

Investigation of triplet fullerene C₇₀ lineshape EPR under continuous light illumination: zero field splitting parameters distribution

Uvarov M.N.^{1*}, Kulik L.V.¹, Pichugina T.I.¹, Dzuba S.A.^{1,2}

¹Institute of Chemical Kinetics and Combustion, 630090, Institutskaya 3, Novosibirsk, Russia

²Novosibirsk State University, 630090, Pirogova 2, Novosibirsk, Russia

*e-mail: uvarov@kinetics.nsc.ru

Continuous wave (CW) and pulse electron paramagnetic resonance (EPR) spectra of triplet state of fullerene C₇₀ in various glassy matrices were obtained at temperatures 5K÷260K. At temperatures below 30K the emission region appeared at EPR spectra because populations of ³C₇₀ spin sublevels are non-equilibrium immediately after photoexcitation. At low temperatures spin-lattice relaxation time of ³C₇₀ becomes comparable with triplet ³C₇₀ lifetime. At temperatures higher 50K EPR spectra contained only absorptive part.

Transversal relaxation rate was obtained by pulse EPR methods. It does not substantially depend on EPR spectrum position. So, exchange process within EPR spectrum due to rotations or pseudorotations of ³C₇₀ molecule around its long symmetry axis has not appreciably influence the EPR lineshape below 77K.

CW EPR lineshape of ³C₇₀ at 77K was simulated supposing the equilibrium population of ³C₇₀ spin sublevels. The zero field splitting parameters *D* and *E* were revealed to have probability distributions. EPR lineshape of ³C₇₀ was simulated successfully assuming Gaussian probability distribution of *D* value, whereas *E* value probability distribution function was different. It had a property: at *E* = 0 the probability value is 0. At work [1] EPR lineshape of ³C₇₀ was simulated assuming rectangular probability density of *E* value.

With temperature increasing higher 100K the rapid rising of the transversal relaxation rate of ³C₇₀ was obtained from pulse EPR data. The phenomenon can be explained by ³C₇₀ molecule motion due to glass matrix softening. CW EPR lineshape narrowing with temperature increasing confirmed the suggestion about ³C₇₀ motions.

D and *E* values distribution can be explained by dependence of molecular ³C₇₀ Jahn-Teller distortion on local surrounding of each molecule. We can conclude that ³C₇₀ symmetry is not higher than D_{2h}.

- [1] M.N. Uvarov, L.V. Kulik, T.I. Pichugina, S.A. Dzuba, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, DOI: 10.1016/j.saa.2011.01.047 (2011)