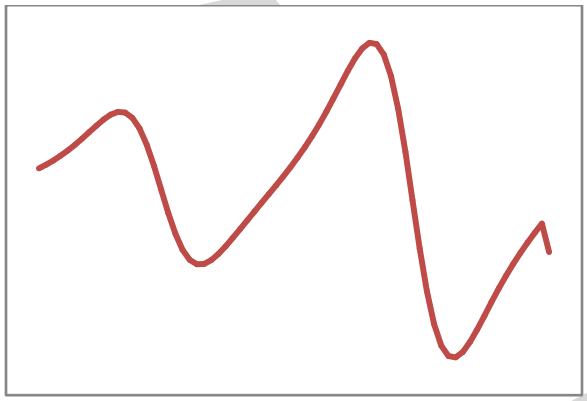
Curve 1



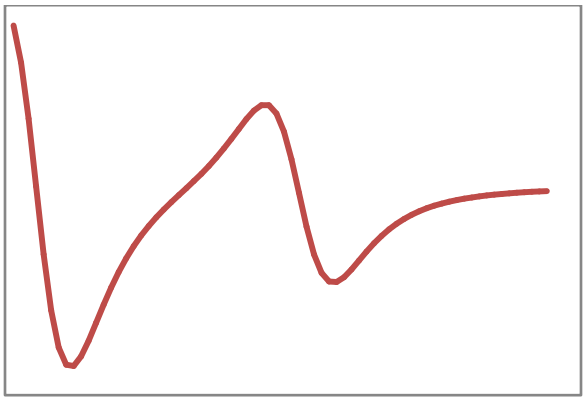
Curve 2.



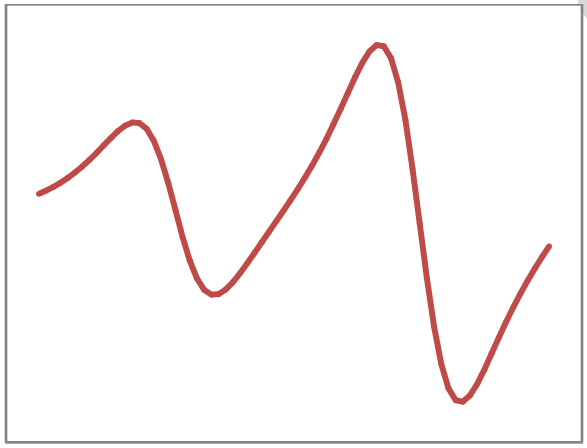
Curve 5.



Curve 3.



Curve 6.



Curve 4.

Figures: Triplet spectra stimulates with different values of magnetic parameters

Line separation is found to depend on the A_i and B_i values. Tf the other splitting constant is zero no change in hyperfine spacing is observed.

Conclusion

In conclusion hyperfine interactions are dependent on the magnetic parameters. The (a/y) value determines spectral resolution, while A,B value determines spectral separation.

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