Supplementary Material (ESI) for Chemical Communications


# The Influence of the Cage Size on the Reactivity of Trimetallic Nitride Metallofullerenes: A Mono and Bisadduct of $Gd_3N@C_{80}$ and A Monoadduct of $Gd_3N@C_{84}$

Manuel N. Chaur[a], Frederic Melin[a], Andreas J. Athans[a], Bevan Elliott[a], Kenneth Walker[b], Brian C. Holloway[b] and Luis Echegoyen[a*]

*Contribution from the Department of Chemistry, Clemson University, Clemson, South Carolina 29634,*

*and Luna Innovations, Inc. (NanoWorks division), 521 Bridge street, Danville, Virginia 24541*

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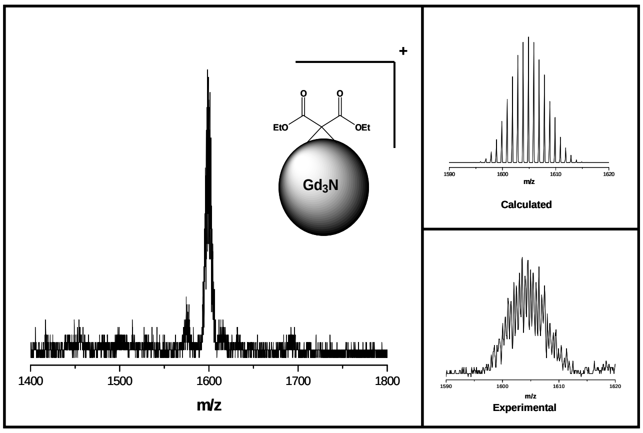
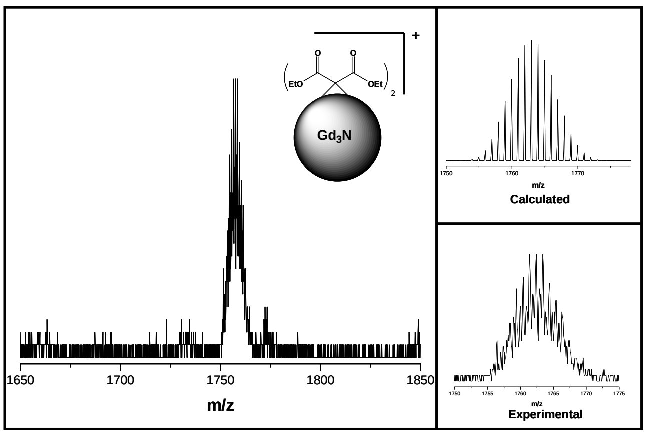
SUPPORTING INFORMATION

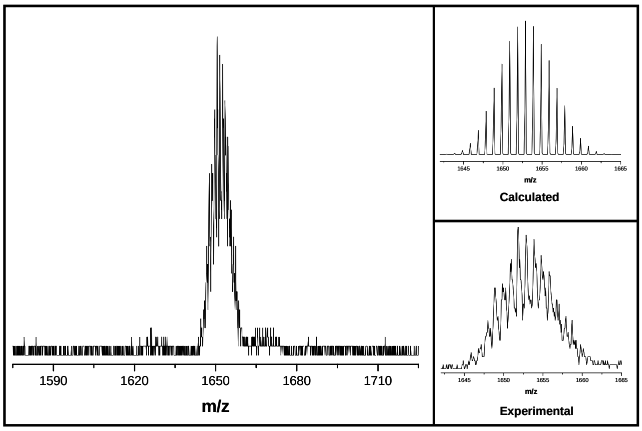
## I. Simulated and experimental mass spectra of isolated monoadduct $Gd_3N@C_{80}$-$C(CO_2Et)_2$



