Supplementary Information

Stability of [10-12]cycloparaphenylene complexes with pristine fullerenes $C_{76, 78, 84}$ and endohedral metallofullerenes $M_3N@C_{78, 80}$

Markus Freiberger†, Olga A. Stasyuk†, Eugenia M. Pérez-Ojeda, Luis A. Echegoyen, Miquel Solà* and Thomas Drewello*

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1. Experimental Section

Chemicals: [n]CPPs and the fullerene C_{84} were purchased from TCI (Belgium, HPLC grad) while trifluoroacetic acid (TFA) and the fullerenes $C_{76/78}$ were purchased from Merck (Germany, HPLC grade). The solvents acetonitrile (ACN), dichloromethane (DCM) and toluene (tol) were purchased from VWR (Belgium, HPLC grade). Isomerically pure $M_3N@I_h$-C_{80} (M = Y, Gd, Lu) were purchased from Luna Innovations (Roanoke, VA, USA). The $Sc_3N@C_{2n}$ (n = 39, 40) isomers of this family were synthesized in an arc-discharge reactor using ammonia as a reactive-gas atmosphere and graphite rods packed with a mixture of Sc_2O_3 and graphite powder.[1] Starting with a mixture of $Sc_3N@C_{2n}$ (n = 34, 39, 40), large quantities of isomerically pure $Sc_3N@I_h$-C_{80} were separated in a single step by selective chemical oxidation/reduction using acetylferrocenium $[Fe(COCH_3C_5\text{-}H_{44})Cp]^+$ as an oxidizing agent and CH_3SNa as a reducing agent.[2] $Sc_3N@D_{3h}$-C_{78} was purified by three cycles of selective oxidative/reductive steps.[2] Finally, $Sc_3N@D_{5h}$-C_{80} was purified using a combination of two non-chromatographic methods, selective oxidative/reductive removal and reactivity differences.[2-3]

Sample preparation: Stock solutions of [n]CPPs were prepared in DCM (0.2 g l^{-1}) while the stock solutions of C_{84} and all EMFs were prepared in tol (0.2 – 0.5 g l^{-1}). For the ESI experiments a solvent mixture of ACN/DCM/tol (3:2:1, v:v:v) was used to which a small amount of TFA was added to enhance ionization.[4] The analyte concentrations was 1 x 10^{-5} mol l^{-1} in case of [n]CPPs while the concentration of the EMFs was up to three times the CPP concentration to enhance complex formation. The total concentration of C_{84} was unknown due to solubility issues.

Instrumentation: All mass spectrometry experiments were performed on a quadrupole time-of-flight mass spectrometer (microTOF-Q II, Bruker Daltonics, Bremen) equipped with an electrospray ionization (ESI) source. The analyte solutions were directly injected into the ESI source with a syringe pump at a flow rate of 180 µl h^{-1}. The temperature of the nitrogen heating gas was set to 180 °C and a capillary voltage of −4.5 kV was applied. Prior to each experiment, the instrument parameters were optimized to obtain good signal intensities. MS^2 experiments were carried out with N_2 as collision gas which was generated by a Parker LCMS64 nitrogen generator with a purity of 99.999% and a flow rate of 0.2 l min^{-1}.

Breakdown graphs: Breakdown graphs are a plot of the survival yield (SY) as a function of the collision energy. The SY is the ratio of precursor ions surviving the collision event at a given

collision energy against the total amount of ions observed. The collision energy is given as the laboratory energy (E_{lab}) divided by the degrees of freedom (DoF) of the hosting CPP. This approach of defining the collision energy is based on previous studies of our group.[5-7] However, the importance of considering DoF in the description of the collision event has also been addressed in several other publications.[8-17] The number of DoF was calculated according to Eqn. 1:

$$DoF = (3 * n) - 6 \quad (1)$$

With *n* corresponding to the number of atoms of the CPP.

All SY curves were recorded under multiple collision conditions and fitted with a sigmoid Boltzmann function. The collision energy, E_{50}, at which 50% of the parent ions have dissociated into their fragment ions is chosen as a relative measure of stability. The fragmentation energies obtained represent relative rather than absolute values with respect to the actual energy demand of the dissociation processes.

2. Additional mass spectrometry results

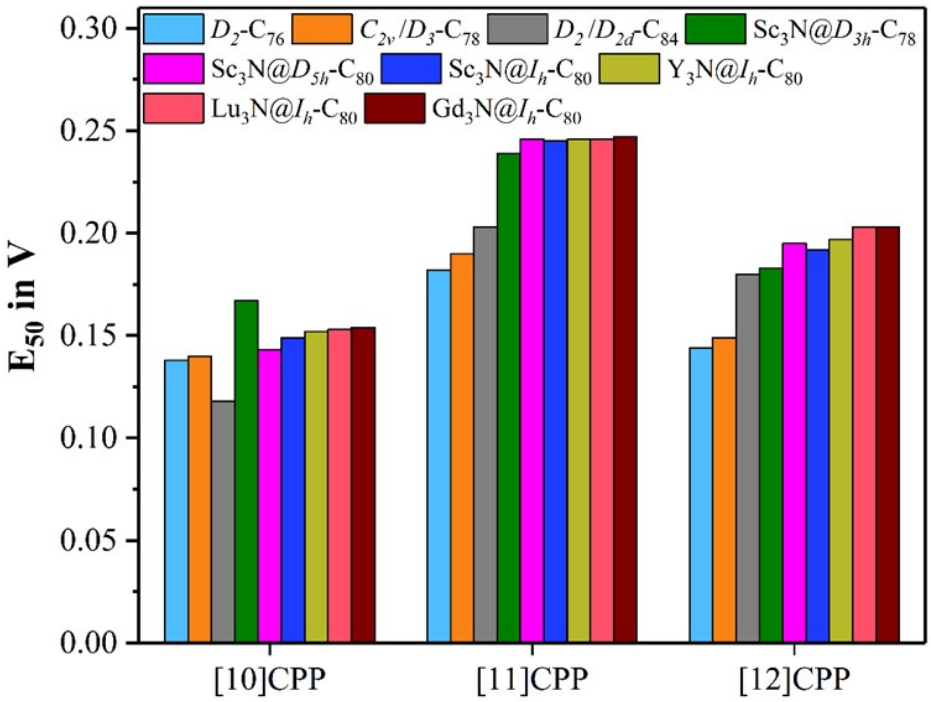


Figure S1. Collision energy, E_{50}, at which 50% of the parent ions have dissociated, for the studied host-guest complexes between [10]-, [11]- and [12]CPP and various fullerenes.

2.1 MS[1] spectra

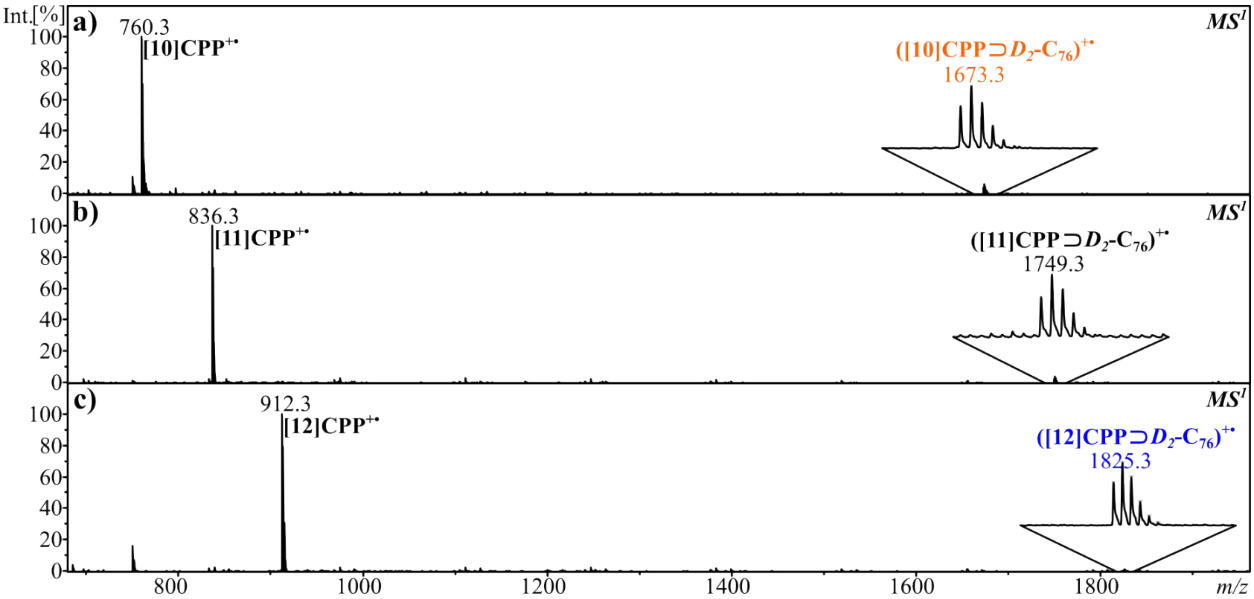


Figure S2. Positive-ion mode ESI MS[1] spectra of solutions containing C_{76} and **a)** [10]CPP, **b)** [11]CPP or **c)** [12]CPP.

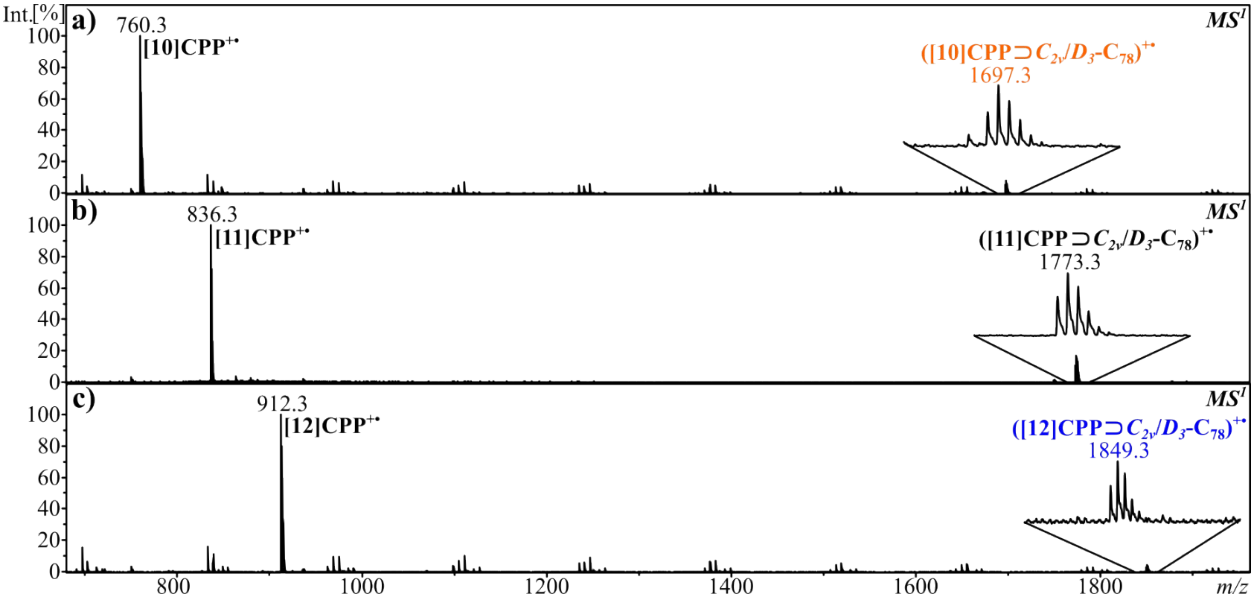


Figure S3. Positive-ion mode ESI MS[1] spectra of solutions containing C_{78} and **a)** [10]CPP, **b)** [11]CPP or **c)** [12]CPP.

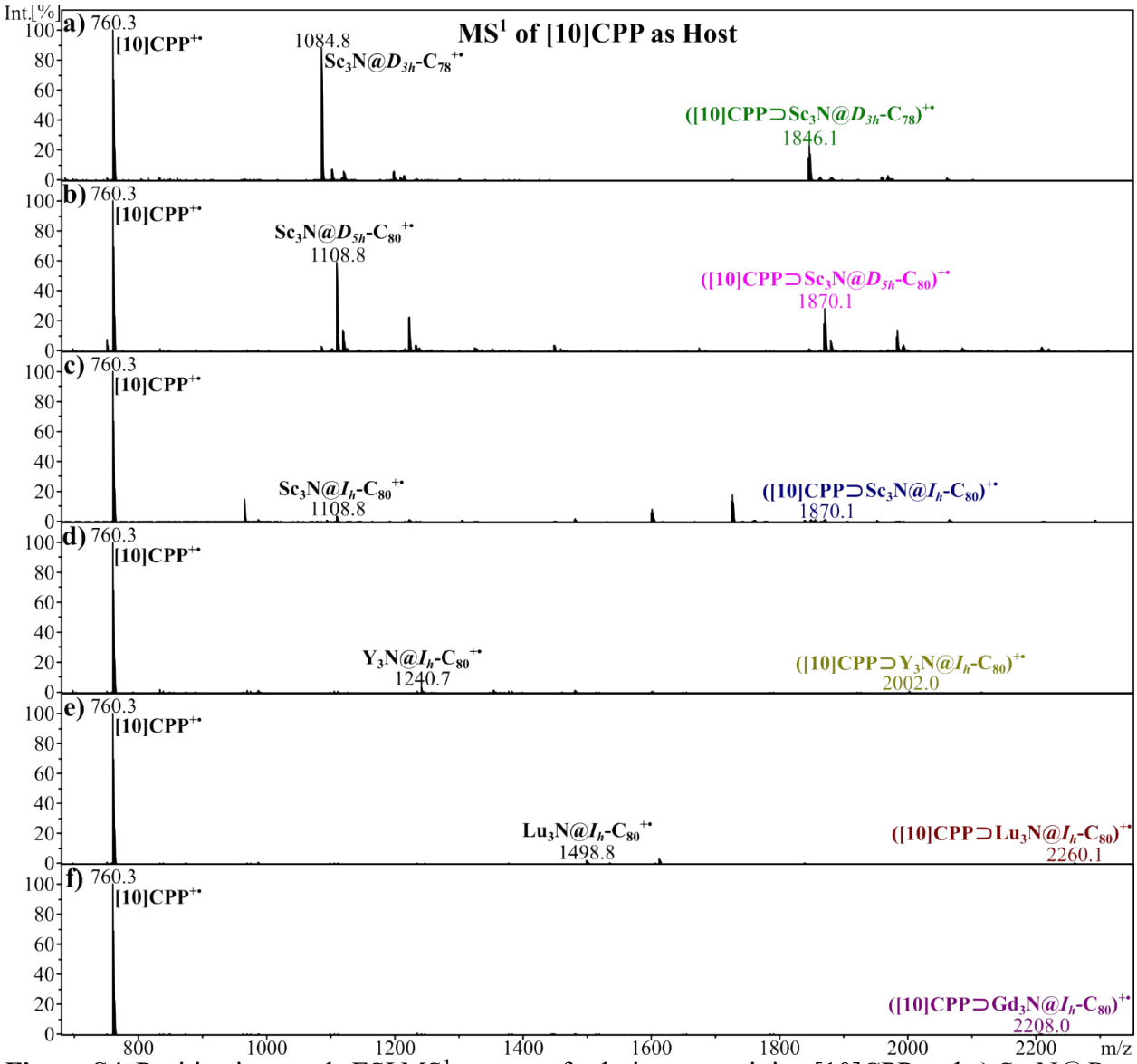


Figure S4. Positive ion-mode ESI MS^1 spectra of solutions containing [10]CPP and **a)** $Sc_3N@D_{3h}$-C_{78}, **b)** $Sc_3N@D_{5h}$-C_{80}, **c)** $Sc_3N@I_h$-C_{80}, **d)** $Y_3N@I_h$-C_{80}, **e)** $Lu_3N@I_h$-C_{80} and **f)** $Gd_3N@I_h$-C_{80}.

