Electronic Supplementary Material (ESI) for Dalton Transactions.

Magnetic moments and exchange coupling in nitride clusterfullerenes $Gd_xSc_{3-x}N@C_{80}$ (x = 1–3)

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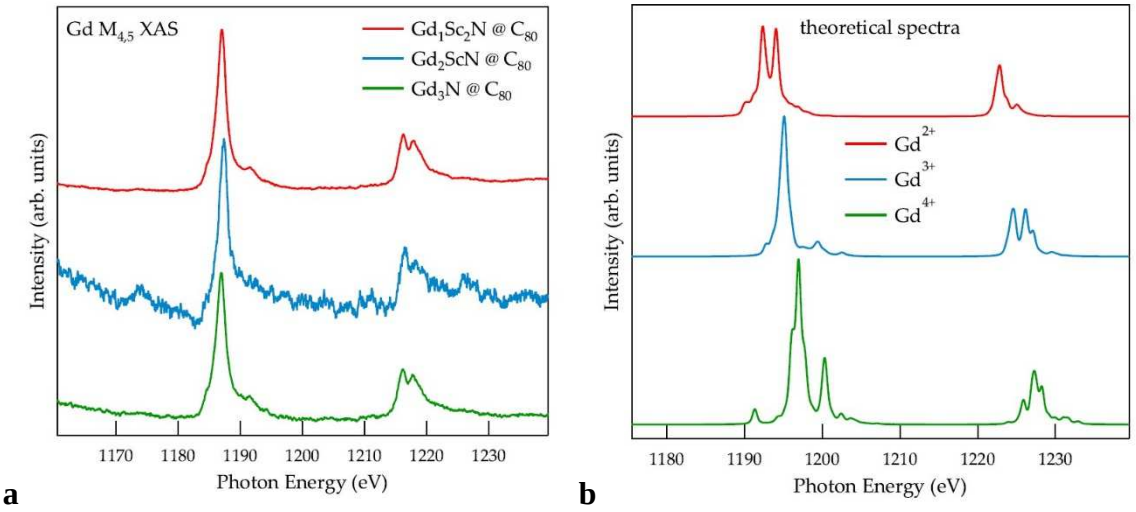

Figure S1 Experimental X-ray absorption spectra of $Gd_1Sc_2N@C_{80}$, $Gd_2Sc_1N@C_{80}$, $Gd_3N@C_{80}$ (a) and theoretical XAS spectra for Gd-ions: Gd^{2+}, Gd^{3+} and Gd^{4+}(b).

Synthesis and separation of Gd-Lu NCFs

Synthesis of Gd-Lu mixed nitride clusterfullerenes was performed using the same condition as for Sc-Gd NCFs, using melamine as a solid source of nitrogen. Figure S2 shows HPLC of the fullerene extract obtained in a typical synthesis. Mass spectrum of the main fraction shows that it consists mainly of $Lu_3N@C_{80}$, $GdLu_2N@C_{80}$, and $Gd_2LuN@C_{80}$. This fraction was further subjected to recycling HPLC, which allowed removal of $Gd_2LuN@C_{80}$. $GdLu_2N@C_{80}$ and $Lu_3N@C_{80}$ could not be separated at this step. Since $Lu_3N@C_{80}$ is non-magnetic, further separation was not performed. Instead, we added more $Lu_3N@C_{80}$ to achieve 1:10 ratio of $GdLu_2N@C_{80}$ and $Lu_3N@C_{80}$ in the sample to achieve high dilution of $GdLu_2N@C_{80}$ and minimize intermolecular interaction between Gd-containing molecules. Mixing $GdLu_2N@C_{80}$ and $Lu_3N@C_{80}$ ensures that after drying the sample, there is no phase separation (i.e. fullerenes with different carbon cages may crystallize separately, and hence mixing may not be efficient way to reduce intermolecular interaction between Gd-NCFs).