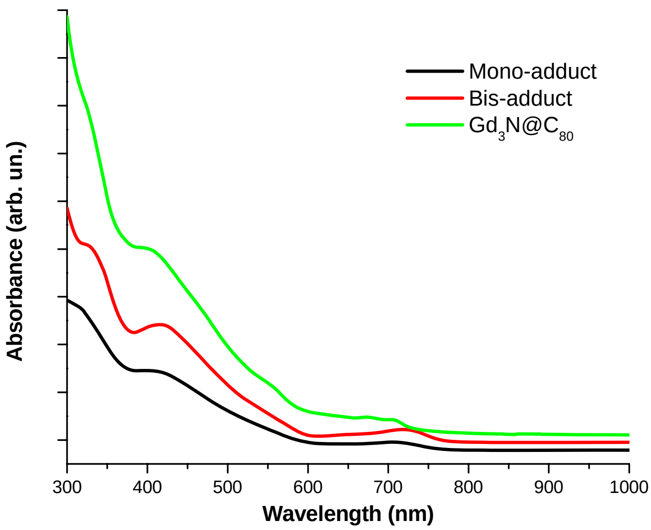

## II. Simulated and experimental mass spectra of isolated bisadduct $Gd_3N@C_{80}$-$[C(CO_2Et)_2]_2$



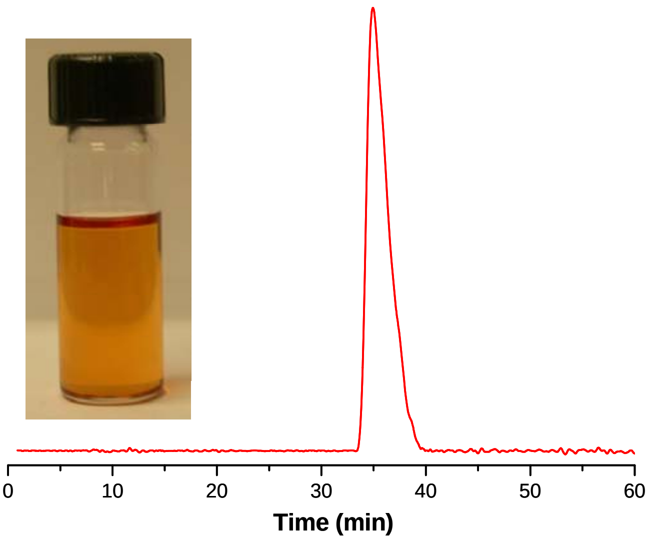
III. Simulated and experimental mass spectra of isolated monoadduct $Gd_3N@C_{84}$-$C(CO_2Et)_2$



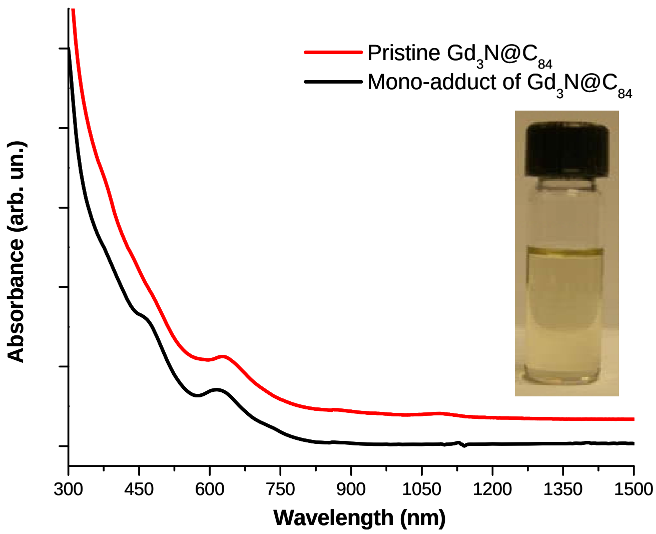

IV. UV-vis-NIR spectra of pure $Gd_3N@C_{80}$ ($I_h$), monoadduct $Gd_3N@C_{80}$-$(C(CO_2Et)_2)$, and bisadduct $Gd_3N@C_{80}$-$[C(CO_2Et)_2]_2$.



V. Two stage HPLC chromatogram of bisadduct $Gd_3N@C_{80}$-[C($CO_2$Et)$_2$]$_2$. Eluent: Toluene; Flow rate: 2.0 mL/min; Buckyprep and Buckyprep-M columns; Detection: 372 nm.




VI. UV-vis-NIR spectra of pure $Gd_3N@C_{84}$ and monoadduct $Gd_3N@C_{84}$-(C($CO_2$Et)$_2$).



VII. Relevant redox potentials for pristine $Gd_3N@C_{80}$ and $Gd_3N@C_{84}$ and their methano derivatives (V vs $Fc^+/Fc$).

| compound | $E_{1/2}$ ox$_1$ | $E_{pc}$ red$_1$ | $E_{pc}$ red$_2$ | $E_{pc}$ red$_3$ |
|---|---|---|---|---|
| $Gd_3N@C_{80}$ | +0.58 | -1.44 | -1.86 | -2.18 |
| $Gd_3N@C_{80}$-[C(COOEt)$_2$] | +0.58 | -1.39 | -1.83 | -2.17 |
| $Gd_3N@C_{80}$-[C(COOEt)$_2$]$_2$ | +0.59 | -1.40 | -1.88 | |
| $Gd_3N@C_{84}$ | 0.32 | -1.37 | -1.76 | |
| $Gd_3N@C_{84}$-[C(COOEt)$_2$] | 0.28 | -1.43 | -1.77 | -2.38 |