Electronic Supplementary Information for:

Solution phase n-doping of C_{60} and PCBM using tetrabutylammonium fluoride

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I. Materials and experimental procedures

UV-vis-NIR spectroscopy

Spectroscopic experiments were performed on a Perkin Elmer Lambda 1050 spectrometer. Ortho-dichlorobenzene (o-DCB) solutions were prepared from 99 % anhydrous o-DCB (Sigma Aldrich) and deoxygenated via freeze-pump-thaw method. 0.5 mM solutions of C_{60} were prepared from C_{60} (99.5 %, SES Research) and deoxygenated o-DCB. Solutions were subsequently deoxygenated to remove any O_2 introduced during transfer. Spectroscopy of solutions was carried out using a custom designed airfree cuvette. Equivalents of tetrabutylammonium fluoride trihydrate (Fluka) were added to the cell as solid prior to introduction of C_{60} solution under N_2. PCBM (99%, SES Research) solutions were prepared using deoxygenated CH_2Cl_2 (Omnisolv spectroscopic grade) under airfree conditions.

Electrochemistry

Electrochemical measurements were performed using a standard 3-electrode geometry with a glassy carbon working electrode, platinum coil counter electrode, and silver wire pseudo reference separated from the analyte solution via a vycor frit. Subsequent to experiments, the reference was calibrated versus ferrocene under identical conditions. Electrolyte solution was 0.1 M tetrabutylammonium tetrafluoroborate (Sigma Aldrich) in deoxygenated o-DCB. All experiments were performed under airfree conditions (active N_2 atmosphere) and data collected using a custom designed potentiostat.

^{19}F NMR

The ^{19}F NMR spectra were collected on a Bruker-Advance-III-HD 600MHz NMR spectrometer equipped with a 5mm Prodigy CryoProbe. The samples were prepared in 99.8% $CDCl_3$ (Cambridge Isotope Laboratories).

FTIR

FTIR experiments were performed using a Nicolet FTIR spectrometer. Thin films were cast onto KBr substrates under airfree conditions and measurements conducted under airfree conditions utilizing a custom design chamber equipped with CaF optical windows. Spectra were recorded at 2 cm^{-1} resolution for 16 scans.

II. Figures

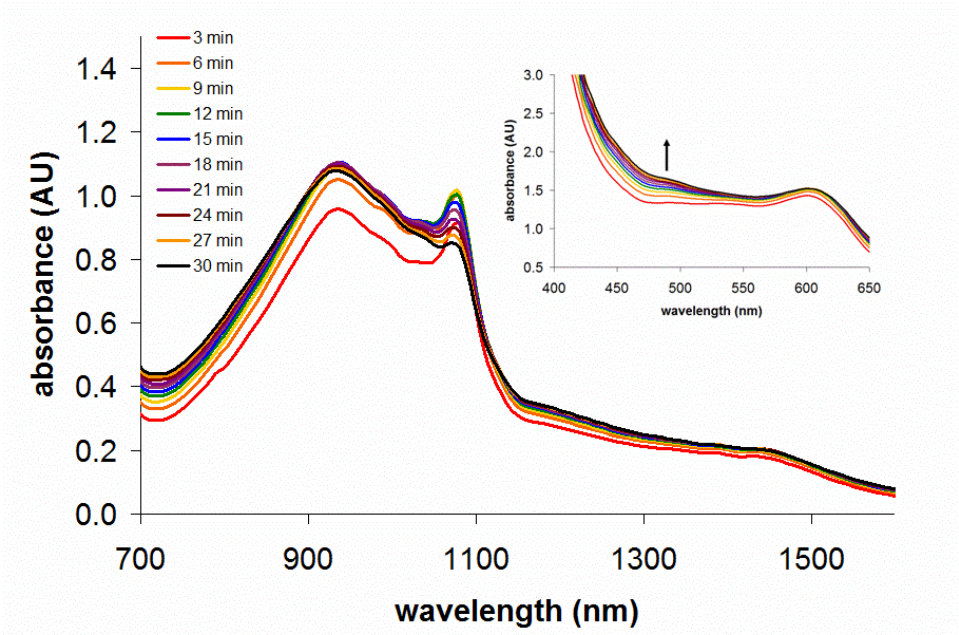

Figure S1. UV-vis-NIR time progression (180 s intervals) of 0.5 mM C_{60} solution with 4 eq TBAF. Inset shows high energy portion of the spectrum.

