Electronic supplementary information for

Addition of CF_2 group to endohedral fullerene $Sc_3N@I_h$-C_{80}

Anastasia D. Pykhova, Olesya O. Semivrazhskaya, Nataliya A. Samoylova, Alexey V. Rybalchenko, Marco Rosenkranz, Ilya N. Ioffe, Alexey A. Popov and Alexey A. Goryunkov

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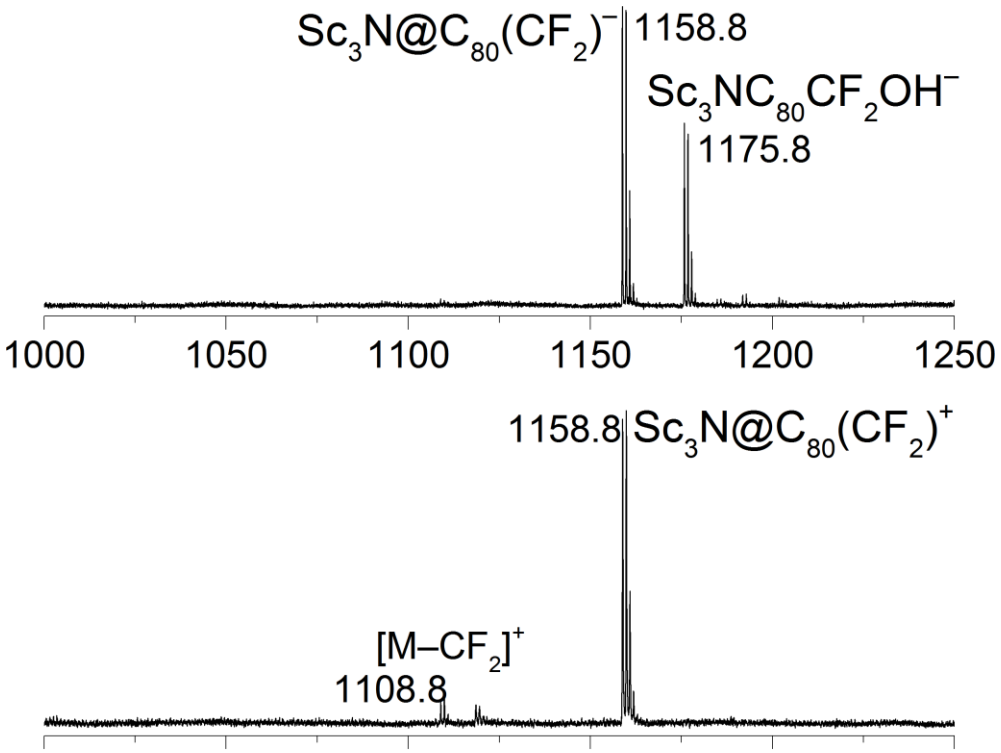

Figure *S*1. Negative ion (top) and positive ion (bottom) MALDI mass spectra of isolated $Sc_3N@C_{80}(CF_2)$.

