

# Supplementary Materials

of

## Non-functionalized fullerenes and endofullerenes in aqueous dispersions as superoxide scavengers

by

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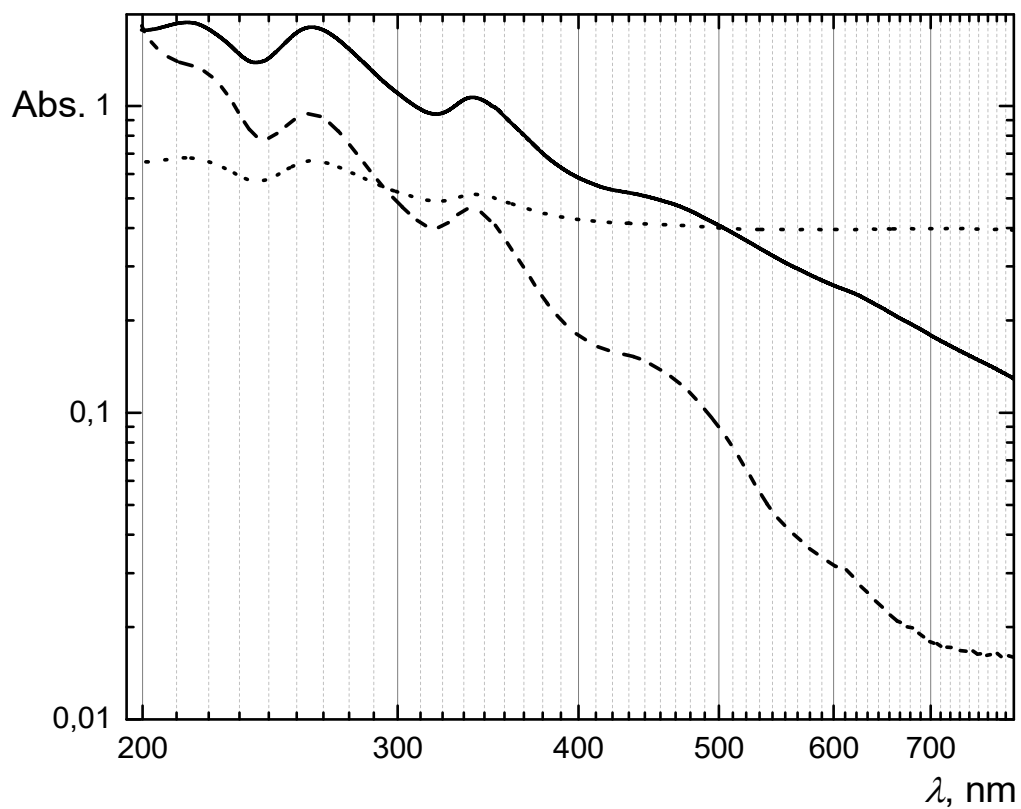
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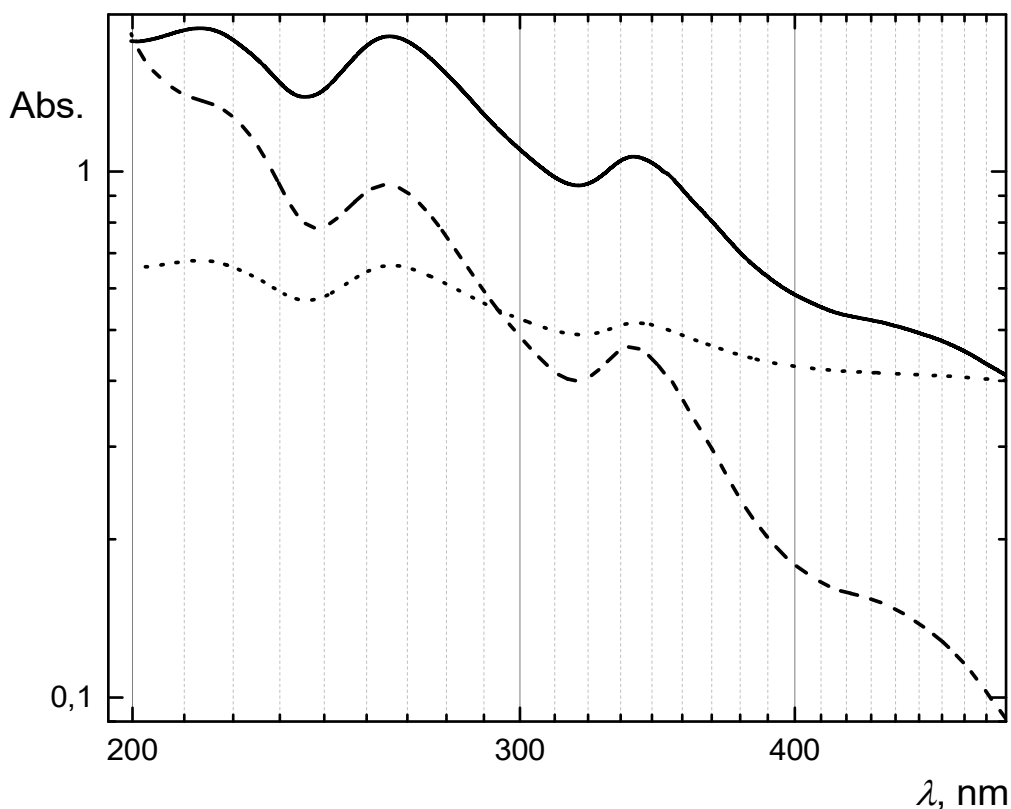
## 1. Ultraviolet-visible absorbance measurements