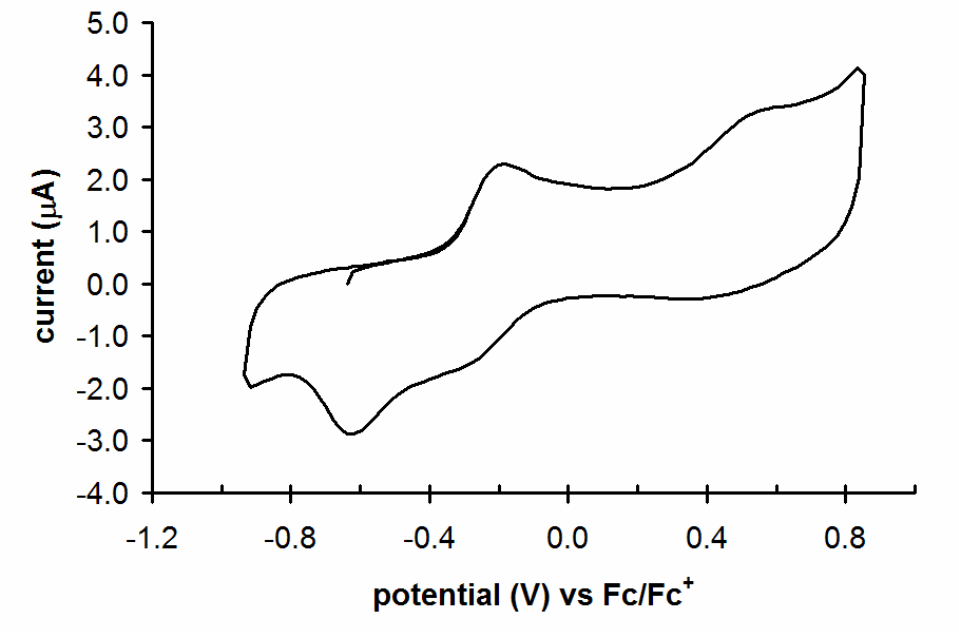

Figure S2. CV of crude product of PCBM / TBAF mixture after evaporation of solvent and re-dissolving in acetonitrile (0.1M $TBABF_4$).

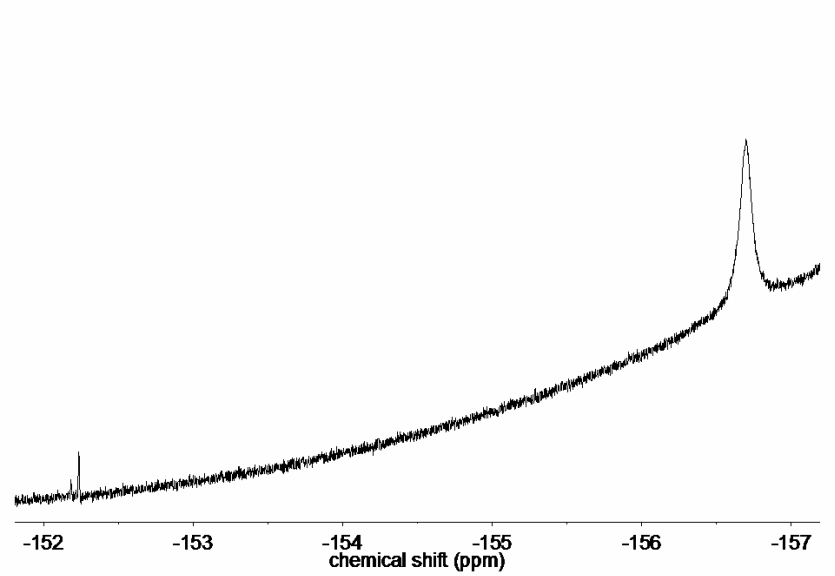

Figure S3. ^{19}F NMR of PCBM / TBAF (5 eq) solution after reaction by evaporating the solvent and rediluting $CDCl_3$. The small peaks at ~152 ppm are assigned to FHF^- impurities detected in control spectra.