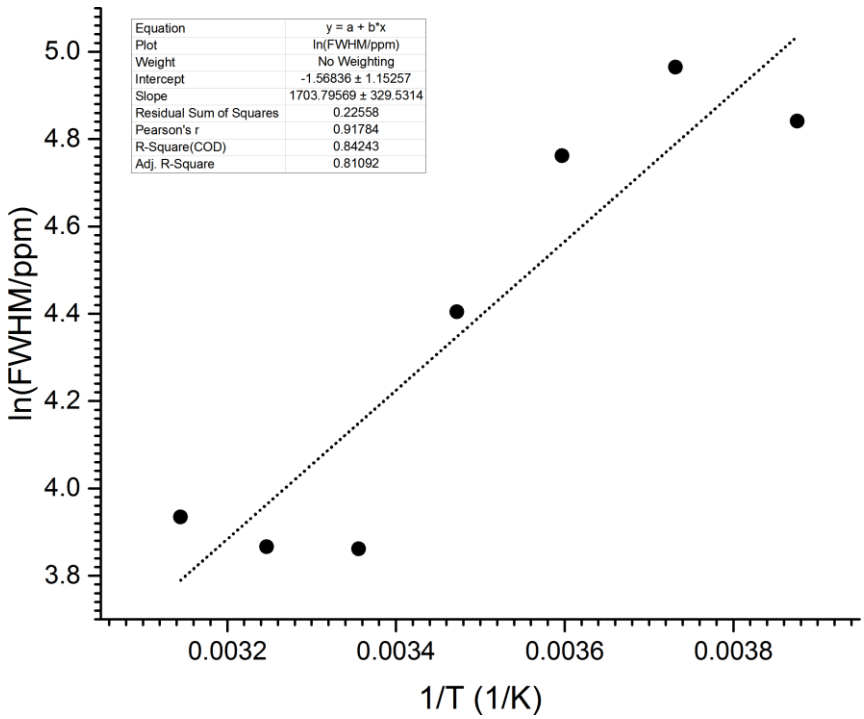

Figure *S*2. The temperature-dependent full width at half-maximum (FWHM) of a peak at ca. 190 ppm of ^{45}Sc NMR spectra of $Sc_3N@C_{80}(CF_2)$

