Change in ESR line-shape with solvent

Product used：Electron Spin Resonance (ESR)

■ Change in ESR signal line-shape of TEMPOL with solvent

The solvent effect in ESR signal of solution sample is known to appear in the g-value, the hyperfine coupling constant (A-value) and the line-width. For example, the effect appears in the isotropic hyperfine splitting when the molecular motion is fast. It is known that in polar solvents, the density of unpaired electron on nitrogen atom increases and the A-value increases[1]. The g-value tends to decrease in polar solvents [2]. The line-width is considered to reflect the interaction with the solvent due to the difference in the rotational correlation time of the sample.

TEMPOL was diluted with each solvent of the benzene, the dimethylformamide (DMF), and the ultrapure water to prepare a solution with the same concentration (10^{-3} mol/L). The same amount of each solution was collected in a capillary tube and measured as shown in Figure. 1. Table 1 summarizes the g-values, A-values and line-widths of the signals for each solvent. Dielectric loss of solvents increases in the order of benzene < DMF < ultrapure water. The ESR signal intensity appears to be the largest when diluted with ultrapure water. On the one hand, when compared by the integrated value of the spectrum, the larger the dielectric loss of the solvent, the smaller the area. As shown above, the g-value, the A-value and the line-width of radicals in solution change depending on the environment.

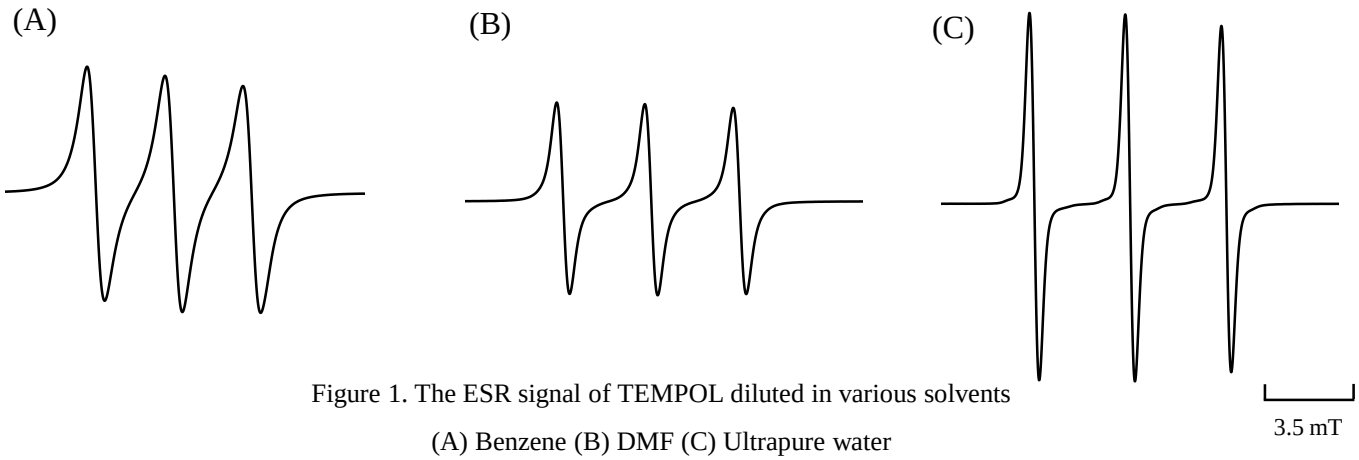

Figure 1. The ESR signal of TEMPOL diluted in various solvents
(A) Benzene (B) DMF (C) Ultrapure water

Table 1. ESR parameters in various solvents

Solvent	g-value	A-value (mT)	Line-width (mT)
Benzene	2.0062	1.53	0.34
DMF	2.0062	1.57	0.23
Ultrapure water	2.0058	1.70	0.17

Reference

[1] Hiroaki Ohya, Jun Yamauchi (1989) : Electron Spin Resonance -Material micro-characterization, Kodansha Inc. , p302.

[2] Kazuhiko Ishizu (1981) : Introduction to Practical ESR -Approach to Life Science-, Kodansha Inc. , p318.

JEOL Ltd.
3-1-2 Musashino Akishima Tokyo 196-8558 Japan Sales Division Tel. +81-3-6262-3560 Fax. +81-3-6262-3577
www.jeol.com ISO 9001 • ISO 14001 Certified
▼ Local office
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