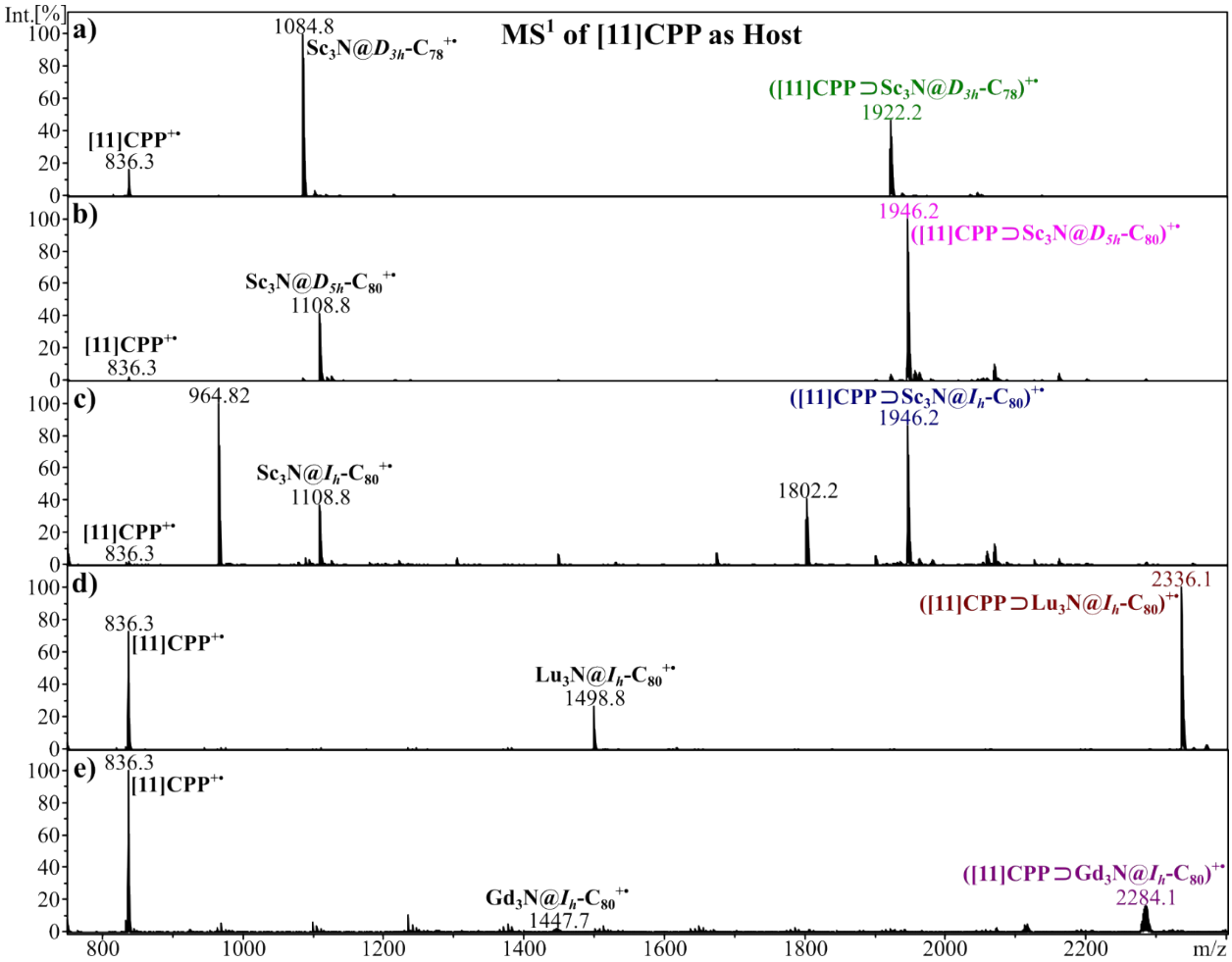


Figure S5. Positive ion-mode ESI MS[1] spectra of solutions containing [11]CPP and **a)** $Sc_3N@D_{3h}$-C_{78}, **b)** $Sc_3N@D_{5h}$-C_{80}, **c)** $Sc_3N@I_h$-C_{80}, **d)** $Lu_3N@I_h$-C_{80} and **e)** $Gd_3N@I_h$-C_{80}.

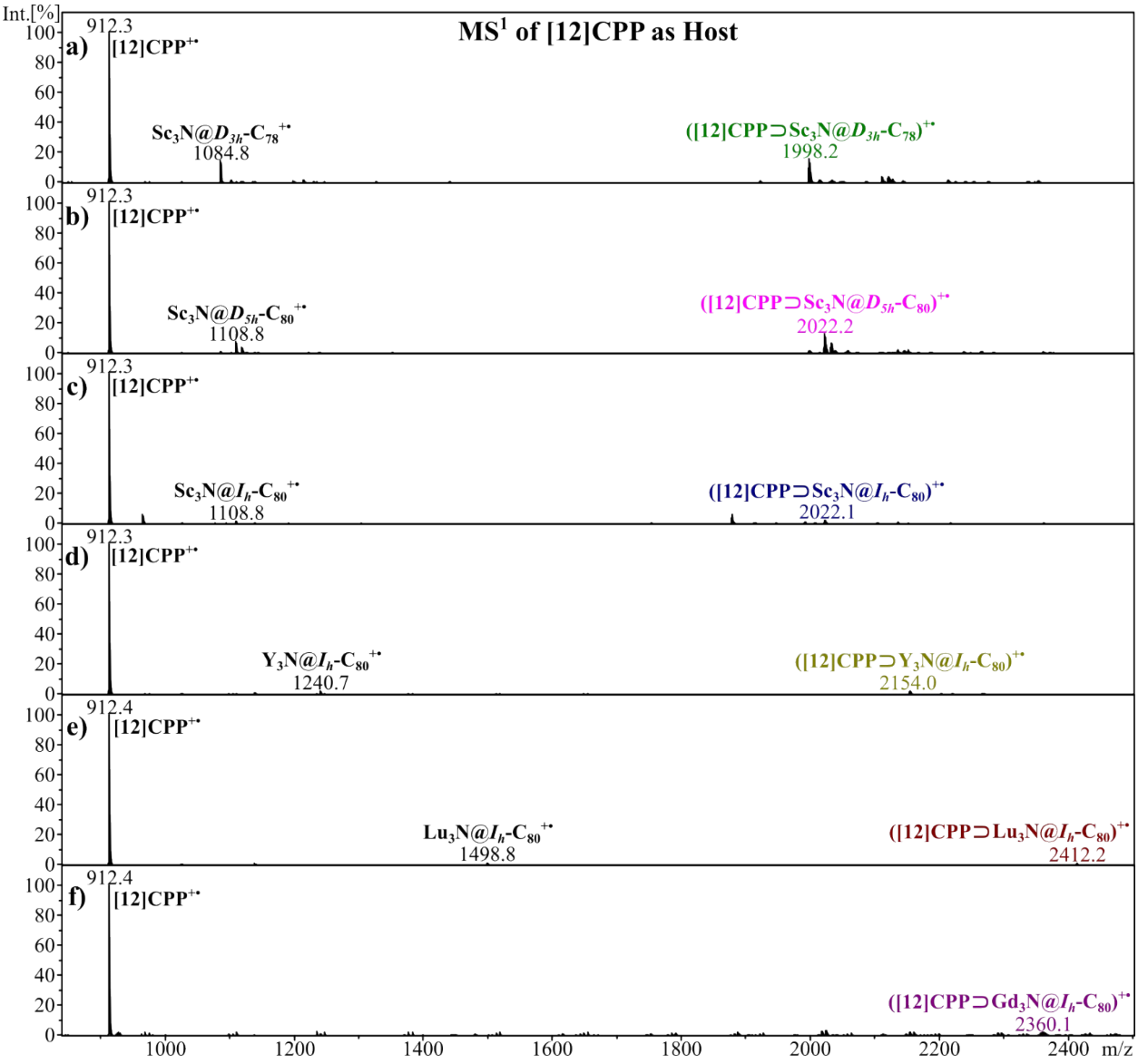


Figure S6. Positive ion-mode ESI MS[1] spectra of solutions containing [12]CPP and **a)** $Sc_3N@D_{3h}$-C_{78}, **b)** $Sc_3N@D_{5h}$-C_{80}, **c)** $Sc_3N@I_h$-C_{80}, **d)** $Y_3N@I_h$-C_{80}, **e)** $Lu_3N@I_h$-C_{80} and **f)** $Gd_3N@I_h$-C_{80}.

We also observe complex formation between the hosts [10] and [12]CPP and the EMF guests. However, the intensities of the corresponding signals are decreased compared to the [11]CPP based host-guest complexes indicating a reduced tendency to complex formation (as already shown for the C_{84} guest, Figure 2).

2.2 MS^2 spectra

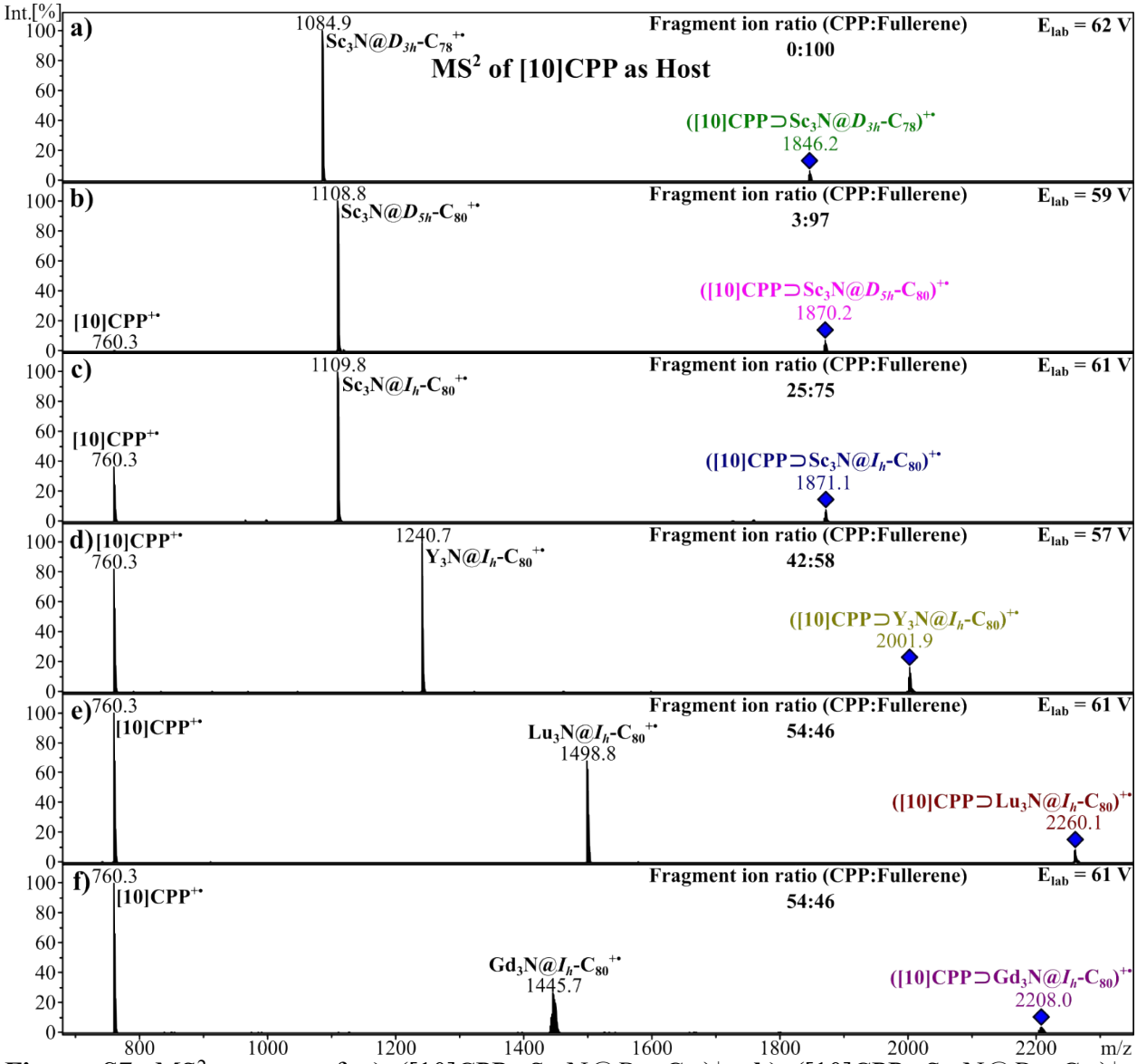


Figure S7. MS^2 spectra of **a)** $([10]CPP \supset Sc_3N@D_{3h}\text{-}C_{78})^{+\bullet}$, **b)** $([10]CPP \supset Sc_3N@D_{5h}\text{-}C_{80})^{+\bullet}$, **c)** $([10]CPP \supset Sc_3N@I_h\text{-}C_{80})^{+\bullet}$, **d)** $([10]CPP \supset Y_3N@I_h\text{-}C_{80})^{+\bullet}$, **e)** $([10]CPP \supset Lu_3N@I_h\text{-}C_{80})^{+\bullet}$ and **f)** $([10]CPP \supset Gd_3N@I_h\text{-}C_{80})^{+\bullet}$.

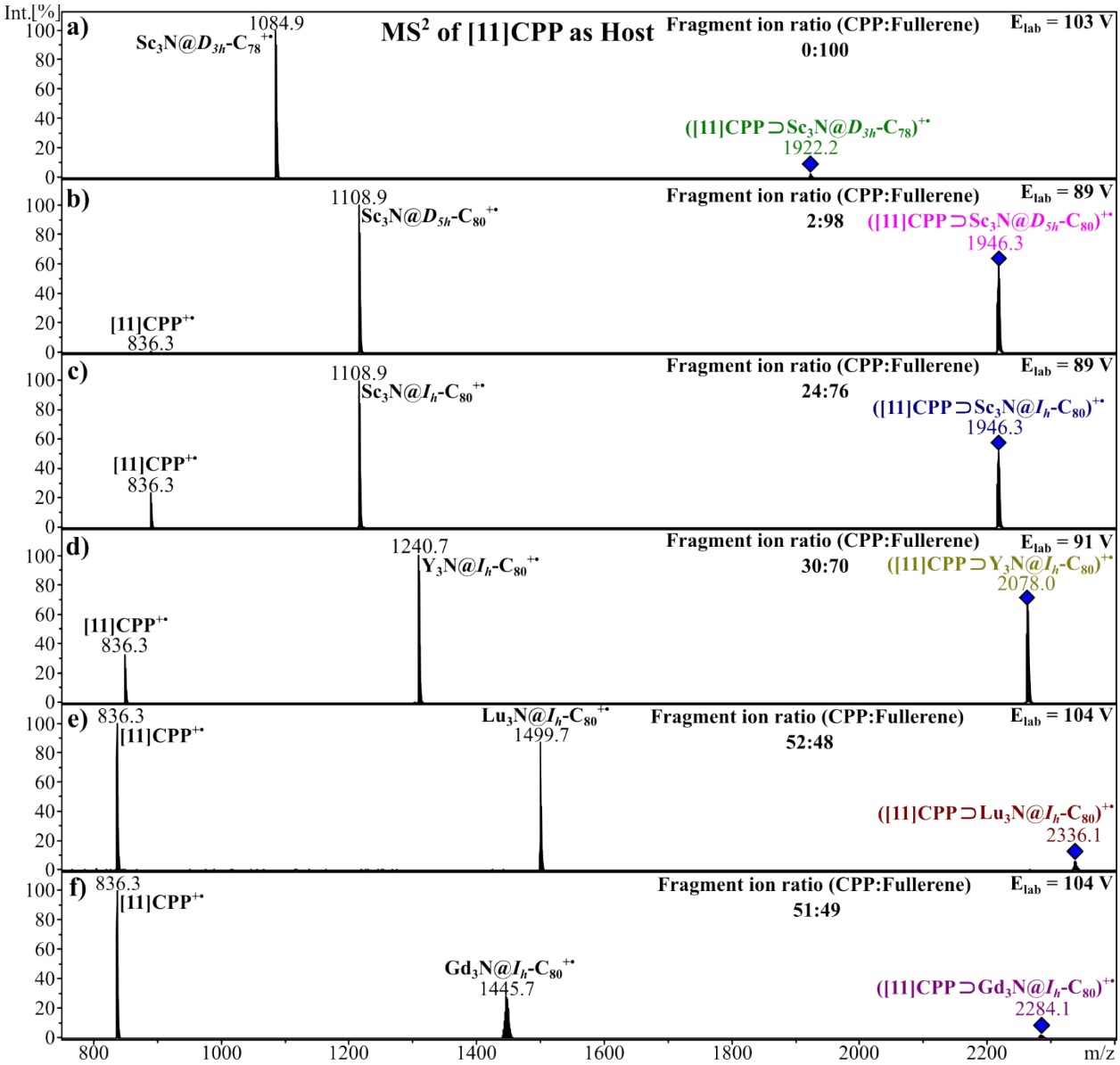


Figure S8. MS^2 spectra of **a)** $([11]CPP \supset Sc_3N@D_{3h}\text{-}C_{78})^{+\bullet}$, **b)** $([11]CPP \supset Sc_3N@D_{5h}\text{-}C_{80})^{+\bullet}$, **c)** $([11]CPP \supset Sc_3N@I_h\text{-}C_{80})^{+\bullet}$, **d)** $([11]CPP \supset Y_3N@I_h\text{-}C_{80})^{+\bullet}$, **e)** $([11]CPP \supset Lu_3N@I_h\text{-}C_{80})^{+\bullet}$ and **f)** $([11]CPP \supset Gd_3N@I_h\text{-}C_{80})^{+\bullet}$.

