

## Investigation of triplet fullerene C<sub>70</sub> lineshape EPR under continuous light illumination: zero field splitting parameters distribution

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Continuous wave (CW) and pulse electron paramagnetic resonance (EPR) spectra of triplet state of fullerene C<sub>70</sub> in various glassy matrices were obtained at temperatures 5K÷260K. At temperatures below 30K the emission region appeared at EPR spectra because populations of <sup>3</sup>C<sub>70</sub> spin sublevels are non-equilibrium immediately after photoexcitation. At low temperatures spin-lattice relaxation time of <sup>3</sup>C<sub>70</sub> becomes comparable with triplet <sup>3</sup>C<sub>70</sub> 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 <sup>3</sup>C<sub>70</sub> molecule around its long symmetry axis has not appreciably influence the EPR lineshape below 77K.

CW EPR lineshape of <sup>3</sup>C<sub>70</sub> at 77K was simulated supposing the equilibrium population of <sup>3</sup>C<sub>70</sub> spin sublevels. The zero field splitting parameters  $D$  and  $E$  were revealed to have probability distributions. EPR lineshape of <sup>3</sup>C<sub>70</sub> 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 <sup>3</sup>C<sub>70</sub> was simulated assuming rectangular probability density of  $E$  value.

With temperature increasing higher 100K the rapid rising of the transversal relaxation rate of <sup>3</sup>C<sub>70</sub> was obtained from pulse EPR data. The phenomenon can be explained by <sup>3</sup>C<sub>70</sub> molecule motion due to glass matrix softening. CW EPR lineshape narrowing with temperature increasing confirmed the suggestion about <sup>3</sup>C<sub>70</sub> motions.

$D$  and  $E$  values distribution can be explained by dependence of molecular <sup>3</sup>C<sub>70</sub> Jahn-Teller distortion on local surrounding of each molecule. We can conclude that <sup>3</sup>C<sub>70</sub> symmetry is not higher than D<sub>2h</sub>.

- [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)