**Figure S1.** Absorbance spectra in the log-log coordinates of aqueous fullerene dispersions of C<sub>60</sub> in the range 190–800 nm:

- (i) native (dotted line) with a significant scattering component (pathlength 0.2 cm,  $37.9 \pm 0.5$  ppm);
- (ii) filtered through 0.22  $\mu\text{m}$  (dashed line) with a lower scattering component (pathlength 1.0 cm,  $15.7 \pm 0.6$  ppm);
- (iii) sample after sedimentation during 24h (solid line) with an appropriate scattering component (pathlength 1.0 cm,  $6.8 \pm 0.7$  ppm);

scanning rate 40 nm/min, data interval 0.067 nm, integration time in each point 1.0 s.



**Figure S2.** Absorbance spectra in the log–log coordinates of aqueous fullerene dispersions of C<sub>60</sub> in the range 190–500 nm:

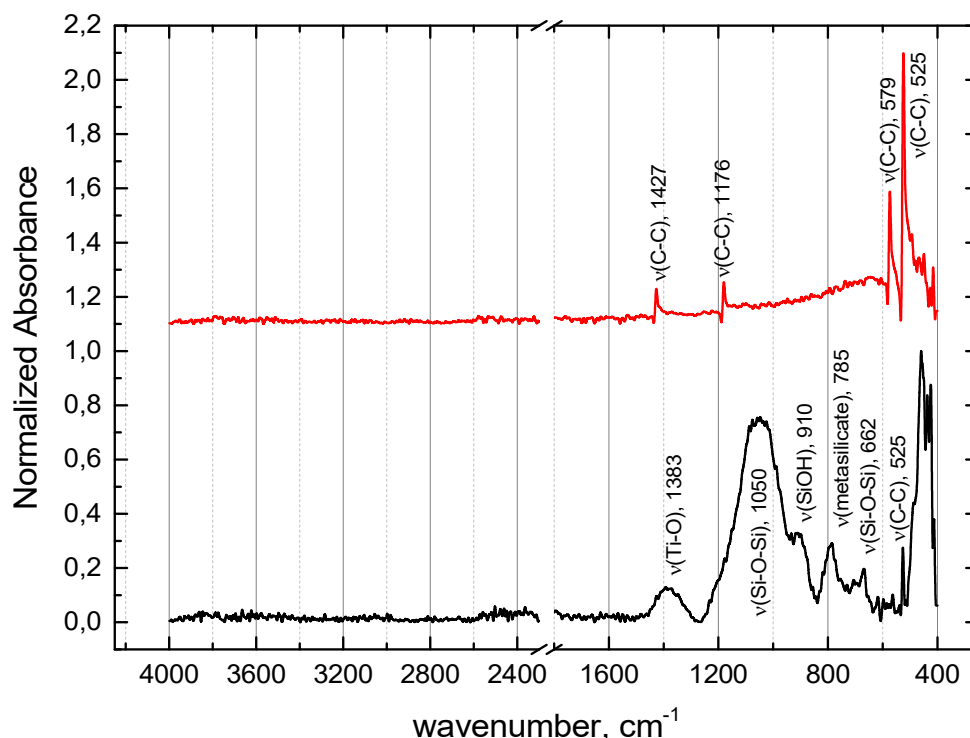
- (iv) native (dotted line) with a significant scattering component (pathlength 0.2 cm,  $37.9 \pm 0.5$  ppm);
- (v) filtered through 0.22  $\mu\text{m}$  (dashed line) with a lower scattering component (pathlength 1.0 cm,  $15.7 \pm 0.6$  ppm);
- (vi) sample after sedimentation during 24h (solid line) with an appropriate scattering component (pathlength 1.0 cm,  $6.8 \pm 0.7$  ppm);

scanning rate 40 nm/min, data interval 0.067 nm, integration time in each point 1.0 s.