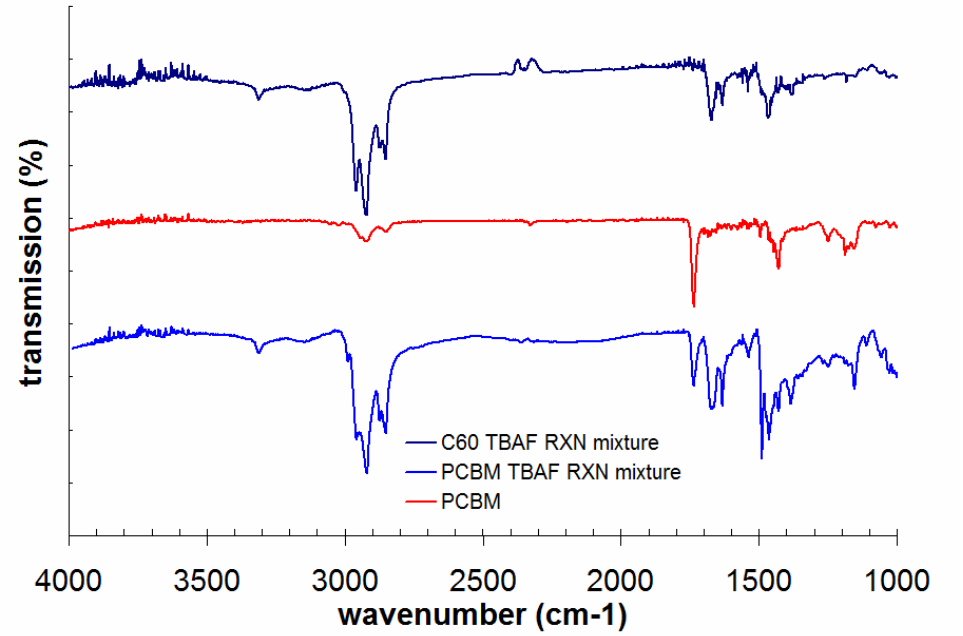

Figure S4. FTIR of C_{60} / TBAF (7 eq TBAF) reaction solution (top), PCBM control (middle), and PCBM / TBAF (5 eq TBAF) reaction solution (bottom).

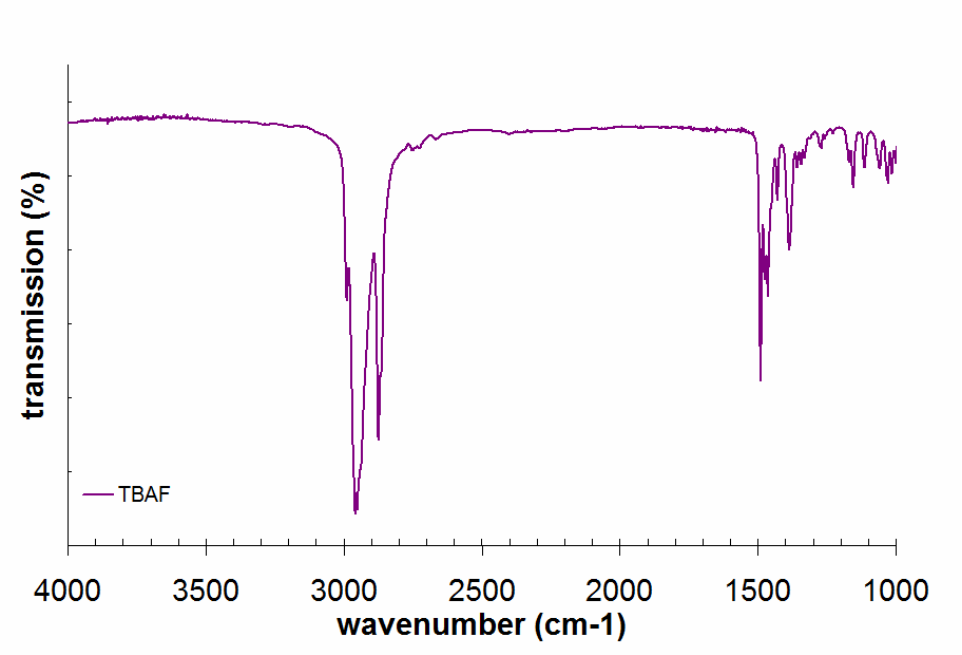

Figure S5. FTIR of TBAF film cast from CH_2Cl_2 onto KBR.