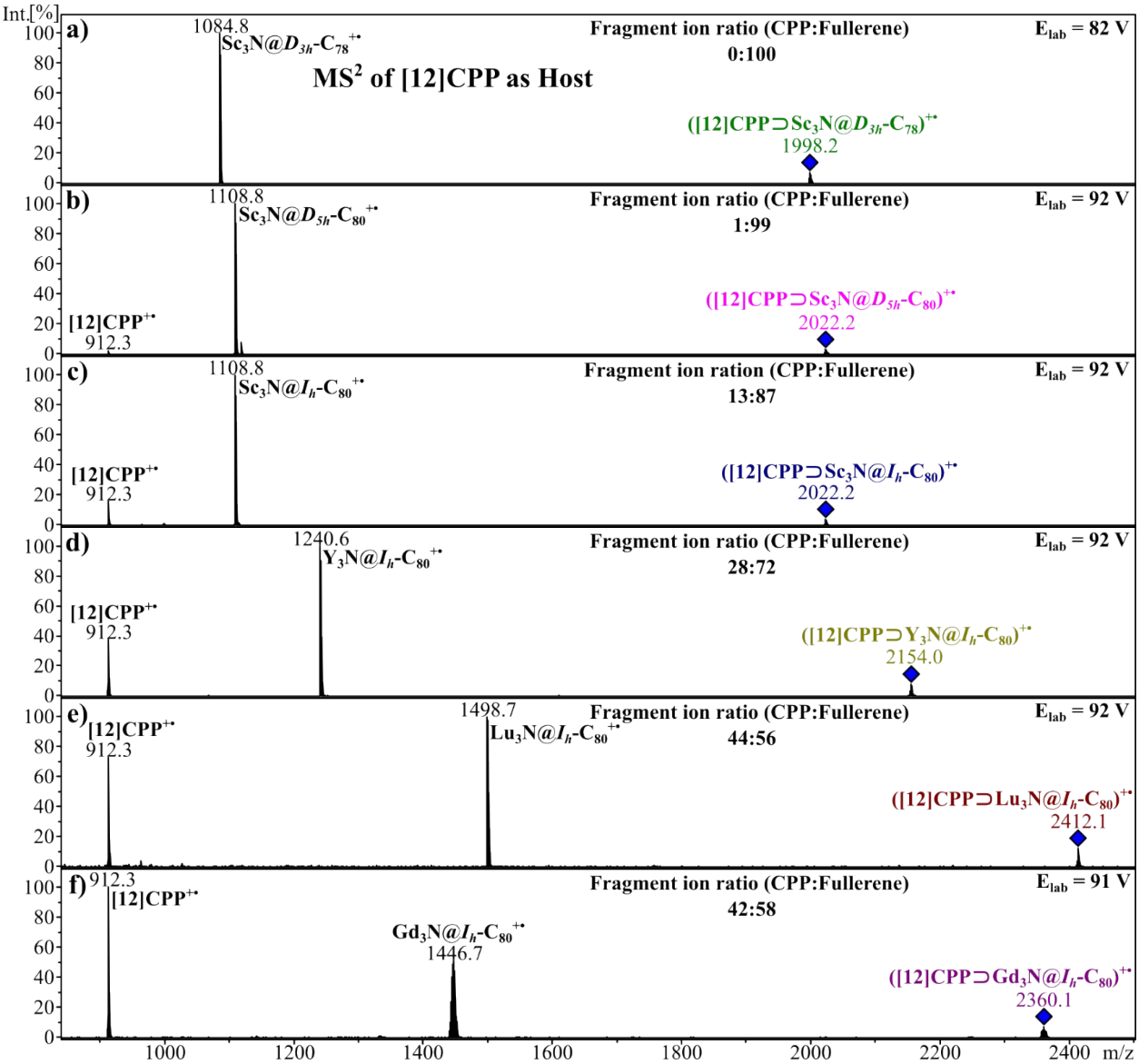


Figure S9. MS^2 spectra of **a)** $([12]CPP⊃Sc_3N@D_{3h}\text{-}C_{78})^{+\bullet}$, **b)** $([12]CPP⊃Sc_3N@D_{5h}\text{-}C_{80})^{+\bullet}$, **c)** $([12]CPP⊃Sc_3N@I_h\text{-}C_{80})^{+\bullet}$, **d)** $([12]CPP⊃Y_3N@I_h\text{-}C_{80})^{+\bullet}$, **e)** $([12]CPP⊃Lu_3N@I_h\text{-}C_{80})^{+\bullet}$ and **f)** $([12]CPP⊃Gd_3N@I_h\text{-}C_{80})^{+\bullet}$.

By and large the same charge distributions and trends as observed and discussed for [11]CPP (main article) are found.

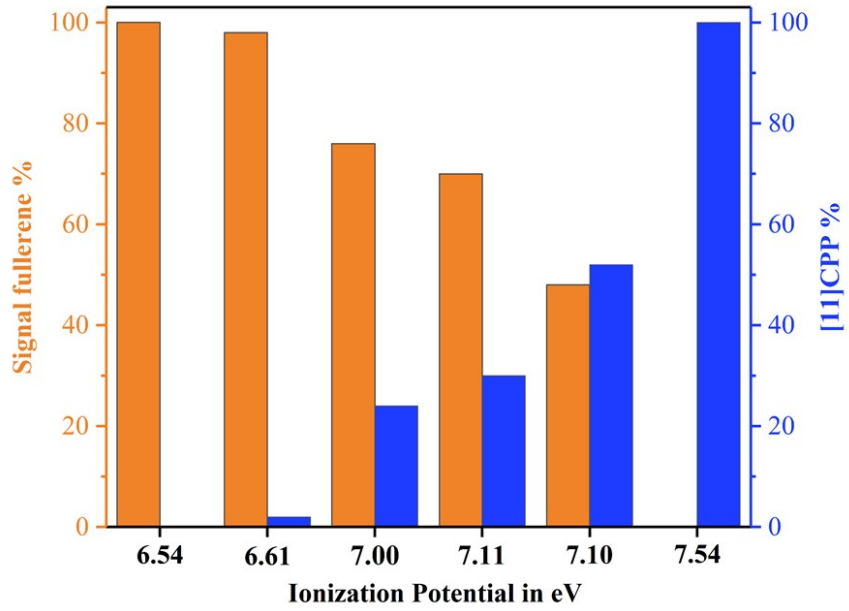


Figure S10. Trends in the intensities of fullerene and [11]CPP signals in MS^2 spectra depending on the ionization potential (IP) of the fullerene.

2.3 Breakdown Graphs

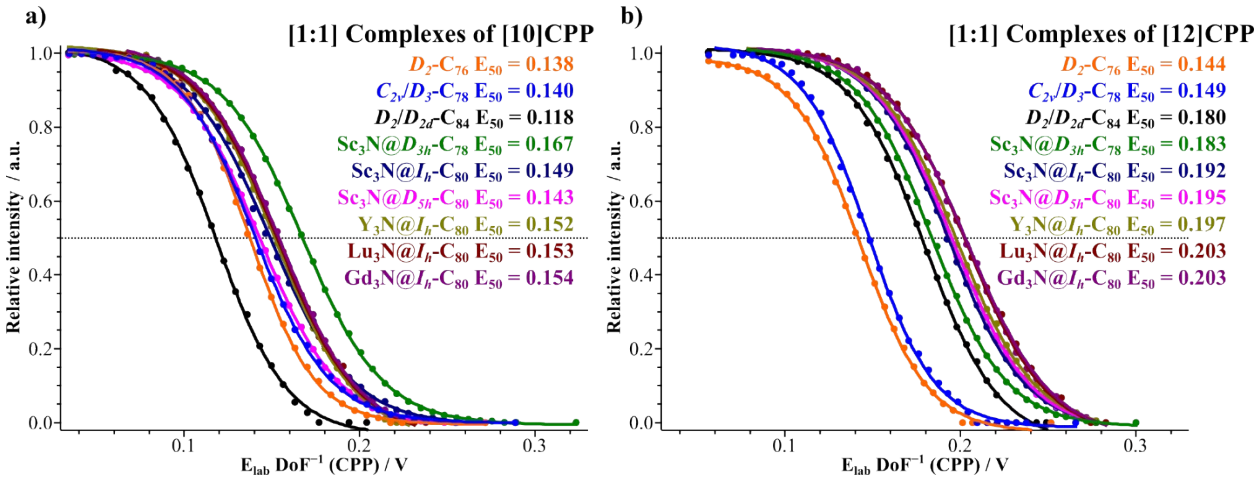


Figure S11. Energy-resolved collision-induced dissociation graphs (breakdown graphs) of host-guest complexes between **a)** [10]CPP and D_2-C_{76}, C_{2v}/D_3-C_{78}, D_2/D_{2d}-C_{84}, $Sc_3N@D_{3h}$-C_{78}, $M_3N@C_{80}$ (I_h, M = Sc, Y, Gd, Lu; D_{5h}, M = Sc) and **b)** [12]CPP and D_2-C_{76}, C_{2v}/D_3-C_{78}, D_2/D_{2d}-C_{84}, $Sc_3N@D_{3h}$-C_{78}, $M_3N@C_{80}$ (I_h, M = Sc, Y, Gd, Lu; D_{5h}, M = Sc).

As already observed for [11]CPP, the complexes of [10/12]CPP (Figure S7) with EMFs are more stable than the complexes with pristine fullerenes. In case of [10]CPP as host (Figure S10a), we find a different order of stabilities within the EMF based complexes (compared to [11]CPP and [12]CPP). Here, $Sc_3N@C_{78}$ forms the most stable complex and not the EMFs with a C_{80} core. We relate this observation to the size of [10]CPP. [10]CPP is not an ideal host for any of the studied fullerenes due to its rather small cavity.[18] Therefore, [10]CPP prefers to bind the smallest fullerene in the tested series, which is $Sc_3N@C_{78}$. This observation is also consistent with the fragmentation energies of complexes between [10]CPP and pristine fullerenes (E_{50}: $C_{84} < C_{76} = C_{78}$).

The relative order of stabilities for the [12]CPP host follows the order of [11]CPP based complexes. However, the complex with C_{84} is not significantly less stable than the complexes with EMFs. We relate this observation to the diameter of [12]CPP. C_{84} offers a larger fullerene core than the EMFs and, hence, more stabilization with the [12]CPP host via dispersion interactions is possible while complexes with EMFs suffer more severely from a size mismatch.

Comparing the complex stabilities of different CPP sizes ([10/11/12]CPP⊃EMF), we find the following order: [11]CPP > [12]CPP > [10]CPP.

This observation is in good agreement with the expected interaction strengths based on the breakdown graphs of the respective complexes with $C_{76/78/84}$.

3. DFT calculations

3.1 Methodology

Geometry optimization of the complexes was performed using the DFT BLYP functional[19-20] with D3(BJ) dispersion correction[21-22] and def2-SVP basis set.[23-24] For efficient calculations, effective core potentials for heavy atoms (ECP28MWB for Y and Lu,[25-26] ECP54MWB for Gd[27-28] and resolution of identity (RI) approximation were used as implemented in the ORCA 4.1.2 program.[29-30] The complexes were treated in the form of radical cations (charge +1, multiplicity 2 for all [11]CPP⊃$M_3N@C_{80}$, except for [11]CPP⊃$Gd_3N@C_{80}$ with charge +1, multiplicity 7). Open-shell species were treated with the unrestricted formalism.

For the assessment of the fragmentation energy, single point energy calculations at the ω-B97M-V/def2-TZVPP level were additionally performed on the BLYP-D3(BJ)/def2-SVP optimized geometries. Such multi-level approach is common in computational chemistry and allows for large savings in computational resources without significant loss of accuracy. Two fragmentation schemes were taken into account:

([11]CPP⊃$M_3N@C_{80}$)$^{+\bullet}$ → [11]CPP$^{+\bullet}$ + $M_3N@C_{80}$ and

([11]CPP⊃$M_3N@C_{80}$)$^{+\bullet}$ → [11]CPP + $M_3N@C_{80}^{+\bullet}$

The fragmentation energy was calculated as the energy difference between the sum of energies of [n]CPP and fullerene and the energy of [n]CPP⊃fullerene complex.

Vertical ionization potential (IP) was calculated using two DFT functionals: ωB97M-V and CAM-B3LYP. VIP refers to the amount of energy required to remove one electron from the species to form a positive charge (IP = E_{cation} - $E_{neutral}$). The cation was taken in the same geometry as the BLYP-D3(BJ)/def-SVP optimized geometry for the neutral system. The molecular structures and orbitals were visualized with Chemcraft 1.8.[31] The NCI analysis was carried out using Critic2 program.[32]

3.2 Computational results

Table S1. HOMO energy (in eV) and ionization potential (IP, in eV) of fullerenes and [11]CPP in isolated form and in their neutral complexes calculated at the ωB97M-V/def2-TZVPP level.

System	HOMO (isolated)	IP (isolated)	HOMO (complex)	IP (complex)
$Sc_3N@I_h$-C_{80}	-7.30	7.00	-7.11	6.74
$Sc_3N@D_{5h}$-C_{80}	-6.92	6.61	-6.69	6.28
$Y_3N@I_h$-C_{80}	-7.39	7.11	-7.15	6.77
$Lu_3N@I_h$-C_{80}	-7.37	7.10	-7.13	6.76
D_{2d}-C_{84}	-7.87	7.54	-7.59	7.12
[11]CPP	-7.21	7.07	n/a	n/a

Table S2. Energy of selected occupied molecular orbitals (in eV) located on fullerene or CPP fragments of neutral complexes calculated at the ωB97M-V/def2-TZVPP level.

Complex	Located on C_{80}/C_{84} fragment	Located on [11]CPP fragment
[11]CPP⊃$Sc_3N@I_h$-C_{80}	-7.11 HOMO	-7.51 HOMO-4
[11]CPP⊃$Y_3N@I_h$-C_{80}	-7.15 HOMO	-7.48 HOMO-4
[11]CPP⊃$Lu_3N@I_h$-C_{80}	-7.13 HOMO	-7.48 HOMO-4
[11]CPP⊃D_{2d}-C_{84}	-7.59 HOMO-1	-7.43 HOMO

Table S3. Hirshfeld spin density (ρ, a.u.) and ionization potential (IP, eV) of fullerene and CPP fragments of [n]CPP⊃fullerene ions calculated at the ωB97M-V/def2-TZVPP level.

Complex	**ρ on fullerene fragment**	**ρ on CPP fragment**	**IP of fullerene fragment**	**IP of CPP fragment**
([11]CPP⊃$Sc_3N@I_h$-C_{80})$^{+\bullet}$	0.995	0.005	-7.06	-7.08
([11]CPP⊃$Y_3N@I_h$-C_{80})$^{+\bullet}$	0.994	0.006	-7.12	-6.88
([11]CPP⊃$Lu_3N@I_h$-C_{80})$^{+\bullet}$	0.994	0.006	-7.10	-6.88
([11]CPP⊃I_h-C_{80})$^{+\bullet}$	0.972	0.028	-6.69	-7.04
([11]CPP⊃D_{2d}-C_{84})$^{+\bullet}$	0.976	0.024	-7.50	-6.90
([11]CPP⊃C_{2v}-C_{78})$^{+\bullet}$	0.988	0.012	-7.13	-6.92
([11]CPP⊃D_2-C_{76})$^{+\bullet}$	0.985	0.015	-7.30	-7.02
([10]CPP⊃$Sc_3N@I_h$-C_{80})$^{+\bullet}$	0.979	0.021	-7.07	-6.91
([10]CPP⊃$Y_3N@I_h$-C_{80})$^{+\bullet}$	0.983	0.017	-7.10	-6.80
([10]CPP⊃$Lu_3N@I_h$-C_{80})$^{+\bullet}$	0.982	0.018	-7.10	-6.80
([10]CPP⊃I_h-C_{80})$^{+\bullet}$	0.977	0.023	-6.65	-6.80
([10]CPP⊃D_{2d}-C_{84})$^{+\bullet}$	0.946	0.054	-7.49	-6.93
([10]CPP⊃C_{2v}-C_{78})$^{+\bullet}$	0.977	0.023	-7.13	-6.90
([10]CPP⊃D_2-C_{76})$^{+\bullet}$	0.984	0.016	-7.30	-6.89
([12]CPP⊃$Sc_3N@I_h$-C_{80})$^{+\bullet}$	0.993	0.007	-7.06	-6.97
([12]CPP⊃$Y_3N@I_h$-C_{80})$^{+\bullet}$	0.995	0.005	-7.11	-7.10
([12]CPP⊃$Lu_3N@I_h$-C_{80})$^{+\bullet}$	0.995	0.005	-7.10	-6.98
([12]CPP⊃I_h-C_{80})$^{+\bullet}$	0.971	0.029	-6.64	-6.94
([12]CPP⊃D_{2d}-C_{84})$^{+\bullet}$	0.967	0.033	-7.49	-6.97
([12]CPP⊃C_{2v}-C_{78})$^{+\bullet}$	0.970	0.030	-7.12	-7.09
([12]CPP⊃D_2-C_{76})$^{+\bullet}$	0.988	0.012	-7.30	-6.93

Table S4. Energies (ΔE_{frag}, in kcal/mol) for fragmentation of [10]CPP⊃fullerene ions calculated at the ωB97M-V/def2-TZVPP level and experimental ratio of signals.

Complex	**ΔE_{frag} (channel 1)**	**ΔE_{frag} (channel 2)**	**Difference[a]**	**Experimental ratio of ions (CPP:fullerene)**
([10]CPP⊃$Sc_3N@I_h$-C_{80})$^{+\bullet}$	63.54	67.15	3.61	25:75
([10]CPP⊃$Y_3N@I_h$-C_{80})$^{+\bullet}$	64.25	71.24	6.99	42:58
([10]CPP⊃$Lu_3N@I_h$-C_{80})$^{+\bullet}$	67.07	73.85	6.78	54:46
([10]CPP⊃D_{2d}-C_{84})$^{+\bullet}$	51.18	64.12	12.94	100:0

[a] – Difference = ΔE_{frag}(channel 2) - ΔE_{frag}(channel 1)

Table S5. Energies (ΔE_{frag}, in kcal/mol) for fragmentation of [12]CPP⊃fullerene ions calculated at the ωB97M-V/def2-TZVPP level and experimental ratio of signals.

