Fullerene C_{70} triplet zero-field splitting parameters revisited from light-induced EPR spectra at thermal equilibrium

Uvarov M.N.[1]*, Kulik L.V.[1], Pichugina T.I.[1], Dzuba S.A.[1,2]

[1]*Institute of Chemical Kinetics and Combustion, 630090, Institutskaya 3, Novosibirsk, Russia*
[2]*Novosibirsk State University, 630090, Pirogova 2, Novosibirsk, Russia*
**e-mail: uvarov@kinetics.nsc.ru*

X-band continuous wave (CW) electron paramagnetic resonance (EPR) and echo-detected (ED) EPR spectra of triplet state of fullerene C_{70} in decaline, o-terphenyl, toluene and toluene-d_8 molecular glasses, and in polymethylmethacrylate (PMMA) polymer were obtained under continuous light illumination. At temperatures below 30 K EPR spectra correspond to a non-equilibrium polarization within spin sublevels of $^3C_{70}$. Above 30 K the spectra are characteristic for Boltzmann equilibrium. $^3C_{70}$ CW EPR spectra at 77 K were simulated fairly well using distribution of the zero-field splitting *D* and *E* parameters. These distributions may be caused by inhomogeneity of the glassy matrix surrounding, which influences the Jahn-Teller distortions of $^3C_{70}$ molecules (*D*-strain and *E*-strain). In addition to the broad triplet line, a narrow line in the center of CW EPR spectrum was observed, its nature is briefly discussed.

ED EPR spectrum obtained at the same conditions has a narrow hole in the center of the spectrum. With increase of the microwave pulse power this hole transforms into a single narrow absorptive line. Numerical simulations by density matrix formalism confirm that the central hole originates from a simultaneous excitation of both allowed electron spin transitions of the triplet, because of their degeneracy at this spectral position [1].

[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)