Filtering or samples sedimentation improves their spectral characteristics for all aqueous dispersions (C<sub>60</sub>, C<sub>70</sub> and Gd@C<sub>82</sub>). The scattering of the filtering samples (through 0.22  $\mu\text{m}$ ) is decreased, and the peaks (absorbance maxima) become narrower. As well, we isolated a narrow-sized fraction of fullerene nanoparticles with an average cluster diameter *ca.*  $121 \pm 5$  nm. As well, absorbance maxima at 261 and 338 nm have coincided, but still, sample filtering allowed us to observe additional peaks at 447 nm (mid absorption band in a range 400–550 nm) and 607 nm. According to [1] the absorbance spectra coincided with a slight red shift in this work.

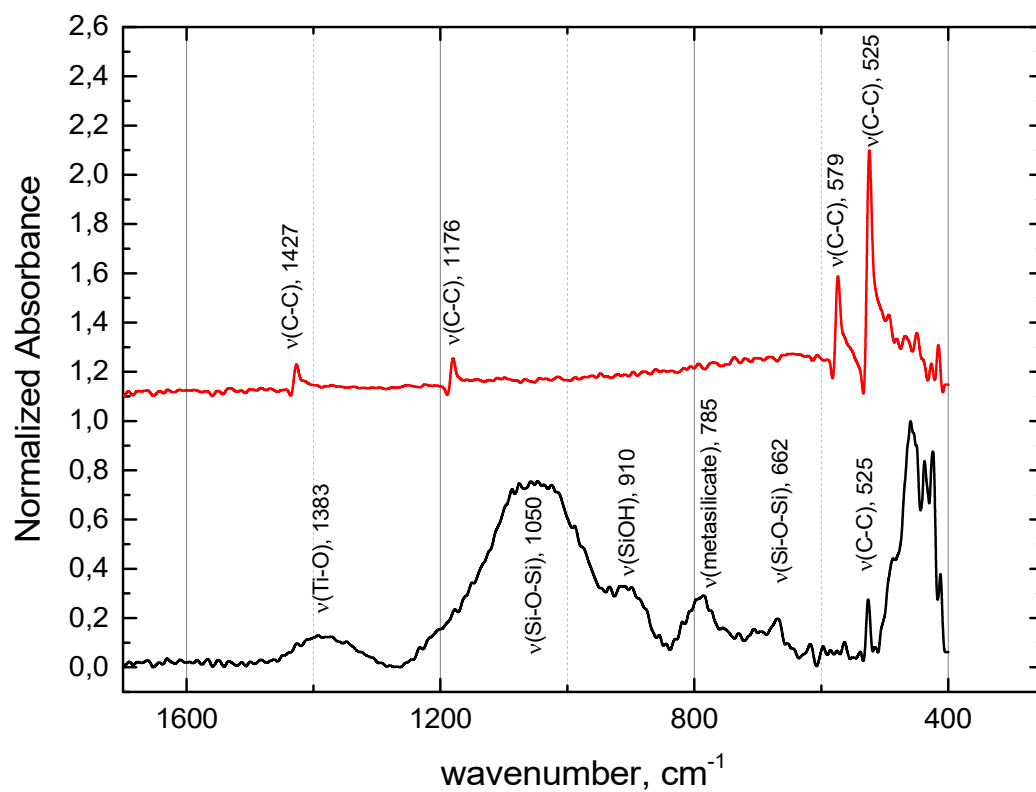
## 2. Fourier-transform infrared spectroscopy

The FTIR spectroscopy was applied to clarify the nature and the state of titanium and silicon particles. According to ICP–AES titanium and silicon was observed after an ultrasound probe sonication of fullerene–water systems. Owing to the possible generation of free radicals by sonolysis of water, it was supposed to check the metal or nonmetal oxide formation.



**Figure S3.** FTIR-Absorbance spectra in the range 4000–400 cm<sup>-1</sup> of pristine C<sub>60</sub> (red line), concentrated AFD C<sub>60</sub> (black line) by centrifugation, scans — 64, baseline scans — 64 data interval — 1 cm<sup>-1</sup>.

The FTIR-ATR spectra of pristine C<sub>60</sub> include all C–C bands [2], as for AFD C<sub>60</sub> obtained by a direct probe sonication of water–fullerene suspension, additional signals are observed. Figure S3 shows of AFD C<sub>60</sub> FTIR spectra. The bands of SiO<sub>2</sub>, TiO<sub>2</sub> NPs are present. In Figure S3 (line) the FTIR spectrum of TiO<sub>2</sub> NPs band clearly shows the signal at 1383 cm<sup>-1</sup> related to Ti–O modes [3-5]; band at 1050 cm<sup>-1</sup> correspond to silicon oxide, Si–OH or Si–O–Si modes [6,7]. For more detail, the figure with a narrower range is given (Figure S4)



**Figure S4.** FTIR-Absorbance spectra in the range 1650–400 cm<sup>-1</sup> of pristine C<sub>60</sub> (red line), concentrated AFD C<sub>60</sub> (black line) by centrifugation, scans — 64, baseline scans — 64 data interval — 1 cm<sup>-1</sup>.

### 3. References in supplementary materials

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