Complex	**ΔE_{frag} (channel 1)**	**ΔE_{frag} (channel 2)**	**Difference[a]**	**Experimental ratio of ions (CPP:fullerene)**
([12]CPP⊃$Sc_3N@I_h$-C_{80})$^{+\bullet}$	54.31	56.41	2.10	13:87
([12]CPP⊃$Y_3N@I_h$-C_{80})$^{+\bullet}$	56.04	56.32	0.28	28:72
([12]CPP⊃$Lu_3N@I_h$-C_{80})$^{+\bullet}$	56.81	59.65	2.84	44:56
([12]CPP⊃D_{2d}-C_{84})$^{+\bullet}$	45.16	57.22	12.06	100:0

[a] – Difference = ΔE_{frag}(channel 2) - ΔE_{frag}(channel 1)

Table S6. BSSE-corrected binding energies ($\Delta E_{binding}$, in kcal/mol) for neutral [11]CPP⊃fullerene complexes calculated at the ωB97M-V/def2-TZVPP level.

Complex	**$\Delta E_{binding}$**	**BSSE correction**	**$\Delta E_{binding}$ BSSE corrected**
[11]CPP⊃$Sc_3N@I_h$-C_{80}	-63.573	1.760	-61.813
[11]CPP⊃$Y_3N@I_h$-C_{80}	-64.482	1.799	-62.683
[11]CPP⊃$Lu_3N@I_h$-C_{80}	-64.227	1.974	-62.253
[11]CPP⊃$Gd_3N@I_h$-C_{80}	-62.162	4.002	-58.160
[11]CPP⊃I_h-C_{80}*	-59.497	1.629	-57.868
[11]CPP⊃D_{2d}-C_{84}	-62.929	1.641	-61.288
[11]CPP⊃C_{2v}-C_{78}	-60.928	1.611	-59.317
[11]CPP⊃D_2-C_{76}	-58.115	1.664	-56.451

* hypothetical structure, not observed experimentally

Table S7. Energies (ΔE_{frag}, in kcal/mol) for fragmentation of [11]CPP⊃Sc_3N@fullerene ions calculated at the ωB97M-V/def2-TZVPP level and experimental ratio of signals.

Complex	**ΔE_{frag} (channel 1)**	**ΔE_{frag} (channel 2)**	**Difference[a]**	**Experimental ratio of ions (CPP:fullerene)**
([11]CPP⊃$Sc_3N@I_h$-C_{80})$^{+\bullet}$	67.93	67.60	-0.33	24:76
([11]CPP⊃$Sc_3N@D_{5h}$-C_{80})$^{+\bullet}$	83.45	72.13	-11.32	2:98
([11]CPP⊃$Sc_3N@D_{3h}$-C_{78})$^{+\bullet}$	83.76	69.03	-14.74	0:100

[a] – Difference = ΔE_{frag}(channel 2) - ΔE_{frag}(channel 1)

Table S8. Energies (ΔE_{frag}, in kcal/mol) for fragmentation of hypothetical [n]CPP⊃I_h-C_{80} ions calculated at the ωB97M-V/def2-TZVPP level.

Complex	ΔE_{frag} (pathway 1)	ΔE_{frag} (pathway 2)	Difference[a]
([10]CPP⊃I_h-C_{80})$^{+\bullet}$	74.43	71.06	-3.37
([11]CPP⊃I_h-C_{80})$^{+\bullet}$	78.08	70.00	-8.09
([12]CPP⊃I_h-C_{80})$^{+\bullet}$	63.15	56.27	-6.87

[a] – Difference = ΔE_{frag}(channel 2) - ΔE_{frag}(channel 1)

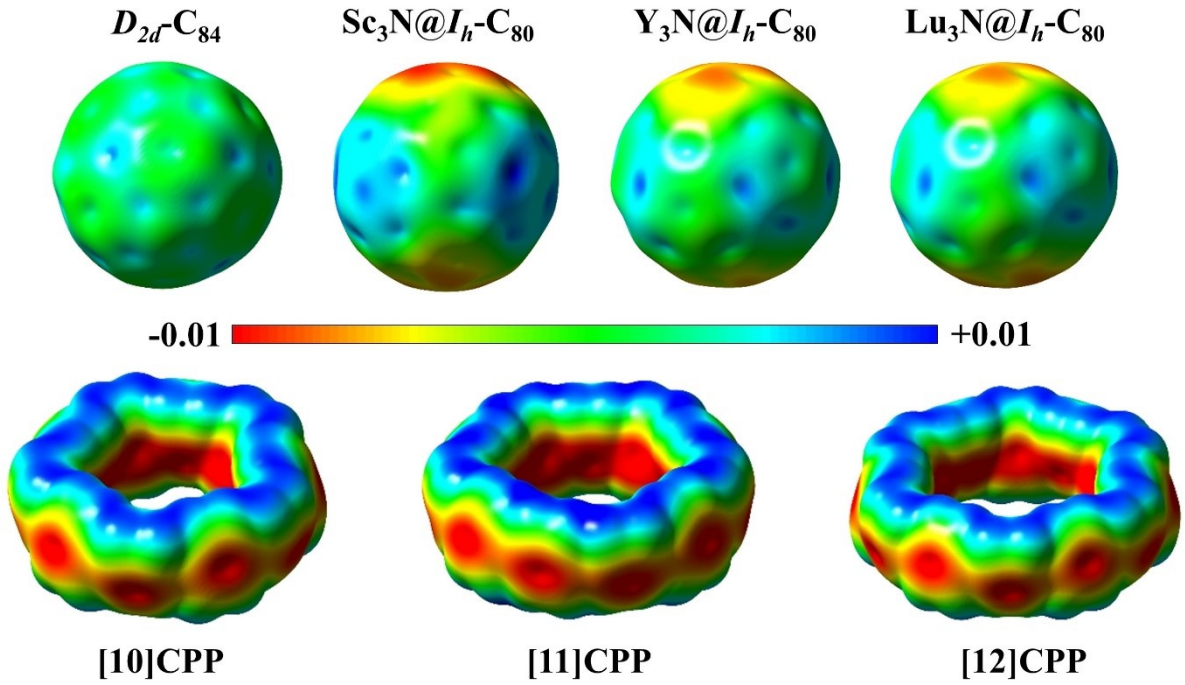
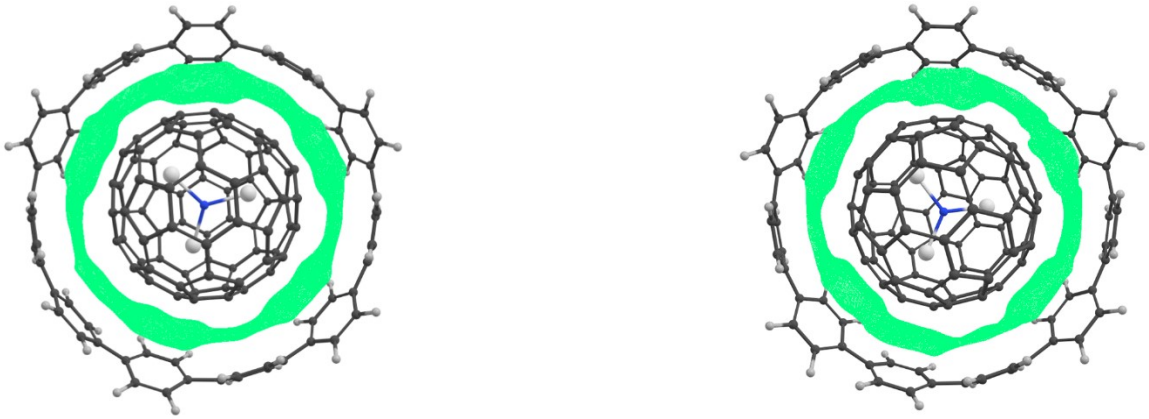


Figure S12. Molecular electrostatic potential (MEP) of fullerenes and CPPs mapped on 0.0001 a.u. isosurfaces of the electron density.



[11]CPP⊃$Sc_3N@I_h$-C_{80} **[11]CPP⊃$Sc_3N@D_{5h}$-C_{80}**

Figure S13. NCI isosurfaces of van der Waals interactions for [11]CPP⊃$Sc_3N@I_h$-C_{80} and [11]CPP⊃$Sc_3N@D_{5h}$-C_{80} complexes. Isosurfaces were generated for RDG = 0.5 a.u.

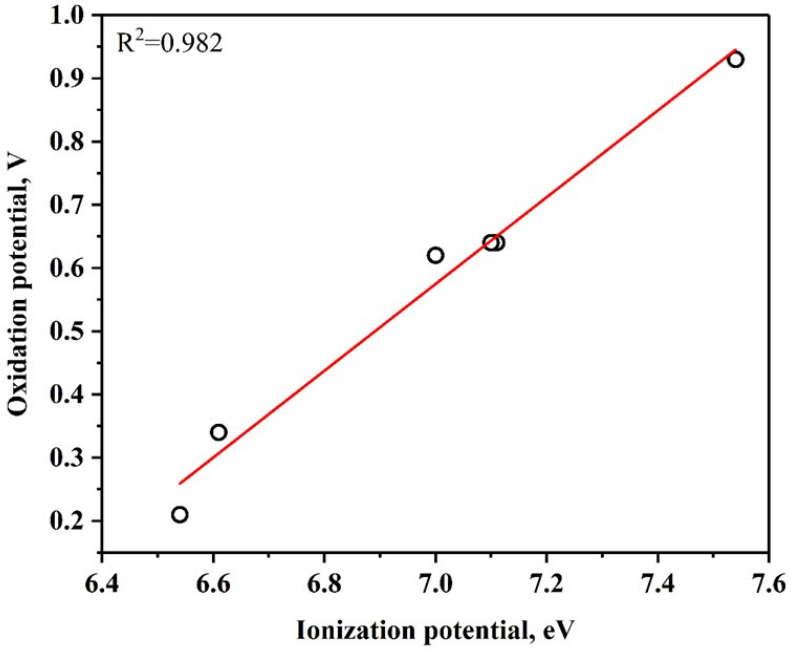


Figure S14. Correlation between experimentally measured oxidation potential and calculated IPs of EMFs.

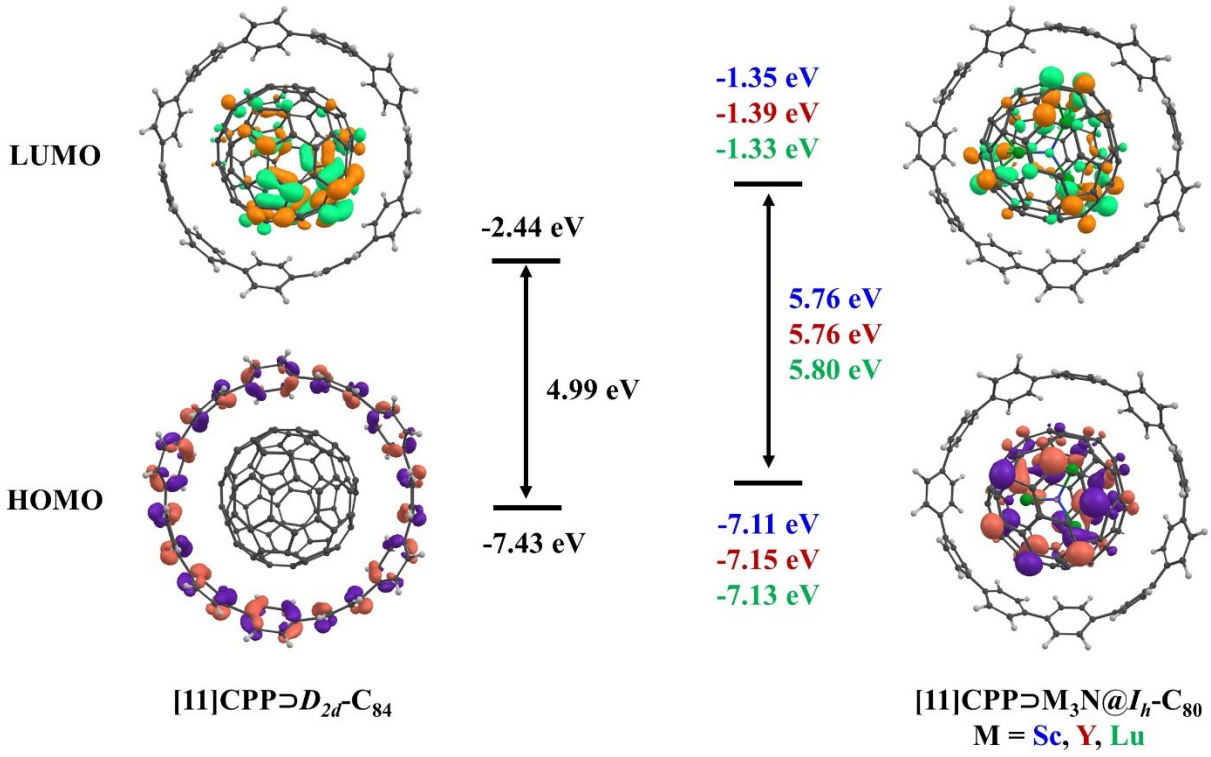


Figure S15. HOMO and LUMO of complexes formed by [11]CPP with EMFs and pristine C_{84} fullerene at the ωB97M-V/def2-TZVPP level. Color scheme for fullerenes: C_{84} – black, $Sc_3N@I_h$-C_{80} – blue, $Y_3N@I_h$-C_{80} – red, $Lu_3N@I_h$-C_{80} – green.

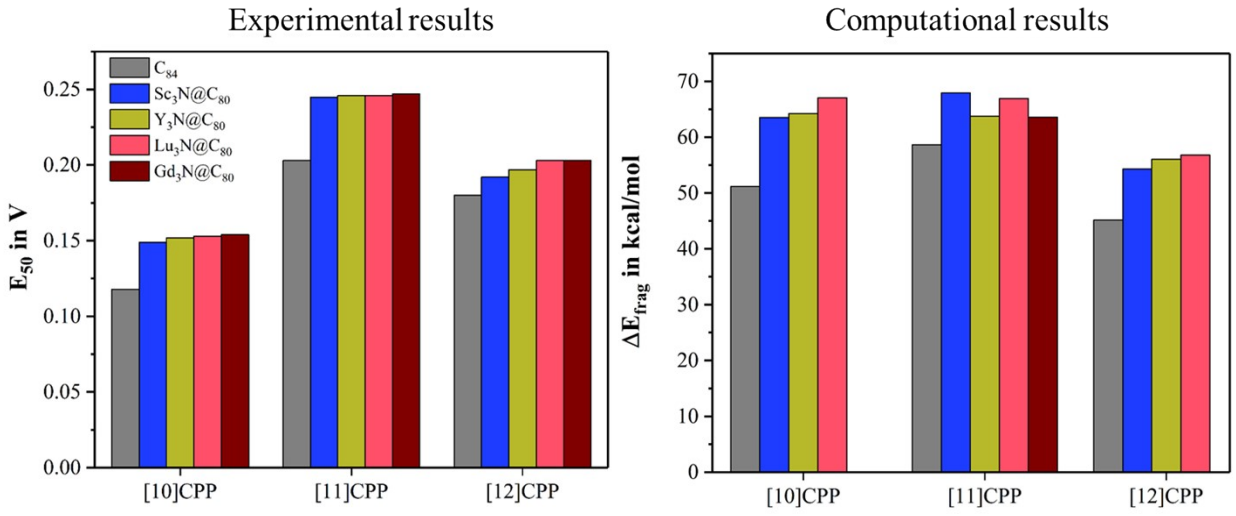


Figure S16. Histograms for experimental (E_{50}) and computational (ΔE_{frag}) results of C_{84} fullerene and $M_3N@I_h$-C_{80} with [n]CPPs (n=10, 11, 12).

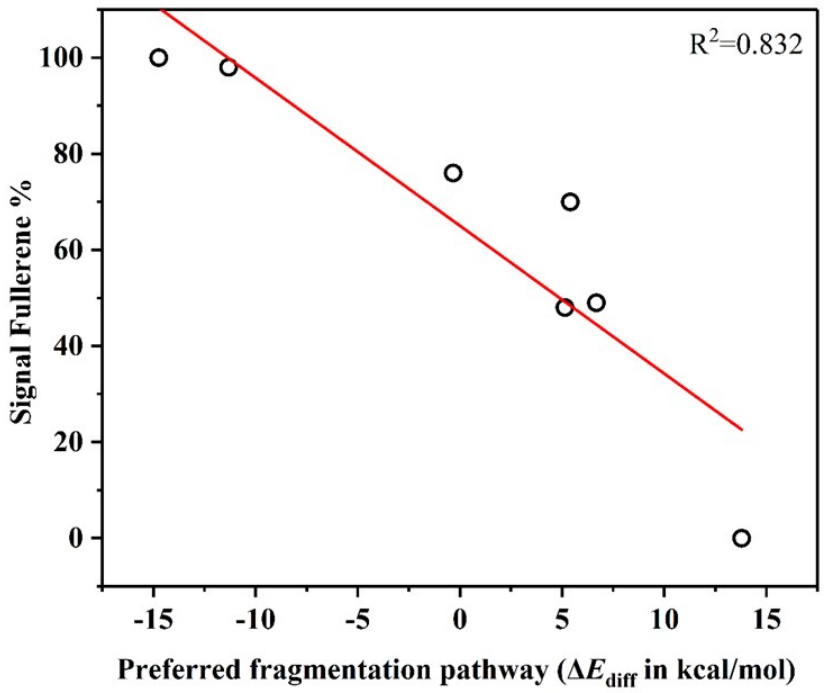


Figure S17. Correlation between the intensity of the fullerene signal in MS^2 spectra and preferred fragmentation pathway (ΔE_{diff}) of [11]CPP⊃fullerene complexes.

