Fluorination and Hydrogenation of Aza[60]fullerene

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Hydrogenation of aza[60]fullerene with Zn/HCl gives  $C_{59}NH_5$ . Fluorination with either MnF<sub>3</sub>, CeF<sub>4</sub> or K<sub>2</sub>PtF<sub>6</sub> gives  $C_{59}NF$ ,  $C_{59}NF_5$ ,  $C_{59}NF_{17}$ , and  $C_{59}NF_{33}$  with the highest fluorination level detected being in C<sub>59</sub>NF<sub>37</sub>. Various trifluoromethyl derivatives, especially of C<sub>59</sub>NF<sub>5</sub> viz. C<sub>59</sub>NF<sub>4</sub>CF<sub>3</sub>, C<sub>59</sub>NF<sub>3</sub>(CF<sub>3</sub>)<sub>2</sub> and C<sub>59</sub>NF<sub>2</sub>(CF<sub>3</sub>)<sub>3</sub>, and oxide derivatives of the highest fluorinated species, are formed also. In general, the higher the fluorination level, the shorter the HPLC retention times; trifluoromethylation reduces, and oxide formation increases, the HPLC retention times as is the case with the all-carbon fullerenes. C<sub>59</sub>NF<sub>33</sub> is the main product of the reaction, and is extremely volatile so that it gives an intense EI mass spectrum even at room temperature. It appears to be retained substantially on the HPLC Cosmosil Buckyprep column, which makes purification for NMR analysis difficult. The formation of most of the derivatives is interpreted in terms of their increased aromaticity compared to that of the  $C_{59}N$ .