



# Photo-induced charge separation process in (PCBM-C<sub>120</sub>O)/(M3EH-PPV) blend solid film studied by means of X and K-bands ESR at 77 and 120 K

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## ABSTRACT

The new fullerene dimer adduct PCBM-C<sub>120</sub>O was studied as an electron acceptor by light-induced ESR (LESR) when blended with the electron donor-conjugated polymer M3EH-PPV in a thin solid film. ESR parameters for the PCBM-C<sub>120</sub>O anion radical and the M3EH-PPV polaron (triaxial  $g_{x,y,z}$  factors) were determined by X- and K-band ESR techniques at temperatures of 77 and 120 K. It was found that isotropic  $g_0$  of PCBM-C<sub>120</sub>O anion radical ESR spectra obtained in this blend under illumination is close to  $g$ -factor of electrochemically reduced (C<sub>120</sub>O)<sup>-•</sup> and does not coincide with the analogous parameter of (C<sub>120</sub>O)<sup>2-••</sup> (reported in literature). Spin relaxation parameters ( $T_1$  and  $T_2$ ) of the PCBM-C<sub>120</sub>O anion radical and M3EH-PPV positive polaron are similar to  $T_1$ ,  $T_2$  for light-induced ion radicals in the P3HT/PCBM blend.

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## 1. Introduction

The search for and study of new effective donor/acceptor compounds for photovoltaics continues to be one of the most important goals for the application and understanding of the fundamental aspects of electron transfer in solid organic semiconductors. Mono-fullerene anion radicals and their various mono-adducts exhibit good properties as electron acceptors in mediums with conjugated polymers. The photovoltaic properties of the most effective fullerene derivatives for solar cell applications, including the mono-fullerene adduct 1-(3-methoxycarbonyl)propyl-1-phenyl-[6,6]-methano fullerene (PCBM), have been widely introduced in numerous literature sources (for example, discussed in [1a,b]); this is, however, not the case for the fullerene dimer composites. The unique possibility of mono-fullerene and its derivatives to accept not only one, but several electrons and create poly-anions C<sub>60</sub><sup>(n-)</sup> where  $n=2$  through 5 (theoretically  $n=6$ ) has already been established experimentally by electrochemical methods (partly with the use of ESR). This has been reported in the references sum-

marized in review [2a] and also in some other recently published works [2b,c]. However, the above properties for  $n \geq 2$  have not been demonstrated in any experiments where the photo-induced charge separation processes (CSP) is expected in the donor-acceptor composites medium. Regarding the most stable poly-anion radical C<sub>60</sub><sup>(2-)</sup>, one can see that an alternative for the di-anion of mono-fullerene and its derivatives could be the di-anion of di-fullerene and its derivatives. The study of di-fullerene reduction/oxidation properties has already been performed [3a,b]. The reduction of C<sub>120</sub>O to (C<sub>120</sub>O)<sup>6-</sup> was successfully demonstrated electrochemically [3a] and the reduction to (C<sub>120</sub>O)<sup>4-•</sup> and (C<sub>120</sub>OS)<sup>3-•</sup> was recorded by ESR in [3a] and [3b], respectively. Concerning ESR, it should be pointed out that its application to the electrochemical reduction/oxidation process study can give unique information about the spin states of di-fullerene ions (doublet, triplet state [3a,b]). Nevertheless, it should be noted that contrary to the electrochemical method in previous ESR and LESR studies, the number of charges cannot be established reliably from the ESR spectra in all cases. Therefore, from now on only the sign of charge will be denominated for the anion radical in this report. Although as an example of CSP with di-fullerene has already been demonstrated for solar cell applications [4a], we report here what is most likely one of the first experiments of photo-induced CSP registration by LESR in (fullerene dimer)/(conjugated polymer) blends.

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