3.3 Cartesian coordinates

Coordinates for [11]CPP⊃fullerene complexes optimized at BLYP-D3(BJ)/def2-SVP in the form of radical cations (charge +1, multiplicity 2 for all complexes except for $([11]CPP⊃Gd_3N@C_{80})^{+\bullet}$ with charge +1, multiplicity 7).

$([11]CPP⊃Sc_3N@I_h\text{-}C_{80})^{+\bullet}$				$([11]CPP⊃Y_3N@I_h\text{-}C_{80})^{+\bullet}$			
6	26.314471000	-25.029031000	-6.636552000	6	7.596094000	-1.388237000	-2.265878000
6	26.540296000	-23.651433000	-6.532897000	6	7.944225000	-0.368643000	-1.381090000
6	26.295464000	-22.960613000	-5.319427000	6	7.779758000	-0.527416000	0.023289000
6	25.970066000	-23.736973000	-4.179109000	6	7.443962000	-1.824905000	0.495146000
6	25.743802000	-25.111877000	-4.282700000	6	7.097746000	-2.845630000	-0.389630000
6	25.833383000	-25.776046000	-5.531600000	6	7.068852000	-2.622308000	-1.792660000
6	26.105647000	-21.491660000	-5.267574000	6	7.686574000	0.629403000	0.932633000
6	25.525814000	-20.827293000	-6.377143000	6	7.282477000	1.892942000	0.422279000
6	24.953639000	-19.558851000	-6.238499000	6	6.799526000	2.890808000	1.267342000
6	24.936917000	-18.898942000	-4.984436000	6	6.689216000	2.676562000	2.667876000
6	25.664544000	-19.490471000	-3.920834000	6	7.258779000	1.483333000	3.193243000
6	26.237929000	-20.758967000	-4.060288000	6	7.747356000	0.487483000	2.347876000
6	23.967289000	-17.801155000	-4.761965000	6	5.801415000	3.541145000	3.464554000
6	23.566100000	-16.916216000	-5.794558000	6	5.480254000	4.867442000	3.062777000
6	22.381237000	-16.179324000	-5.691557000	6	4.358511000	5.520587000	3.569552000
6	21.531561000	-16.304475000	-4.560614000	6	3.487831000	4.881577000	4.498330000
6	22.027148000	-17.056771000	-3.465561000	6	3.919434000	3.635740000	5.031576000
6	23.216443000	-17.783240000	-3.561244000	6	5.046244000	2.985001000	4.531897000
6	20.105864000	-15.893676000	-4.596203000	6	2.114065000	5.364043000	4.733816000
6	19.444904000	-15.661550000	-5.830536000	6	1.510599000	6.306681000	3.854254000
6	18.049968000	-15.639314000	-5.917949000	6	0.131350000	6.504085000	3.835435000
6	17.237285000	-15.871367000	-4.779163000	6	-0.733162000	5.763240000	4.687886000
6	17.897027000	-15.941288000	-3.525854000	6	-0.112870000	4.956481000	5.683062000
6	19.291263000	-15.939531000	-3.436043000	6	1.267065000	4.766458000	5.708144000
6	15.813907000	-16.269752000	-4.900172000	6	-2.178397000	5.648596000	4.418656000
6	15.334966000	-16.832094000	-6.110271000	6	-2.708998000	6.020580000	3.152942000
6	14.147106000	-17.567342000	-6.147762000	6	-3.955370000	5.563099000	2.728076000
6	13.383401000	-17.783774000	-4.974545000	6	-4.741370000	4.705480000	3.545019000
6	13.767312000	-17.075357000	-3.807894000	6	-4.299996000	4.501853000	4.882343000
6	14.950813000	-16.330690000	-3.774132000	6	-3.055549000	4.962503000	5.307014000
6	12.425209000	-18.913200000	-4.934670000	6	-5.798283000	3.879126000	2.936129000
6	11.731686000	-19.358343000	-6.088894000	6	-6.418766000	4.227995000	1.703799000
6	11.165012000	-20.636589000	-6.140064000	6	-7.086008000	3.271733000	0.939310000
6	11.267726000	-21.526807000	-5.040438000	6	-7.169240000	1.915976000	1.365596000
6	11.818677000	-21.019144000	-3.837485000	6	-6.712702000	1.618801000	2.678320000
6	12.384223000	-19.741439000	-3.785458000	6	-6.046634000	2.574748000	3.443311000
6	11.060230000	-22.987278000	-5.186921000	6	-7.486471000	0.818888000	0.433246000
6	11.376162000	-23.615488000	-6.416796000	6	-7.253402000	0.979865000	-0.959152000
6	11.564413000	-24.998529000	-6.493227000	6	-7.173864000	-0.122449000	-1.809491000
6	11.443449000	-25.818738000	-5.344098000	6	-7.321396000	-1.446256000	-1.312831000
6	10.970999000	-25.209906000	-4.153553000	6	-7.724895000	-1.592180000	0.043640000
6	10.784185000	-23.825557000	-4.076548000	6	-7.807218000	-0.489346000	0.892631000
6	12.038326000	-27.176582000	-5.354135000	6	-6.849060000	-2.588692000	-2.115877000

6	12.168636000	-27.934530000	-6.546317000	6	-6.726130000	-2.514658000	-3.531381000
6	13.064396000	-29.006331000	-6.625899000	6	-5.934279000	-3.422713000	-4.232954000
6	13.871485000	-29.369343000	-5.516695000	6	-5.221547000	-4.451178000	-3.555804000
6	13.612745000	-28.720421000	-4.283543000	6	-5.494425000	-4.632328000	-2.172912000
6	12.717946000	-27.648960000	-4.204047000	6	-6.286393000	-3.723845000	-1.471147000
6	15.106054000	-30.176612000	-5.668252000	6	-4.061241000	-5.126842000	-4.164417000
6	15.844020000	-30.097629000	-6.875533000	6	-3.301517000	-4.447404000	-5.154696000
6	17.190008000	-30.472459000	-6.924937000	6	-1.991839000	-4.827077000	-5.443171000
6	17.860563000	-30.945094000	-5.769729000	6	-1.374633000	-5.909964000	-4.760599000
6	17.074064000	-31.193489000	-4.615516000	6	-2.199767000	-6.703359000	-3.915528000
6	15.727087000	-30.818326000	-4.566189000	6	-3.509264000	-6.320797000	-3.623730000
6	19.341982000	-30.913637000	-5.722657000	6	0.095279000	-6.022660000	-4.751921000
6	20.137215000	-31.025578000	-6.891498000	6	0.902425000	-5.437430000	-5.766769000
6	21.472434000	-30.606608000	-6.898995000	6	2.261612000	-5.203927000	-5.559498000
6	22.073304000	-30.059665000	-5.736913000	6	2.885924000	-5.550962000	-4.330017000
6	21.324459000	-30.094960000	-4.534079000	6	2.116142000	-6.285838000	-3.388743000
6	19.990168000	-30.512822000	-4.527313000	6	0.756360000	-6.514883000	-3.594082000
6	23.316271000	-29.255086000	-5.793324000	6	4.190272000	-4.994293000	-3.929326000
6	23.574363000	-28.455140000	-6.933959000	6	4.599079000	-3.725432000	-4.421046000
6	24.493396000	-27.402985000	-6.883588000	6	5.626525000	-3.012266000	-3.803720000
6	25.199111000	-27.106030000	-5.691023000	6	6.299006000	-3.529998000	-2.663141000
6	25.060034000	-28.007796000	-4.605255000	6	6.002057000	-4.867502000	-2.281267000
6	24.137427000	-29.058124000	-4.654621000	6	4.972783000	-5.579760000	-2.896310000
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1	26.865624000	-23.090761000	-7.420250000	1	8.303985000	0.587057000	-1.784168000
1	25.764198000	-23.236947000	-3.223831000	1	7.322593000	-2.000627000	1.571220000
1	25.367181000	-25.653850000	-3.405665000	1	6.717596000	-3.789232000	0.020970000
1	25.402135000	-21.364074000	-7.326735000	1	7.226763000	2.051841000	-0.661506000
1	24.395822000	-19.130852000	-7.082002000	1	6.379730000	3.800693000	0.820900000
1	25.735584000	-18.967736000	-2.956715000	1	7.280141000	1.322252000	4.279321000
1	26.753028000	-21.214610000	-3.203250000	1	8.145073000	-0.436885000	2.786903000
1	24.167695000	-16.844219000	-6.711572000	1	6.100147000	5.374398000	2.311506000
1	22.084174000	-15.538803000	-6.532387000	1	4.126697000	6.528145000	3.202611000
1	21.416036000	-17.182843000	-2.564382000	1	3.302481000	3.108489000	5.768285000
1	23.494472000	-18.453973000	-2.737684000	1	5.267684000	1.970061000	4.885541000
1	20.026657000	-15.584181000	-6.757727000	1	2.120500000	6.834812000	3.111711000
1	17.586272000	-15.508510000	-6.904496000	1	-0.286575000	7.201787000	3.099564000
1	17.314981000	-16.096930000	-2.608683000	1	-0.727234000	4.397735000	6.399101000
1	19.750358000	-16.052517000	-2.445975000	1	1.687480000	4.091377000	6.463344000
1	15.961505000	-16.809405000	-7.010415000	1	-2.089497000	6.572561000	2.436714000
1	13.882276000	-18.097705000	-7.071744000	1	-4.265070000	5.768236000	1.695754000
1	13.153931000	-17.153397000	-2.899384000	1	-4.925251000	3.932993000	5.582935000
1	15.237454000	-15.832029000	-2.838674000	1	-2.736277000	4.743178000	6.333471000
1	11.679457000	-18.708985000	-6.973992000	1	-6.336787000	5.254571000	1.322910000
1	10.673694000	-20.970881000	-7.064331000	1	-7.517232000	3.567445000	-0.025993000
1	11.923534000	-21.679815000	-2.967378000	1	-6.769200000	0.591228000	3.057302000
1	12.921129000	-19.435902000	-2.877687000	1	-5.598917000	2.265419000	4.395769000
1	11.608612000	-23.000888000	-7.296280000	1	-7.007934000	1.970723000	-1.360775000
1	11.939086000	-25.430325000	-7.430373000	1	-6.871261000	0.038548000	-2.851610000
1	10.793525000	-25.826638000	-3.261694000	1	-7.942827000	-2.591450000	0.443019000
1	10.462309000	-23.378702000	-3.125762000	1	-8.089141000	-0.645686000	1.941995000
1	11.593344000	-27.647680000	-7.437425000	1	-7.230312000	-1.708732000	-4.080796000

1	13.177339000	-29.541700000	-7.578782000	1	-5.828718000	-3.311701000	-5.320244000
1	14.218231000	-28.968863000	-3.402295000	1	-4.974363000	-5.419834000	-1.613577000
1	12.647704000	-27.087286000	-3.263684000	1	-6.367243000	-3.828189000	-0.382054000
1	15.400969000	-29.606795000	-7.751783000	1	-3.693856000	-3.528498000	-5.607440000
1	17.763568000	-30.263344000	-7.837323000	1	-1.397624000	-4.195317000	-6.114727000
1	17.540808000	-31.639004000	-3.726112000	1	-1.789727000	-7.607274000	-3.446100000
1	15.159582000	-30.974669000	-3.638394000	1	-4.102517000	-6.929639000	-2.928588000
1	19.687430000	-31.403937000	-7.819882000	1	0.445561000	-5.126539000	-6.715442000
1	22.049532000	-30.662468000	-7.832457000	1	2.848049000	-4.714679000	-6.348467000
1	21.751523000	-29.669525000	-3.616790000	1	2.559915000	-6.573851000	-2.427816000
1	19.407846000	-30.406480000	-3.603021000	1	0.173210000	-6.974777000	-2.786909000
1	22.952034000	-28.571672000	-7.830456000	1	4.023841000	-3.239346000	-5.218919000
1	24.568144000	-26.724148000	-7.742903000	1	5.829134000	-1.987037000	-4.136839000
1	25.650466000	-27.852650000	-3.691756000	1	6.563881000	-5.339064000	-1.464305000
1	24.015318000	-29.710094000	-3.778600000	1	4.745502000	-6.597385000	-2.552210000
21	20.693690000	-23.238113000	-5.068686000	39	-0.968776000	-1.457345000	-1.196850000
21	17.795073000	-25.212091000	-5.254077000	39	2.107328000	0.016725000	-0.191603000
21	17.560825000	-21.712936000	-5.480233000	39	-0.916612000	0.892517000	1.486718000
7	18.682817000	-23.388208000	-5.275912000	7	0.075395000	-0.202205000	0.055375000
6	15.424885000	-21.909667000	-3.057779000	6	-0.067986000	3.907853000	0.848619000
6	14.796358000	-22.326952000	-4.275843000	6	0.742541000	3.443282000	1.933954000
6	15.018271000	-21.493749000	-5.445936000	6	0.042231000	2.768327000	3.026159000
6	22.218696000	-22.099057000	-6.825190000	6	-2.486028000	-3.441021000	-0.271191000
6	15.926748000	-22.869098000	-2.095328000	6	0.439398000	3.928414000	-0.511344000
6	16.880605000	-25.132055000	-1.884300000	6	1.998570000	2.819326000	-2.076920000
6	15.820188000	-24.282317000	-2.352905000	6	1.776404000	3.476627000	-0.819185000
6	15.110737000	-24.699971000	-3.533824000	6	2.634362000	3.094291000	0.271781000
6	14.689383000	-24.317600000	-5.814858000	6	2.768087000	1.975339000	2.321684000
6	14.980159000	-23.521131000	-6.970348000	6	2.056876000	1.224648000	3.319538000
6	15.130607000	-22.100351000	-6.755545000	6	0.701258000	1.642895000	3.661230000
6	15.739640000	-24.105205000	-8.035236000	6	2.382101000	-0.160607000	3.444029000
6	15.254526000	-25.648661000	-5.684489000	6	3.732570000	1.347256000	1.412596000
6	17.110540000	-27.162164000	-6.293426000	6	4.348529000	-0.775884000	0.226485000
6	16.066727000	-26.239602000	-6.720963000	6	4.030310000	-0.074578000	1.486904000
6	16.291898000	-25.444924000	-7.906429000	6	3.321303000	-0.805550000	2.523558000
6	17.273393000	-26.322704000	-2.624882000	6	2.995887000	1.756961000	-2.218341000
6	16.591146000	-26.745501000	-3.826387000	6	3.905176000	1.365183000	-1.148994000
6	15.515132000	-25.889576000	-4.268504000	6	3.662470000	2.053419000	0.124090000
6	17.369602000	-27.427498000	-4.861067000	6	4.304114000	-0.067847000	-1.095195000
6	18.498201000	-19.283675000	-5.682706000	6	-3.472425000	0.716409000	2.115262000
6	17.822883000	-19.688830000	-6.892746000	6	-2.648995000	0.290729000	3.237108000
6	16.031017000	-21.298404000	-7.547717000	6	-0.315228000	0.699018000	4.077904000
6	16.443163000	-20.143914000	-6.757139000	6	-1.644037000	1.246518000	3.756427000
6	17.869046000	-19.407109000	-4.370823000	6	-3.256132000	2.009869000	1.450902000
6	16.307017000	-20.743507000	-3.040085000	6	-1.503462000	3.601816000	0.807913000
6	16.529208000	-19.926578000	-4.211408000	6	-2.214383000	2.939700000	1.891388000
6	15.794495000	-20.258112000	-5.431451000	6	-1.424592000	2.576602000	3.094243000
6	19.784456000	-21.293066000	-1.760478000	6	-2.722222000	1.847698000	-2.287305000
6	18.687602000	-20.497781000	-2.249753000	6	-2.876552000	2.509220000	-1.013025000
6	18.922432000	-19.662260000	-3.398111000	6	-3.583355000	1.815679000	0.031769000
6	17.354832000	-21.002243000	-2.061687000	6	-1.857912000	3.434953000	-0.601242000
6	21.342420000	-25.469693000	-2.810202000	6	0.398023000	-1.014787000	-4.022477000