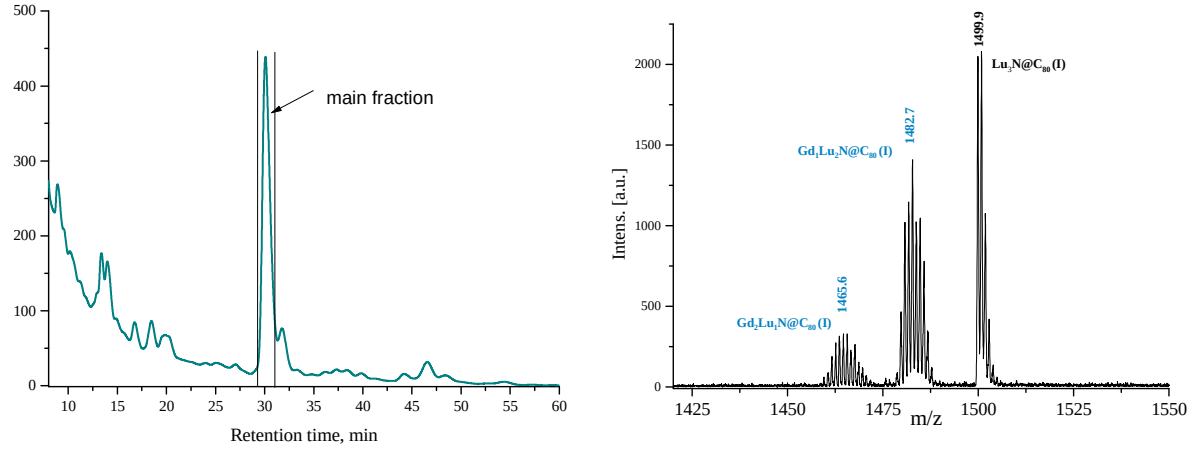

Figure S2. HPLC trace of Gd-Lu extract (left) and mass-spectrum of the main fraction (right).

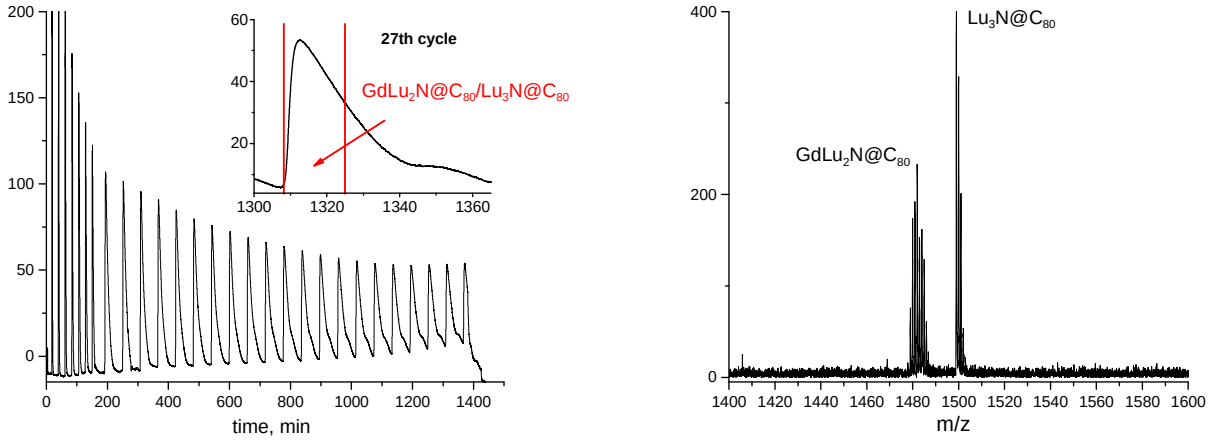

Figure S3. Recycling HPLC of the man Gd-Lu NCF fraction (left). The inset shows 27 cycles and marks collected part. Mass-spectrum of the sample after removal of $Gd_2LuN@C_{80}$ (right).