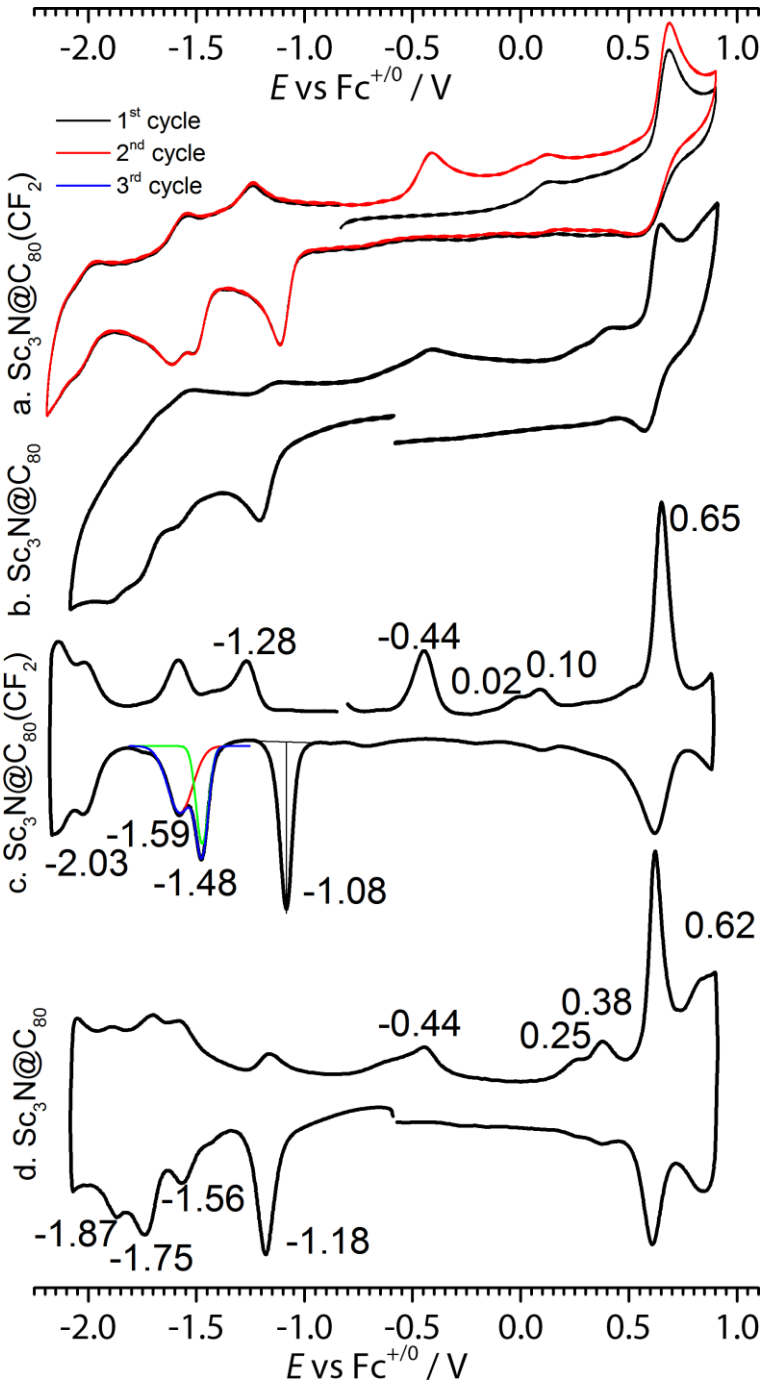

Figure *S*3. CV curves of (a) $Sc_3N@C_{80}(CF_2)$ and (b) $Sc_3N@I_h$-C_{80} (Pt, oDCB, 0.15 M Bu_4NBF_4, vs $Fc^{+/0}$, 100 mV s^{-1}, 30 °C). The deconvoluted CV curves are shown for (c, 2nd scan) $Sc_3N@C_{80}(CF_2)$ and (d) $Sc_3N@I_h$-C_{80} (the redox potentials are shown for deconvoluted curves).

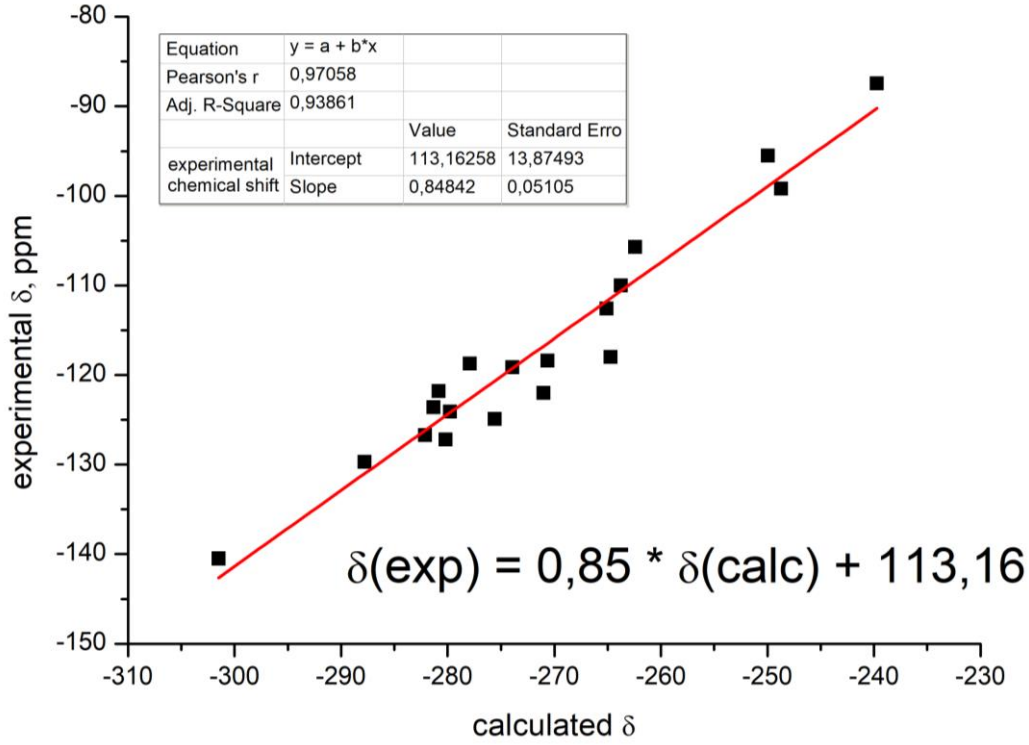

Figure *S*4. Experimental and calculated ^{19}F NMR chemical shifts correlation for CF_2-derivitized fullerenes: $C_{60}(CF_2)$, *cis*-2-$C_{60}(CF_2)_2$, $C_{60}(CF_2)H_2$, $C_{70}(CF_2)$, C_s-$C_{70}(CF_3)_8(CF_2)$, C_s-$C_{70}(CF_3)_8(CF_2)(OH)_2$, $C_{70}(CF_3)_8(CF_2)H(OH)$.