6	19.516626000	-27.042354000	-3.498315000	6	2.728033000	-0.585352000	-3.106822000
6	20.861526000	-26.552608000	-3.648234000	6	1.683769000	-1.497490000	-3.544527000
6	18.819961000	-27.475633000	-4.698763000	6	3.630993000	-0.998382000	-2.033394000
6	22.267695000	-24.668753000	-3.597949000	6	-0.637468000	-2.007974000	-3.706545000
6	22.775141000	-22.432622000	-4.548316000	6	-2.768529000	-2.429278000	-2.417625000
6	22.437067000	-23.249170000	-3.382187000	6	-2.021880000	-1.621929000	-3.414357000
6	21.606124000	-22.666200000	-2.354127000	6	-2.260392000	-0.186068000	-3.417906000
6	21.919340000	-24.870820000	-7.320516000	6	0.187791000	-4.226920000	-0.812005000
6	22.586215000	-24.459255000	-6.107007000	6	-0.648839000	-3.849819000	-1.938585000
6	22.345540000	-25.260682000	-4.931555000	6	0.031310000	-3.103523000	-2.987264000
6	22.839912000	-23.037604000	-5.897788000	6	-2.073207000	-3.537834000	-1.681332000
6	19.441324000	-27.308667000	-5.993617000	6	3.335375000	-2.241338000	-1.347614000
6	20.772925000	-26.774151000	-6.155050000	6	2.256468000	-3.135728000	-1.753582000
6	21.476211000	-26.424447000	-4.956383000	6	1.458743000	-2.768573000	-2.891385000
6	21.036134000	-26.027270000	-7.347580000	6	1.618286000	-3.914895000	-0.741113000
6	18.401265000	-27.081858000	-6.966033000	6	3.739586000	-2.099726000	0.033583000
6	17.564071000	-25.469187000	-8.622850000	6	2.851932000	-2.174758000	2.331983000
6	18.656003000	-26.262674000	-8.138539000	6	3.014127000	-2.830969000	1.065861000
6	19.992201000	-25.773336000	-8.326808000	6	1.988948000	-3.757663000	0.653279000
6	22.098928000	-21.146578000	-4.691267000	6	-3.562736000	-1.693725000	-1.409686000
6	21.247671000	-20.558539000	-3.669498000	6	-3.798925000	-0.250656000	-1.428264000
6	21.044798000	-21.321410000	-2.474553000	6	-3.179365000	0.484545000	-2.488171000
6	20.188451000	-19.687699000	-4.104016000	6	-4.020112000	0.444974000	-0.172757000
6	19.553422000	-22.614721000	-1.206920000	6	-1.519297000	2.031444000	-3.073193000
6	18.223603000	-23.156947000	-1.101076000	6	-0.458346000	2.894024000	-2.621528000
6	17.122501000	-22.312734000	-1.488693000	6	-0.664438000	3.628753000	-1.400219000
6	18.065820000	-24.579576000	-1.260144000	6	0.892698000	2.534563000	-2.968426000
6	20.675774000	-23.459452000	-1.563680000	6	-1.234055000	0.794197000	-3.771057000
6	18.713233000	-26.499373000	-2.443042000	6	2.466558000	0.818186000	-3.217714000
6	20.502684000	-24.864396000	-1.809585000	6	0.119206000	0.397186000	-4.039749000
6	19.194664000	-25.427777000	-1.596121000	6	1.180801000	1.306521000	-3.678540000
6	21.801447000	-20.930231000	-6.089847000	6	-3.417009000	-2.341438000	-0.121145000
6	20.073720000	-20.447527000	-7.764147000	6	-2.826836000	-2.074919000	2.265614000
6	20.713061000	-20.089125000	-6.533446000	6	-3.590124000	-1.632018000	1.142366000
6	19.932132000	-19.454385000	-5.511500000	6	-3.939231000	-0.237078000	1.098979000
6	21.408206000	-23.903175000	-8.288085000	6	-0.308235000	-4.250011000	0.561892000
6	20.468319000	-21.635046000	-8.504585000	6	-1.858065000	-3.146039000	2.123057000
6	21.516364000	-22.495591000	-8.034747000	6	-1.641445000	-3.810566000	0.861845000
6	14.596854000	-23.735818000	-4.489004000	6	2.111070000	3.060488000	1.628888000
6	17.791266000	-24.156281000	-9.189035000	6	1.654316000	-2.367237000	3.127370000
6	19.282574000	-22.191733000	-9.133045000	6	-0.755208000	-2.868633000	3.024234000
6	19.122225000	-23.614717000	-9.288110000	6	0.593280000	-3.226731000	2.674917000
6	20.223496000	-24.460864000	-8.905926000	6	0.797459000	-3.962844000	1.455670000
6	16.664972000	-23.312564000	-8.828389000	6	1.363695000	-1.124917000	3.818512000
6	18.640188000	-20.267200000	-7.934713000	6	-2.332131000	-1.127647000	3.267210000
6	16.853360000	-21.912828000	-8.576663000	6	0.006705000	-0.725391000	4.095175000
6	18.156653000	-21.352095000	-8.783707000	6	-1.042167000	-1.633052000	3.726675000
([11]CPP⊃Lu_3N@I_h-C_{80})$^{+\bullet}$				**([11]CPP⊃Gd_3N@I_h-C_{80})$^{+\bullet}$**			
6	7.440441000	-1.216015000	-2.400553000	6	7.480429000	-1.580588000	-2.099097000
6	7.777865000	-0.233214000	-1.469401000	6	7.786395000	-0.550282000	-1.226292000
6	7.570702000	-0.437527000	-0.076463000	6	7.534935000	-0.674327000	0.157904000

6	7.163898000	-1.735197000	0.336911000	6	7.113351000	-1.931714000	0.639941000
6	6.829249000	-2.718239000	-0.592818000	6	6.803754000	-2.960951000	-0.232885000
6	6.881297000	-2.457867000	-1.988926000	6	6.905200000	-2.782136000	-1.629213000
6	7.532051000	0.677779000	0.887355000	6	7.486167000	0.492286000	1.042392000
6	7.215192000	1.991854000	0.447828000	6	7.109300000	1.749092000	0.524274000
6	6.754301000	2.958722000	1.341473000	6	6.698177000	2.770220000	1.365233000
6	6.582635000	2.659713000	2.720273000	6	6.639813000	2.580145000	2.762644000
6	7.099546000	1.417630000	3.184923000	6	7.191901000	1.388860000	3.285589000
6	7.563034000	0.453228000	2.292379000	6	7.604219000	0.369011000	2.445549000
6	5.681639000	3.482622000	3.546562000	6	5.800649000	3.464333000	3.574325000
6	5.336677000	4.818264000	3.197853000	6	5.495096000	4.786013000	3.178367000
6	4.201779000	5.430489000	3.727846000	6	4.393308000	5.445933000	3.693670000
6	3.343502000	4.740839000	4.631615000	6	3.529199000	4.814321000	4.620065000
6	3.793906000	3.481044000	5.112339000	6	3.960660000	3.582324000	5.159964000
6	4.931485000	2.871392000	4.587985000	6	5.069438000	2.926451000	4.654028000
6	1.965207000	5.190052000	4.898980000	6	2.153043000	5.276838000	4.830545000
6	1.324997000	6.129814000	4.043511000	6	1.557810000	6.207571000	3.947781000
6	-0.057366000	6.302226000	4.060913000	6	0.186468000	6.386439000	3.905413000
6	-0.887736000	5.538362000	4.927574000	6	-0.675006000	5.629418000	4.729670000
6	-0.229303000	4.729521000	5.896382000	6	-0.069872000	4.822511000	5.719812000
6	1.153711000	4.564195000	5.885140000	6	1.302568000	4.660550000	5.776298000
6	-2.340699000	5.419107000	4.704705000	6	-2.107638000	5.505258000	4.444273000
6	-2.919914000	5.836307000	3.474581000	6	-2.610484000	5.825086000	3.164547000
6	-4.182227000	5.396140000	3.082645000	6	-3.847016000	5.363189000	2.745764000
6	-4.934994000	4.504328000	3.894497000	6	-4.639563000	4.551804000	3.584395000
6	-4.442104000	4.249055000	5.204625000	6	-4.220972000	4.391719000	4.924552000
6	-3.183337000	4.698904000	5.599943000	6	-2.990136000	4.862885000	5.345052000
6	-6.006540000	3.697460000	3.285462000	6	-5.713413000	3.741045000	3.006519000
6	-6.661016000	4.098255000	2.086977000	6	-6.394434000	4.128518000	1.830911000
6	-7.321439000	3.169610000	1.284580000	6	-7.116956000	3.206779000	1.092327000
6	-7.361707000	1.790858000	1.637285000	6	-7.183383000	1.851903000	1.488799000
6	-6.885131000	1.436189000	2.928499000	6	-6.648374000	1.510641000	2.749504000
6	-6.225258000	2.365843000	3.732225000	6	-5.932750000	2.434440000	3.492410000
6	-7.647473000	0.742269000	0.641283000	6	-7.542578000	0.786613000	0.548378000
6	-7.395435000	0.995579000	-0.734533000	6	-7.285323000	0.963193000	-0.827652000
6	-7.290989000	-0.047602000	-1.653065000	6	-7.187847000	-0.125197000	-1.678258000
6	-7.430423000	-1.400903000	-1.244273000	6	-7.346992000	-1.440446000	-1.192350000
6	-7.842769000	-1.641415000	0.095647000	6	-7.799968000	-1.597507000	0.137290000
6	-7.950074000	-0.597004000	1.014116000	6	-7.896566000	-0.509086000	0.987578000
6	-6.935147000	-2.477645000	-2.120514000	6	-6.824212000	-2.565717000	-1.971923000
6	-6.828769000	-2.311116000	-3.528621000	6	-6.687299000	-2.498849000	-3.376707000
6	-6.014883000	-3.147801000	-4.291991000	6	-5.851581000	-3.372754000	-4.050812000
6	-5.268600000	-4.195302000	-3.685699000	6	-5.115913000	-4.355687000	-3.352123000
6	-5.514680000	-4.465265000	-2.312137000	6	-5.388895000	-4.529809000	-1.979198000
6	-6.327481000	-3.627689000	-1.548787000	6	-6.224589000	-3.654861000	-1.304563000
6	-4.115288000	-4.823020000	-4.355660000	6	-3.955094000	-5.021192000	-3.948346000
6	-3.367448000	-4.079170000	-5.307833000	6	-3.172803000	-4.332416000	-4.898851000
6	-2.074943000	-4.462323000	-5.664310000	6	-1.891217000	-4.757892000	-5.207601000
6	-1.463697000	-5.607117000	-5.085232000	6	-1.332800000	-5.890402000	-4.578082000
6	-2.280745000	-6.447010000	-4.278822000	6	-2.178623000	-6.671965000	-3.759634000
6	-3.573526000	-6.064238000	-3.921981000	6	-3.459732000	-6.246616000	-3.450736000
6	0.003980000	-5.745490000	-5.119148000	6	0.119475000	-6.084571000	-4.596880000

6	0.801668000	-5.104975000	-6.107454000	6	0.928857000	-5.572446000	-5.635450000
6	2.168200000	-4.904626000	-5.911224000	6	2.293454000	-5.414838000	-5.460945000
6	2.809221000	-5.334055000	-4.716399000	6	2.912090000	-5.760540000	-4.238662000
6	2.045708000	-6.126303000	-3.816383000	6	2.131032000	-6.437133000	-3.277157000
6	0.679946000	-6.326139000	-4.011877000	6	0.766849000	-6.594369000	-3.451385000
6	4.115106000	-4.797484000	-4.290266000	6	4.217080000	-5.220760000	-3.848383000
6	4.538470000	-3.518919000	-4.743026000	6	4.620436000	-3.962006000	-4.342011000
6	5.540651000	-2.814061000	-4.076108000	6	5.598945000	-3.225145000	-3.695841000
6	6.168448000	-3.350737000	-2.920689000	6	6.219545000	-3.714635000	-2.527385000
6	5.877116000	-4.702836000	-2.587318000	6	5.954489000	-5.051211000	-2.153464000
6	4.877013000	-5.407928000	-3.254841000	6	4.976298000	-5.787855000	-2.799562000
1	7.579779000	-1.009467000	-3.469972000	1	7.662689000	-1.450870000	-3.163819000
1	8.176137000	0.725350000	-1.827226000	1	8.205138000	0.374654000	-1.617405000
1	6.990989000	-1.940044000	1.400355000	1	6.898874000	-2.059949000	1.697801000
1	6.405775000	-3.662818000	-0.229857000	1	6.354741000	-3.867871000	0.164326000
1	7.204632000	2.221718000	-0.624924000	1	7.010877000	1.882535000	-0.549931000
1	6.396241000	3.915248000	0.940693000	1	6.289079000	3.677073000	0.927194000
1	7.091669000	1.190238000	4.258911000	1	7.264332000	1.255639000	4.362872000
1	7.910540000	-0.511804000	2.683559000	1	7.998039000	-0.550470000	2.873573000
1	5.946628000	5.367391000	2.468579000	1	6.110590000	5.280780000	2.429818000
1	3.951550000	6.448017000	3.402219000	1	4.171375000	6.448052000	3.336681000
1	3.182274000	2.911343000	5.821220000	1	3.354149000	3.064662000	5.896612000
1	5.167978000	1.847960000	4.903344000	1	5.283330000	1.919780000	5.003853000
1	1.908181000	6.675401000	3.291944000	1	2.168461000	6.743734000	3.227167000
1	-0.504627000	7.000466000	3.343306000	1	-0.225941000	7.084285000	3.181500000
1	-0.815085000	4.155549000	6.624182000	1	-0.685842000	4.241096000	6.400151000
1	1.605728000	3.890007000	6.622614000	1	1.712687000	3.993297000	6.528694000
1	-2.330495000	6.419367000	2.757629000	1	-1.976337000	6.325881000	2.438996000
1	-4.533274000	5.643298000	2.073261000	1	-4.140659000	5.517958000	1.710403000
1	-5.039309000	3.650676000	5.905358000	1	-4.862358000	3.867005000	5.629651000
1	-2.826195000	4.443013000	6.605208000	1	-2.690290000	4.700888000	6.377175000
1	-6.608265000	5.145200000	1.760272000	1	-6.329901000	5.158642000	1.486156000
1	-7.777826000	3.505255000	0.344202000	1	-7.610846000	3.525372000	0.176831000
1	-6.915957000	0.388683000	3.253458000	1	-6.676643000	0.477569000	3.086217000
1	-5.757398000	2.018315000	4.661720000	1	-5.423169000	2.102254000	4.393402000
1	-7.158191000	2.013197000	-1.067595000	1	-7.015903000	1.946233000	-1.205281000
1	-6.972939000	0.182203000	-2.677319000	1	-6.847457000	0.036371000	-2.697931000
1	-8.047465000	-2.668416000	0.426077000	1	-8.042784000	-2.590560000	0.509759000
1	-8.237970000	-0.823624000	2.049158000	1	-8.211496000	-0.662140000	2.017657000
1	-7.361761000	-1.487231000	-4.021276000	1	-7.222539000	-1.733474000	-3.934758000
1	-5.921857000	-2.967288000	-5.371120000	1	-5.740342000	-3.283338000	-5.129447000
1	-4.965007000	-5.270373000	-1.808693000	1	-4.836561000	-5.273452000	-1.409766000
1	-6.391833000	-3.797144000	-0.466753000	1	-6.306941000	-3.737656000	-0.223888000
1	-3.752957000	-3.119760000	-5.674762000	1	-3.521681000	-3.382961000	-5.297646000
1	-1.484816000	-3.791565000	-6.300819000	1	-1.269507000	-4.131427000	-5.842532000
1	-1.876426000	-7.391386000	-3.891311000	1	-1.810583000	-7.607116000	-3.342789000
1	-4.162578000	-6.714409000	-3.261521000	1	-4.082025000	-6.852162000	-2.794743000
1	0.332141000	-4.724105000	-7.024020000	1	0.471393000	-5.269048000	-6.574854000
1	2.744843000	-4.370478000	-6.677803000	1	2.889271000	-4.987397000	-6.264754000
1	2.501357000	-6.487179000	-2.886160000	1	2.573275000	-6.718821000	-2.325296000
1	0.105570000	-6.835335000	-3.228301000	1	0.176956000	-6.997824000	-2.632572000
1	3.988251000	-3.014613000	-5.546799000	1	4.064939000	-3.496552000	-5.152190000

1	5.745425000	-1.779129000	-4.377389000	1	5.782516000	-2.202971000	-4.017140000
1	6.416264000	-5.189702000	-1.764030000	1	6.500347000	-5.496559000	-1.324276000
1	4.649680000	-6.436022000	-2.943857000	1	4.765012000	-6.802749000	-2.469227000
71	-1.747262000	0.887684000	0.612686000	64	0.895782000	-1.531751000	-1.052289000
71	-0.289340000	-1.905307000	-1.038530000	64	1.278940000	1.252809000	0.923616000
71	1.787935000	0.581190000	0.421617000	64	-1.866697000	0.046823000	0.241561000
7	-0.083941000	-0.140813000	-0.010664000	7	0.135479000	-0.485909000	0.605863000
6	3.169193000	0.857808000	-2.411828000	6	-2.747801000	2.719520000	-0.761044000
6	3.657408000	-0.325623000	-1.766188000	6	-2.823940000	2.703927000	0.661113000
6	4.083578000	-0.185897000	-0.373888000	6	-3.564040000	1.614532000	1.276074000
6	-2.278218000	1.390671000	3.145794000	6	0.837568000	-4.154023000	-0.517065000
6	2.124585000	0.797140000	-3.415792000	6	-1.596332000	3.270983000	-1.438862000
6	0.137075000	-0.480893000	-4.134315000	6	0.825224000	3.679425000	-1.261852000
6	1.531833000	-0.463763000	-3.790297000	6	-0.487167000	3.822117000	-0.715505000
6	2.074964000	-1.662611000	-3.211893000	6	-0.583542000	3.884270000	0.704100000
6	2.925568000	-2.695781000	-1.285300000	6	-1.274344000	2.801569000	2.642492000
6	3.229901000	-2.542927000	0.110374000	6	-1.885931000	1.641185000	3.203848000
6	3.807573000	-1.278218000	0.539225000	6	-3.024793000	1.064964000	2.504511000
6	2.415004000	-3.247759000	1.050248000	6	-1.045117000	0.773052000	3.947920000
6	1.759479000	-3.460829000	-1.725099000	6	0.150106000	3.060062000	2.759115000
6	-0.535166000	-4.269883000	-1.143288000	6	2.394726000	2.036030000	2.977976000
6	0.888494000	-4.139164000	-0.785293000	6	1.017631000	2.154698000	3.456234000
6	1.247921000	-4.010625000	0.612961000	6	0.387414000	1.016155000	4.063041000
6	-0.705930000	-1.636817000	-3.837865000	6	2.001064000	3.541698000	-0.410409000
6	-0.186194000	-2.867771000	-3.271931000	6	1.945890000	3.628964000	1.035983000
6	1.230777000	-2.825438000	-2.934876000	6	0.594567000	3.759991000	1.561826000
6	-1.082014000	-3.644576000	-2.387729000	6	2.895056000	2.782824000	1.795567000
6	2.226876000	2.726744000	1.940375000	6	-3.480904000	-1.996483000	-0.792338000
6	2.762641000	1.533318000	2.563036000	6	-3.579510000	-1.979226000	0.639717000
6	3.564219000	-0.724876000	1.853512000	6	-3.258285000	-0.356642000	2.504360000
6	3.727656000	0.731393000	1.792171000	6	-3.965721000	-0.717261000	1.279615000
6	2.540380000	3.069061000	0.549447000	6	-3.658762000	-0.784893000	-1.578536000
6	3.004552000	2.098964000	-1.648832000	6	-3.280318000	1.616722000	-1.556033000
6	3.425155000	2.245138000	-0.266661000	6	-3.983182000	0.495498000	-0.968108000
6	4.072033000	1.081437000	0.379262000	6	-4.194841000	0.525172000	0.496324000
6	-0.416007000	3.643860000	-1.707834000	6	-0.820562000	0.015159000	-3.887940000
6	0.987081000	3.594645000	-1.379415000	6	-2.111843000	0.216766000	-3.297561000
6	1.365864000	3.750107000	-0.000196000	6	-2.769296000	-0.913056000	-2.731988000
6	1.844722000	2.791193000	-2.204562000	6	-2.404584000	1.487669000	-2.714261000
6	-3.733509000	0.496351000	-1.895670000	6	3.430202000	0.091763000	-2.310185000
6	-2.882472000	-1.780927000	-2.585657000	6	3.744805000	1.728696000	-0.402909000
6	-3.754343000	-0.951904000	-1.779457000	6	4.010351000	0.455681000	-1.035229000
6	-2.365234000	-3.022707000	-2.012533000	6	3.740310000	1.820768000	1.047874000
6	-4.045082000	1.077211000	-0.586881000	6	3.239435000	-1.354760000	-2.356251000
6	-3.249425000	2.544217000	1.295620000	6	1.588778000	-3.232377000	-2.584030000
6	-3.519969000	2.365269000	-0.149414000	6	2.181272000	-1.990773000	-3.126195000
6	-2.599999000	2.984614000	-1.086735000	6	1.283409000	-1.053389000	-3.766222000
6	-3.338734000	-1.119467000	2.359356000	6	2.955950000	-2.988549000	0.965335000
6	-3.876941000	0.076731000	1.744575000	6	3.054769000	-3.011092000	-0.467221000
6	-4.232680000	-0.038031000	0.343965000	6	3.683283000	-1.867713000	-1.068941000
6	-3.421401000	1.389421000	2.229108000	6	2.022737000	-3.707117000	-1.243390000
6	-2.627569000	-3.291770000	-0.610787000	6	3.803313000	0.574108000	1.784386000

6	-3.466151000	-2.437757000	0.217796000	6	4.009496000	-0.717541000	1.148731000
6	-4.052342000	-1.282118000	-0.400638000	6	4.158694000	-0.750637000	-0.268985000
6	-3.159718000	-2.362806000	1.612559000	6	3.441789000	-1.865688000	1.758975000
6	-1.504769000	-4.026585000	-0.069223000	6	2.974603000	0.700290000	2.954546000
6	0.244351000	-3.907190000	1.666589000	6	1.038847000	-0.275379000	4.109132000
6	-1.151997000	-3.866839000	1.337974000	6	2.320988000	-0.465625000	3.514264000
6	-2.014028000	-3.064335000	2.164268000	6	2.600632000	-1.738611000	2.925007000
6	-1.976343000	3.190663000	1.669083000	6	0.114496000	-3.373487000	-2.604603000
6	-1.055492000	3.811308000	0.718713000	6	-0.767277000	-2.389176000	-3.211884000
6	-1.418783000	3.744908000	-0.666701000	6	-0.158046000	-1.269389000	-3.845026000
6	0.356147000	3.849131000	1.040170000	6	-2.092622000	-2.188506000	-2.671454000
6	-0.957090000	2.819254000	-2.769676000	6	0.192635000	1.030815000	-3.801308000
6	-0.109521000	1.950457000	-3.544654000	6	-0.062807000	2.270751000	-3.134365000
6	1.305956000	1.985066000	-3.280208000	6	-1.383365000	2.500356000	-2.633381000
6	-0.673849000	0.713990000	-4.021559000	6	1.029004000	2.903941000	-2.458704000
6	-2.298133000	2.418022000	-2.399273000	6	1.479837000	0.389173000	-3.725797000
6	-2.050298000	-1.125648000	-3.551264000	6	2.909916000	2.639554000	-1.113258000
6	-2.830168000	1.147317000	-2.806780000	6	2.536251000	0.982399000	-2.969267000
6	-2.023580000	0.319751000	-3.670144000	6	2.315630000	2.270591000	-2.378841000
6	-1.415814000	2.505561000	2.817605000	6	-0.320941000	-3.961113000	-1.352435000
6	0.536250000	1.351598000	3.789066000	6	-1.762470000	-3.745098000	0.640619000
6	0.007229000	2.501106000	3.122610000	6	-1.634176000	-3.714549000	-0.772138000
6	0.879214000	3.213507000	2.232334000	6	-2.528707000	-2.855529000	-1.477678000
6	-2.286906000	-1.065882000	3.369574000	6	1.806239000	-3.535791000	1.657178000
6	-0.308935000	0.209993000	4.094429000	6	-0.601598000	-3.918733000	1.480095000
6	-1.705872000	0.190843000	3.747894000	6	0.708604000	-4.081132000	0.927793000
6	3.121234000	-1.595484000	-2.205740000	6	-1.724351000	3.307594000	1.376949000
6	0.787401000	-3.094576000	2.736694000	6	0.024305000	-1.297516000	4.028204000
6	0.502866000	-0.989355000	3.987691000	6	-0.814932000	-3.163572000	2.689929000
6	-0.060426000	-2.224232000	3.508113000	6	0.275974000	-2.531747000	3.357791000
6	-1.475047000	-2.260417000	3.246435000	6	1.592425000	-2.767268000	2.858419000
6	2.129391000	-2.688414000	2.359843000	6	-1.262513000	-0.653678000	3.931898000
6	1.880683000	0.860715000	3.495716000	6	-2.706982000	-2.881092000	1.338381000
6	2.658842000	-1.414012000	2.767539000	6	-2.331938000	-1.242814000	3.186136000
6	1.848333000	-0.592864000	3.621719000	6	-2.105638000	-2.525758000	2.606748000
([11]CPP⊃*D*$_{2d}$-C$_{84}$)$^{+\bullet}$				**([11]CPP⊃*D*$_{2}$-C$_{84}$)$^{+\bullet}$**			
6	7.889436000	-1.699900000	-0.669509000	6	7.954681000	-1.810168000	-0.525200000
6	8.052397000	-0.319814000	-0.557710000	6	8.093503000	-0.424091000	-0.481275000
6	7.639780000	0.381161000	0.611817000	6	7.688656000	0.321896000	0.662488000
6	7.234195000	-0.407826000	1.723859000	6	7.327692000	-0.417010000	1.821935000
6	7.080086000	-1.788304000	1.616056000	6	7.193640000	-1.803735000	1.780233000
6	7.417516000	1.838950000	0.612596000	6	7.415330000	1.768075000	0.591373000
6	7.316914000	2.562537000	-0.609045000	6	7.165841000	2.387781000	-0.664203000
6	6.721692000	3.821561000	-0.658788000	6	6.542539000	3.630020000	-0.746761000
6	6.184052000	4.430651000	0.508933000	6	6.124041000	4.329193000	0.419701000
6	6.465101000	3.794338000	1.750333000	6	6.537562000	3.789692000	1.670689000
6	7.067983000	2.539080000	1.800360000	6	7.164408000	2.547797000	1.754148000
6	5.190405000	5.517153000	0.432721000	6	5.141126000	5.426191000	0.345335000
6	4.471512000	5.742852000	-0.774301000	6	4.440583000	5.690596000	-0.864448000
6	3.280076000	6.465214000	-0.783358000	6	3.280418000	6.461456000	-0.879353000
6	2.735684000	6.994804000	0.417754000	6	2.744379000	7.003735000	0.318966000

6	3.541558000	6.922262000	1.586997000	6	3.533688000	6.884944000	1.496180000
6	4.740029000	6.209156000	1.592116000	6	4.701458000	6.123979000	1.506837000
6	1.310795000	7.364465000	0.468894000	6	1.336259000	7.430977000	0.357769000
6	0.590086000	7.757105000	-0.692265000	6	0.640002000	7.852802000	-0.809094000
6	-0.803989000	7.723672000	-0.718609000	6	-0.753871000	7.869406000	-0.847438000
6	-1.549666000	7.289023000	0.412010000	6	-1.522440000	7.458671000	0.277023000
6	-0.832939000	7.063932000	1.618572000	6	-0.824700000	7.209216000	1.489962000
6	0.560495000	7.102040000	1.646900000	6	0.568121000	7.196587000	1.530095000
6	-2.948557000	6.837853000	0.297101000	6	-2.932848000	7.049181000	0.156111000
6	-3.430035000	6.348571000	-0.947408000	6	-3.419182000	6.552989000	-1.083146000
6	-4.582925000	5.568004000	-1.017652000	6	-4.579503000	5.781710000	-1.143133000
6	-5.313538000	5.230519000	0.153503000	6	-5.315452000	5.468459000	0.031809000
6	-4.927070000	5.859751000	1.368418000	6	-4.932883000	6.125475000	1.234439000
6	-3.776084000	6.644971000	1.437846000	6	-3.772049000	6.894923000	1.295035000
6	-6.254119000	4.096078000	0.122250000	6	-6.244166000	4.323999000	0.028916000
6	-6.879676000	3.670036000	-1.082160000	6	-6.818902000	3.823968000	-1.172573000
6	-7.441788000	2.398525000	-1.190287000	6	-7.343673000	2.533957000	-1.235842000
6	-7.404679000	1.484715000	-0.100916000	6	-7.325428000	1.677285000	-0.100292000
6	-6.940892000	1.978857000	1.148649000	6	-6.922604000	2.244105000	1.138598000
6	-6.379866000	3.251229000	1.257633000	6	-6.393547000	3.532980000	1.200904000
6	-7.582332000	0.033916000	-0.294611000	6	-7.475535000	0.216156000	-0.225096000
6	-7.286024000	-0.548005000	-1.556500000	6	-7.098206000	-0.425807000	-1.435144000
6	-7.045169000	-1.915528000	-1.681123000	6	-6.863905000	-1.799296000	-1.478840000
6	-7.090684000	-2.777134000	-0.552193000	6	-6.994351000	-2.604467000	-0.315178000
6	-7.575968000	-2.223191000	0.666075000	6	-7.537875000	-1.988872000	0.846396000
6	-7.812251000	-0.854780000	0.792566000	6	-7.770862000	-0.614288000	0.891072000
6	-6.431643000	-4.095615000	-0.604958000	6	-6.357923000	-3.933950000	-0.273341000
6	-6.116554000	-4.731807000	-1.838953000	6	-6.056402000	-4.663536000	-1.457239000
6	-5.172048000	-5.755230000	-1.903799000	6	-5.124340000	-5.700279000	-1.446196000
6	-4.491482000	-6.203717000	-0.737628000	6	-4.443843000	-6.063389000	-0.250404000
6	-4.939299000	-5.692284000	0.510392000	6	-4.882559000	-5.456892000	0.957041000
6	-5.881917000	-4.666690000	0.574761000	6	-5.814418000	-4.419566000	0.945956000
6	-3.233076000	-6.967894000	-0.810783000	6	-3.190089000	-6.839596000	-0.268938000
6	-2.410893000	-6.876386000	-1.967005000	6	-2.367192000	-6.830252000	-1.427244000
6	-1.066167000	-7.242496000	-1.927157000	6	-1.030285000	-7.222849000	-1.366031000
6	-0.470039000	-7.716579000	-0.727457000	6	-0.443911000	-7.645651000	-0.143054000
6	-1.338210000	-7.986023000	0.367457000	6	-1.312876000	-7.819807000	0.970078000
6	-2.682964000	-7.621795000	0.326933000	6	-2.649194000	-7.427004000	0.909018000
6	0.995687000	-7.685644000	-0.569621000	6	1.023174000	-7.657235000	0.002429000
6	1.874478000	-7.642965000	-1.688377000	6	1.893965000	-7.751613000	-1.118434000
6	3.196897000	-7.223660000	-1.551793000	6	3.230440000	-7.364189000	-1.026076000
6	3.713304000	-6.815595000	-0.290209000	6	3.767480000	-6.862232000	0.192075000
6	2.886737000	-7.031481000	0.846919000	6	2.945571000	-6.946121000	1.348327000
6	1.566823000	-7.459402000	0.711351000	6	1.609305000	-7.332281000	1.255801000
6	4.931186000	-5.992149000	-0.174415000	6	5.006429000	-6.063685000	0.233171000
6	5.381132000	-5.226819000	-1.284941000	6	5.439211000	-5.363035000	-0.924771000
6	6.266121000	-4.162388000	-1.119882000	6	6.337078000	-4.299965000	-0.829216000
6	6.433005000	-4.673241000	1.248169000	6	6.562934000	-4.704109000	1.554853000
6	5.555055000	-5.742982000	1.080217000	6	5.668034000	-5.768184000	1.458372000
6	6.743119000	-3.800020000	0.168151000	6	6.847892000	-3.881340000	0.429711000
6	7.313335000	-2.459539000	0.385970000	6	7.411166000	-2.527889000	0.576327000
1	8.174772000	-2.197064000	-1.605991000	1	8.231133000	-2.346846000	-1.442463000

1	8.464754000	0.232128000	-1.411656000	1	8.478647000	0.097760000	-1.366580000
1	6.922327000	0.075412000	2.656535000	1	7.020106000	0.108989000	2.733494000
1	6.648065000	-2.335998000	2.462802000	1	6.786200000	-2.318153000	2.659158000
1	7.623128000	2.094411000	-1.552275000	1	7.376819000	1.846852000	-1.594392000
1	6.611396000	4.312394000	-1.633777000	1	6.316863000	4.030909000	-1.741509000
1	6.119646000	4.244485000	2.688806000	1	6.294699000	4.312079000	2.603624000
1	7.204158000	2.063908000	2.779378000	1	7.415066000	2.149414000	2.745351000
1	4.783950000	5.245369000	-1.699488000	1	4.744982000	5.202205000	-1.796431000
1	2.697353000	6.509516000	-1.711612000	1	2.712585000	6.539582000	-1.814708000
1	3.199857000	7.402165000	2.513771000	1	3.201512000	7.367079000	2.425107000
1	5.314184000	6.146984000	2.525340000	1	5.255716000	6.029316000	2.448563000
1	1.136464000	8.054988000	-1.597040000	1	1.204774000	8.133011000	-1.708257000
1	-1.327079000	7.997632000	-1.644136000	1	-1.260443000	8.162213000	-1.776549000
1	-1.367092000	6.729620000	2.516312000	1	-1.378573000	6.894124000	2.382583000
1	1.077922000	6.797930000	2.565389000	1	1.066104000	6.873079000	2.452275000
1	-2.826139000	6.474657000	-1.854236000	1	-2.809979000	6.657147000	-1.989653000
1	-4.848947000	5.107724000	-1.977204000	1	-4.843785000	5.306033000	-2.095547000
1	-5.519571000	5.696594000	2.278426000	1	-5.533616000	5.992107000	2.143766000
1	-3.487287000	7.084706000	2.401527000	1	-3.482931000	7.351700000	2.250724000
1	-6.888202000	4.335225000	-1.955778000	1	-6.814142000	4.443780000	-2.078833000
1	-7.880846000	2.088262000	-2.147591000	1	-7.741151000	2.163993000	-2.190198000
1	-6.902556000	1.311135000	2.018016000	1	-6.902086000	1.621682000	2.041830000
1	-5.916872000	3.543498000	2.208334000	1	-5.973772000	3.882346000	2.152157000
1	-7.111607000	0.095976000	-2.426992000	1	-6.862544000	0.176513000	-2.321231000
1	-6.691448000	-2.296501000	-2.646552000	1	-6.451776000	-2.232461000	-2.398235000
1	-7.724676000	-2.870491000	1.540036000	1	-7.741328000	-2.594225000	1.739507000
1	-8.140331000	-0.456767000	1.761926000	1	-8.152254000	-0.165449000	1.817861000
1	-6.592488000	-4.390329000	-2.767194000	1	-6.531504000	-4.382956000	-2.406415000
1	-4.927537000	-6.192602000	-2.880664000	1	-4.886087000	-6.213653000	-2.386967000
1	-4.451650000	-6.013606000	1.438701000	1	-4.393512000	-5.712016000	1.905077000
1	-6.102952000	-4.221040000	1.552106000	1	-6.025225000	-3.893751000	1.885154000
1	-2.795226000	-6.393518000	-2.873754000	1	-2.743232000	-6.392045000	-2.359827000
1	-0.440150000	-7.030333000	-2.802381000	1	-0.399498000	-7.077022000	-2.251433000
1	-0.939453000	-8.449390000	1.279283000	1	-0.921065000	-8.234770000	1.908020000
1	-3.311941000	-7.807103000	1.207402000	1	-3.280107000	-7.542151000	1.800069000
1	1.500188000	-7.905733000	-2.686332000	1	1.502233000	-8.091816000	-2.086039000
1	3.830995000	-7.168715000	-2.446016000	1	3.861533000	-7.407842000	-1.923386000
1	3.242889000	-6.746167000	1.844050000	1	3.318786000	-6.579086000	2.312126000
1	0.933402000	-7.492260000	1.606252000	1	0.978532000	-7.256716000	2.149935000
1	4.936640000	-5.386431000	-2.274570000	1	4.965833000	-5.564054000	-1.893896000
1	6.484838000	-3.521576000	-1.982987000	1	6.541634000	-3.702367000	-1.726261000
1	6.860808000	-4.484189000	2.241573000	1	7.019642000	-4.475430000	2.526890000
1	5.312984000	-6.372433000	1.946212000	1	5.440135000	-6.356372000	2.356849000
6	-0.123764000	-0.476866000	-4.378219000	6	-0.633938000	-0.789407000	-4.120399000
6	-0.040651000	-1.875979000	-3.975129000	6	0.654731000	-0.164061000	-4.224112000
6	1.342928000	-2.156020000	-3.673903000	6	0.665621000	1.256171000	-4.069047000
6	2.095005000	-0.909422000	-3.862156000	6	-1.796106000	-0.070509000	-3.665715000
6	1.179502000	0.156518000	-4.201607000	6	-1.753453000	1.321944000	-3.358039000
6	-1.290475000	0.229628000	-4.153759000	6	-0.514254000	1.987619000	-3.668375000
6	-2.439965000	-0.407793000	-3.518751000	6	1.856053000	-0.940748000	-3.841836000
6	-2.351529000	-1.725701000	-2.964935000	6	2.988149000	-0.245584000	-3.302405000
6	-1.119341000	-2.491672000	-3.245645000	6	-0.762064000	-2.158185000	-3.634031000