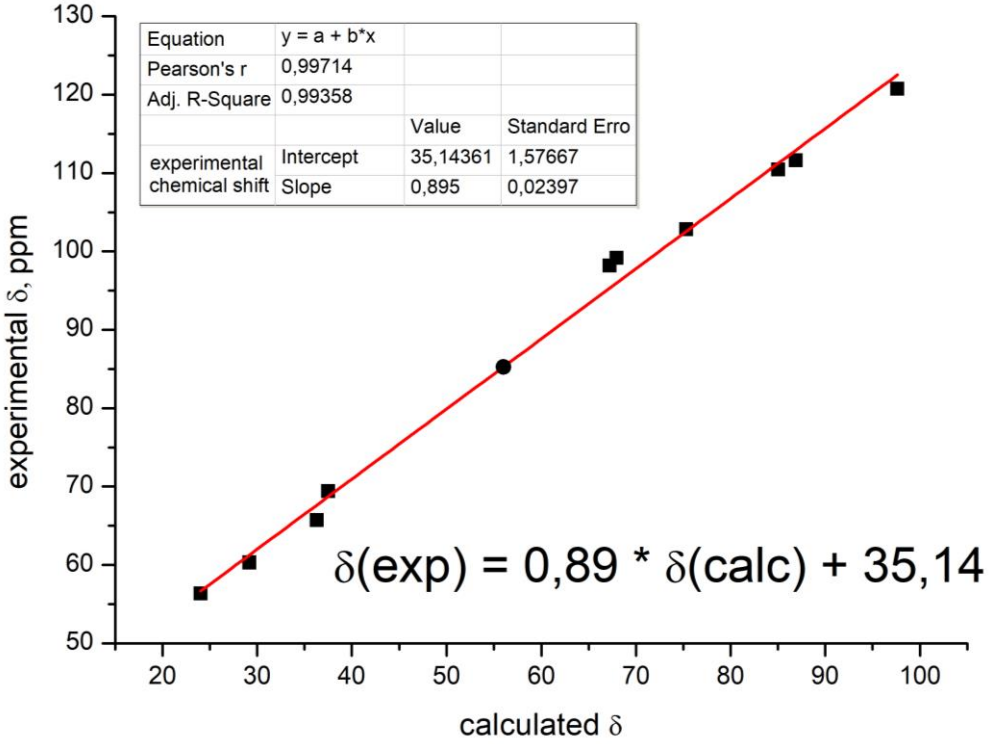

Figure *S*5. Experimental and calculated ^{13}C NMR chemical shifts of bridgehead and CF_2 carbon atoms for CF_2-derivitized fullerenes: $C_{60}(CF_2)$, $C_{60}(CF_2)H_2$, $C_{70}(CF_2)$, C_s-$C_{70}(CF_3)_8(CF_2)$.

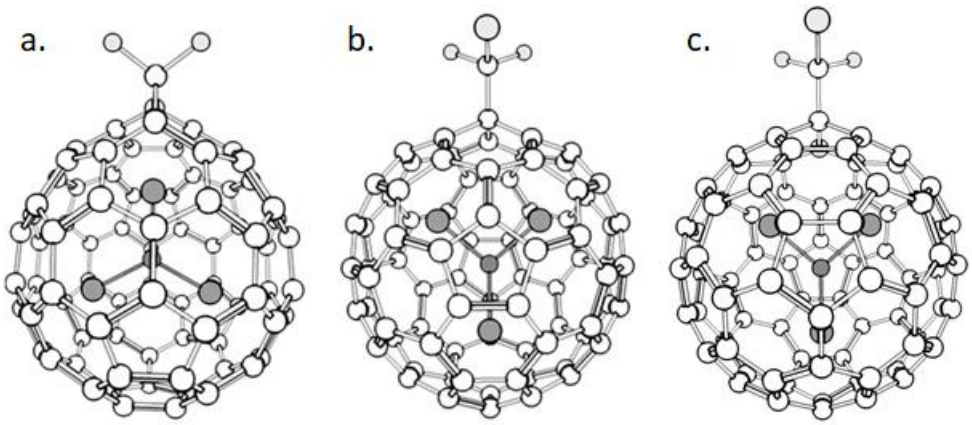

Figure *S*6. The conformers of (a) $Sc_3N@C_{80}(CF_2)$ as well as (b) THJ and (c) PHHJ $Sc_3N@C_{80}(CF_2Cl)^-$ intermediates, respectively.