6	-0.738880000	-3.544823000	-2.362187000	6	0.361022000	-2.893146000	-3.285212000
6	0.641711000	-3.861124000	-2.097591000	6	1.694819000	-2.298954000	-3.404887000
6	1.716923000	-3.090094000	-2.658721000	6	-1.972712000	-2.273910000	-2.837764000
6	2.900171000	-2.797262000	-1.817722000	6	-2.003550000	-3.094768000	-1.655747000
6	3.639018000	-1.594083000	-2.047615000	6	-2.948994000	-2.705399000	-0.666728000
6	3.207854000	-0.636331000	-3.073924000	6	-3.446932000	-0.523218000	-1.819254000
6	3.436293000	0.711504000	-2.601422000	6	-2.632435000	-0.990370000	-2.886455000
6	2.480565000	1.759581000	-2.807782000	6	-3.699481000	-1.477586000	-0.771809000
6	1.302704000	1.469645000	-3.643979000	6	-3.487850000	0.924288000	-1.523847000
6	0.055139000	2.235966000	-3.446522000	6	-2.220349000	3.068401000	-1.657829000
6	-1.217021000	1.624967000	-3.734435000	6	-2.624996000	1.848187000	-2.287692000
6	-2.393334000	1.901504000	-2.945297000	6	-3.886807000	1.308288000	-0.205885000
6	-3.165116000	0.655051000	-2.856915000	6	1.693400000	-3.833446000	-1.628318000
6	-3.908283000	0.372968000	-1.716506000	6	2.519133000	-2.872373000	-2.370261000
6	-3.948362000	-0.979997000	-1.204466000	6	3.533958000	-2.109358000	-1.701436000
6	-3.140267000	-2.025307000	-1.755781000	6	3.800700000	-0.810213000	-2.253450000
6	-2.691657000	-3.089819000	-0.834207000	6	1.924748000	-4.055697000	-0.276330000
6	-1.523719000	-3.841332000	-1.155463000	6	-0.793778000	-3.836227000	-1.245295000
6	-0.628801000	-4.341488000	-0.144170000	6	0.334076000	-3.783583000	-2.124416000
6	0.711062000	-4.361144000	-0.726697000	6	0.803607000	-4.258451000	0.616378000
6	1.821399000	-4.085188000	0.060746000	6	-0.550312000	-4.097035000	0.185733000
6	2.927045000	-3.293913000	-0.472275000	6	2.980002000	-3.317830000	0.426345000
6	3.455799000	-2.512714000	0.615758000	6	3.758902000	-2.331565000	-0.255166000
6	4.034245000	-1.225144000	0.413670000	6	4.212623000	-1.231968000	0.547454000
6	4.211161000	-0.833590000	-0.960485000	6	4.438487000	0.084200000	-0.040835000
6	4.158373000	0.575514000	-1.339227000	6	4.237738000	0.294548000	-1.395437000
6	4.052563000	1.545198000	-0.359269000	6	0.333015000	-3.314878000	2.850900000
6	3.210524000	2.714816000	-0.588489000	6	1.246421000	-3.786098000	1.926023000
6	2.404564000	2.814904000	-1.777160000	6	2.542300000	-3.130236000	1.789767000
6	1.202587000	3.572609000	-1.643072000	6	2.825066000	-1.918621000	2.519023000
6	0.027638000	3.281662000	-2.477435000	6	3.729936000	-1.015806000	1.886947000
6	-1.158321000	3.594150000	-1.721435000	6	-2.721348000	-2.986542000	0.754929000
6	-2.365604000	2.826402000	-1.855179000	6	-1.530421000	-3.637842000	1.191979000
6	-3.157640000	2.525747000	-0.641032000	6	-1.087131000	-3.292113000	2.519187000
6	-3.925235000	1.320919000	-0.595410000	6	1.823962000	1.934974000	-3.480429000
6	-4.055733000	0.549820000	0.617562000	6	2.945144000	1.206929000	-3.098637000
6	-4.154431000	-0.855325000	0.235837000	6	3.632576000	1.540683000	-1.870274000
6	-3.696747000	-1.832217000	1.100452000	6	4.045268000	1.111759000	0.910599000
6	-3.002188000	-3.001020000	0.568610000	6	2.550322000	2.946561000	1.428116000
6	-2.083464000	-3.458209000	1.583414000	6	3.395012000	2.319107000	0.470974000
6	-0.828084000	-4.057752000	1.247635000	6	3.123513000	2.524674000	-0.965035000
6	0.356892000	-3.764910000	2.088500000	6	1.945300000	3.312533000	-1.379320000
6	1.657996000	-3.778261000	1.479927000	6	1.368445000	3.035291000	-2.658070000
6	2.669448000	-2.810770000	1.821776000	6	0.650870000	-2.162662000	3.690535000
6	2.460298000	-1.819809000	2.825631000	6	1.832310000	-1.384872000	3.473881000
6	3.088349000	-0.491075000	2.668230000	6	1.761349000	0.068136000	3.724382000
6	3.875602000	-0.192222000	1.458697000	6	2.667236000	0.980483000	2.997264000
6	3.990816000	1.175723000	1.051760000	6	3.642004000	0.431903000	2.118576000
6	3.254574000	2.235771000	1.706718000	6	2.239824000	2.321703000	2.691402000
6	2.729638000	3.162762000	0.696491000	6	1.394818000	3.756132000	1.018344000
6	1.442480000	3.765157000	0.849991000	6	1.062298000	3.914369000	-0.358652000
6	0.744806000	4.062932000	-0.369195000	6	-0.335898000	4.115662000	-0.643647000

6	-0.716239000	4.083832000	-0.417745000	6	-0.904343000	3.654296000	-1.905483000
6	-1.459729000	3.801169000	0.720484000	6	-0.072806000	3.130556000	-2.878935000
6	-2.687774000	3.014150000	0.624650000	6	0.084698000	1.957888000	3.812001000
6	-2.775491000	2.220407000	1.822389000	6	0.920244000	2.791502000	3.084603000
6	-3.387739000	0.931620000	1.835127000	6	0.381902000	3.653652000	2.038207000
6	-2.859125000	-0.107878000	2.741680000	6	-1.020836000	3.636651000	1.721986000
6	-3.118694000	-1.473297000	2.392807000	6	-1.353967000	3.955959000	0.370472000
6	-2.194624000	-2.536900000	2.721752000	6	-0.617803000	-1.551942000	4.021421000
6	-1.082882000	-2.262422000	3.510414000	6	-0.678273000	-0.186949000	4.277075000
6	0.209726000	-2.890703000	3.210250000	6	0.522416000	0.613326000	4.187327000
6	1.242448000	-1.953898000	3.583095000	6	-3.357006000	-1.949405000	1.529059000
6	0.583356000	-0.777457000	4.138636000	6	-2.788703000	-1.459047000	2.753087000
6	1.189683000	0.460071000	4.029848000	6	-1.688538000	-2.213031000	3.268746000
6	2.481512000	0.603673000	3.365154000	6	-3.537350000	0.853756000	2.109780000
6	2.511116000	1.954334000	2.847139000	6	-4.079484000	0.320059000	0.857150000
6	1.198728000	2.582922000	3.047168000	6	-3.989293000	-1.036333000	0.582995000
6	0.650014000	3.465192000	2.064567000	6	-1.825672000	0.601848000	3.815058000
6	-0.784278000	3.482587000	1.976706000	6	-2.870060000	-0.008659000	3.045247000
6	-1.599045000	2.508383000	2.656367000	6	-2.526310000	3.351286000	-0.272600000
6	-1.036876000	1.509456000	3.504525000	6	-1.354255000	1.935710000	3.539050000
6	-1.680667000	0.182081000	3.577791000	6	-1.915163000	2.739434000	2.489969000
6	-0.862252000	-0.917299000	3.992266000	6	-3.077396000	2.195827000	1.846519000
6	0.374042000	1.639811000	3.763862000	6	-3.356554000	2.491635000	0.437023000
([11]CPP⊃Sc_3N@D_{5h}-C_{80})$^{+\bullet}$				**([11]CPP⊃Sc_3N@D_{3h}-C_{78})$^{+\bullet}$**			
6	26.264554000	-25.100850000	-6.718041000	6	6.258454000	0.650697000	4.858357000
6	26.437897000	-23.716717000	-6.671219000	6	6.773042000	1.412933000	3.806567000
6	26.171271000	-22.986690000	-5.481836000	6	6.172243000	2.644437000	3.430610000
6	25.902690000	-23.731191000	-4.302834000	6	5.122895000	3.137898000	4.247248000
6	25.729014000	-25.115789000	-4.350596000	6	4.607974000	2.376137000	5.297116000
6	25.813338000	-25.821612000	-5.579135000	6	5.116669000	1.081928000	5.583514000
6	25.917353000	-21.532091000	-5.495997000	6	6.452408000	3.295154000	2.134764000
6	25.344002000	-20.938817000	-6.651191000	6	6.815328000	2.505508000	1.013223000
6	24.708254000	-19.697892000	-6.582500000	6	6.733920000	3.017893000	-0.282805000
6	24.617978000	-18.990327000	-5.355665000	6	6.283798000	4.343419000	-0.518528000
6	25.349674000	-19.500753000	-4.248833000	6	6.079151000	5.179768000	0.610766000
6	25.983181000	-20.742705000	-4.316971000	6	6.162737000	4.667267000	1.906870000
6	23.611354000	-17.921246000	-5.201741000	6	5.808583000	4.712073000	-1.866454000
6	23.112095000	-17.190910000	-6.313827000	6	6.311760000	4.093899000	-3.042017000
6	21.919265000	-16.471468000	-6.225148000	6	5.585930000	4.120479000	-4.234080000
6	21.169451000	-16.442880000	-5.018324000	6	4.314183000	4.753601000	-4.306668000
6	21.753255000	-17.036762000	-3.868624000	6	3.915156000	5.530939000	-3.186724000
6	22.943979000	-17.759378000	-3.958940000	6	4.645053000	5.513853000	-1.997736000
6	19.749233000	-16.044820000	-4.987263000	6	3.337946000	4.426414000	-5.366235000
6	18.938148000	-16.266082000	-6.130235000	6	3.475058000	3.235638000	-6.131536000
6	17.547259000	-16.295549000	-6.029439000	6	2.403611000	2.707191000	-6.851524000
6	16.895675000	-16.098819000	-4.782809000	6	1.126885000	3.329310000	-6.834033000
6	17.703122000	-15.692765000	-3.684424000	6	1.042266000	4.605461000	-6.211808000
6	19.094943000	-15.671294000	-3.782673000	6	2.119153000	5.142713000	-5.506973000
6	15.494995000	-16.531591000	-4.607655000	6	-0.098529000	2.602245000	-7.222972000
6	14.639074000	-16.762897000	-5.717466000	6	-0.100351000	1.182302000	-7.267471000
6	13.481206000	-17.529737000	-5.589070000	6	-1.293414000	0.459929000	-7.236536000

6	13.103536000	-18.098941000	-4.341806000	6	-2.543844000	1.123111000	-7.141242000
6	13.855121000	-17.701290000	-3.203429000	6	-2.550594000	2.534867000	-7.288747000
6	15.022378000	-16.948412000	-3.333373000	6	-1.356552000	3.256173000	-7.337271000
6	12.148370000	-19.226092000	-4.286550000	6	-3.711308000	0.383977000	-6.622315000
6	11.368007000	-19.606114000	-5.414586000	6	-3.883996000	-1.010720000	-6.830348000
6	10.804897000	-20.879758000	-5.509126000	6	-4.755215000	-1.753685000	-6.031308000
6	10.978829000	-21.834172000	-4.471600000	6	-5.486680000	-1.141829000	-4.977158000
6	11.582166000	-21.386254000	-3.267768000	6	-5.427966000	0.273673000	-4.877335000
6	12.154984000	-20.117291000	-3.179894000	6	-4.564684000	1.018659000	-5.682526000
6	10.803294000	-23.282930000	-4.692959000	6	-6.086374000	-1.928619000	-3.879828000
6	11.101391000	-23.828854000	-5.968679000	6	-5.551292000	-3.200052000	-3.546115000
6	11.357829000	-25.192450000	-6.123535000	6	-5.806876000	-3.787577000	-2.305962000
6	11.320208000	-26.073827000	-5.011832000	6	-6.612858000	-3.135866000	-1.335811000
6	10.844643000	-25.555196000	-3.777165000	6	-7.293371000	-1.957022000	-1.743703000
6	10.595797000	-24.190658000	-3.619622000	6	-7.036697000	-1.368441000	-2.983355000
6	11.981260000	-27.391555000	-5.101767000	6	-6.526927000	-3.540147000	0.083130000
6	12.147360000	-28.072930000	-6.336872000	6	-6.070110000	-4.828693000	0.471489000
6	13.079022000	-29.105305000	-6.469925000	6	-5.620302000	-5.073296000	1.770316000
6	13.891516000	-29.503746000	-5.375128000	6	-5.608121000	-4.042436000	2.747628000
6	13.606614000	-28.932219000	-4.107456000	6	-6.224280000	-2.811007000	2.406112000
6	12.674544000	-27.902062000	-3.973539000	6	-6.672063000	-2.566162000	1.105998000
6	15.139214000	-30.273959000	-5.559585000	6	-4.794613000	-4.139366000	3.977057000
6	15.854141000	-30.176167000	-6.781317000	6	-3.595789000	-4.898242000	3.962457000
6	17.200485000	-30.539484000	-6.858382000	6	-2.623085000	-4.727906000	4.949583000
6	17.895724000	-31.019274000	-5.717802000	6	-2.801684000	-3.791588000	6.000754000
6	17.130849000	-31.289235000	-4.551425000	6	-4.067392000	-3.153799000	6.101126000
6	15.785143000	-30.926614000	-4.474753000	6	-5.039449000	-3.322259000	5.112349000
6	19.371996000	-30.984774000	-5.693381000	6	-1.627980000	-3.339449000	6.776763000
6	20.150799000	-31.054099000	-6.879616000	6	-0.465414000	-4.143410000	6.917378000
6	21.484920000	-30.642724000	-6.888991000	6	0.764365000	-3.576971000	7.259344000
6	22.105401000	-30.138200000	-5.713732000	6	0.890343000	-2.178457000	7.477245000
6	21.375890000	-30.229518000	-4.499599000	6	-0.305623000	-1.415505000	7.522246000
6	20.042724000	-30.642949000	-4.489846000	6	-1.535526000	-1.982336000	7.181507000
6	23.341872000	-29.331843000	-5.764853000	6	2.191322000	-1.482650000	7.387533000
6	23.648286000	-28.590822000	-6.935789000	6	3.214549000	-2.018725000	6.562482000
6	24.559054000	-27.534112000	-6.902003000	6	4.253942000	-1.214347000	6.089361000
6	25.207098000	-27.163713000	-5.695153000	6	4.317239000	0.163654000	6.420196000
6	25.032227000	-28.015895000	-4.571086000	6	3.408299000	0.644488000	7.400611000
6	24.123189000	-29.074815000	-4.605957000	6	2.370382000	-0.160302000	7.874161000
1	26.437965000	-25.631058000	-7.664002000	1	6.727429000	-0.311806000	5.103647000
1	26.743895000	-23.182145000	-7.580631000	1	7.639236000	1.037302000	3.245379000
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