Electronic Supplementary Material (ESI) for Nanoscale.

Mixed dysprosium-lanthanide nitride clusterfullerenes $DyM_2N@C_{80}$-I_h and $Dy_2MN@C_{80}$-I_h (M = Gd, Er, Tm, and Lu): synthesis, molecular structure, and quantum motion of the endohedral nitrogen atom

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Supporting Information

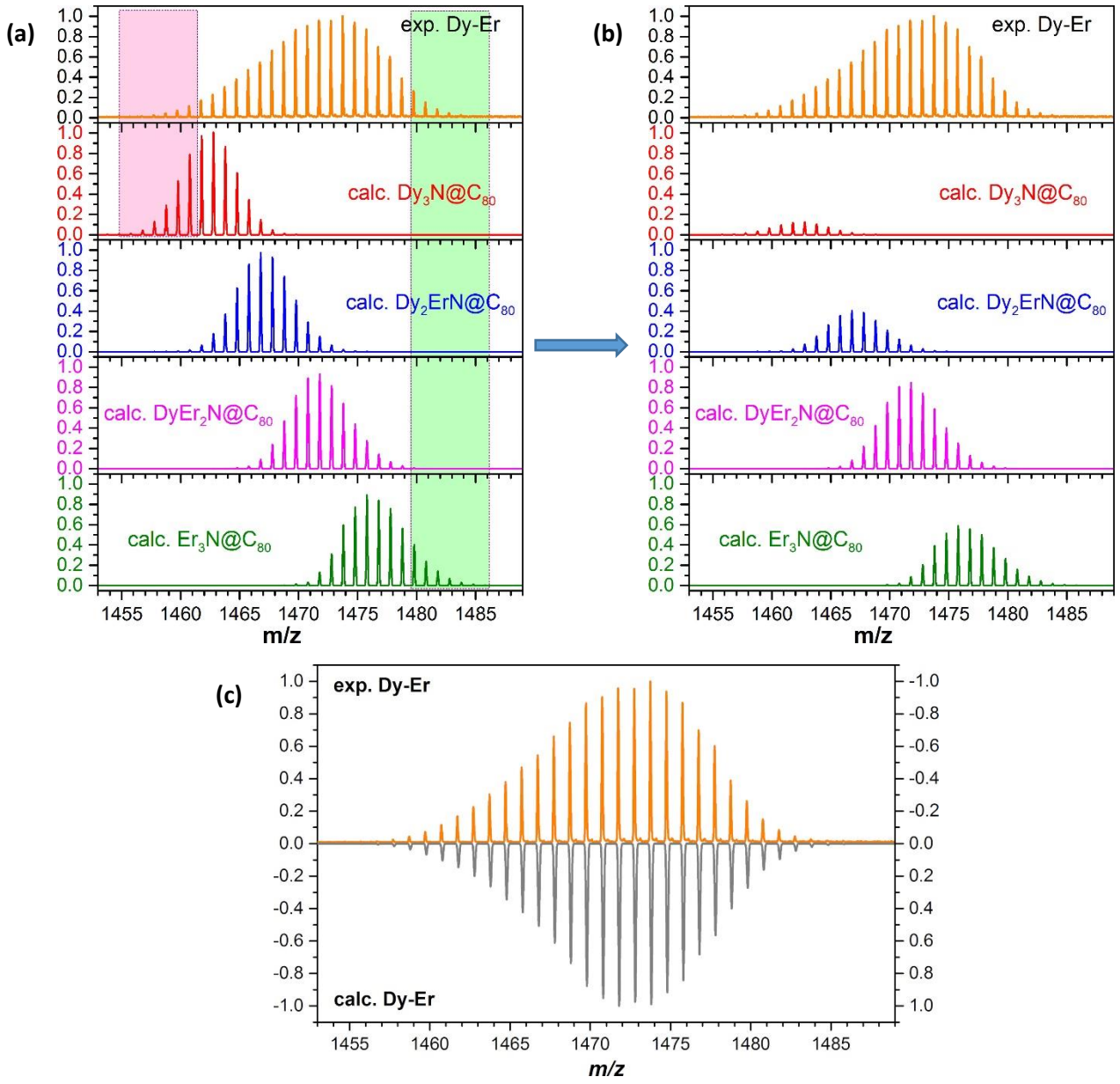

Figure S1. Determination of the sample composition based on mass-spectra. (a) Experimental mass-spectrum of the $Dy_xEr_{3-x}N@C_{80}$ mixture compared to the calculated mass-spectra of all individual molecules. The calculated spectra are normalized to have the same *integral* intensity. Pink and light green rectangles mark the fragments of the mass-spectra of $Dy_3N@C_{80}$ and $Er_3N@C_{80}$, which do not overlap with the spectra of other species. These regions allow determination of the content of these two NCFs in the mixture. After that, content of $DyEr_2N@C_{80}$ and $Dy_2ErN@C_{80}$ can be estimated straightforwardly. (b) The same as (a), but with the intensities of individual components scaled according to their content in the sample. (c) Sum of the calculated mass-spectra of individual components scaled with their content and compared to the experimental mass-spectrum. Good agreement between experimental and calculated spectra ensures that the procedure provides reasonable determination of the sample composition. Compositions of other mixtures were determined in a similar way. The data are listed in Table S1.

Table S1. Relative composition of $Dy_xM_{3-x}N@C_{80}$ mixtures determined based on the positive-ion LDI mass-spectra using the procedure outlines in Fig. S1 (relative concentration of $Dy_3N@C_{80}$ in each mixture is assumed to be equal 1). The graphical representation of these data is shown in Fig. 4.

	M = Sc	M = Lu	M = Tm	M = Er	M = Gd	Binominal distribution
$Dy_3N@C_{80}$	1	1	1	1	1	1
$Dy_2MN@C_{80}$	18	7.3	0.44	3.4	0.92	3
$DyM_2N@C_{80}$	42	19.7	0.30	7.4	0.42	3
$M_3N@C_{80}$	28	18.9	0.18	5.4	0.11	1

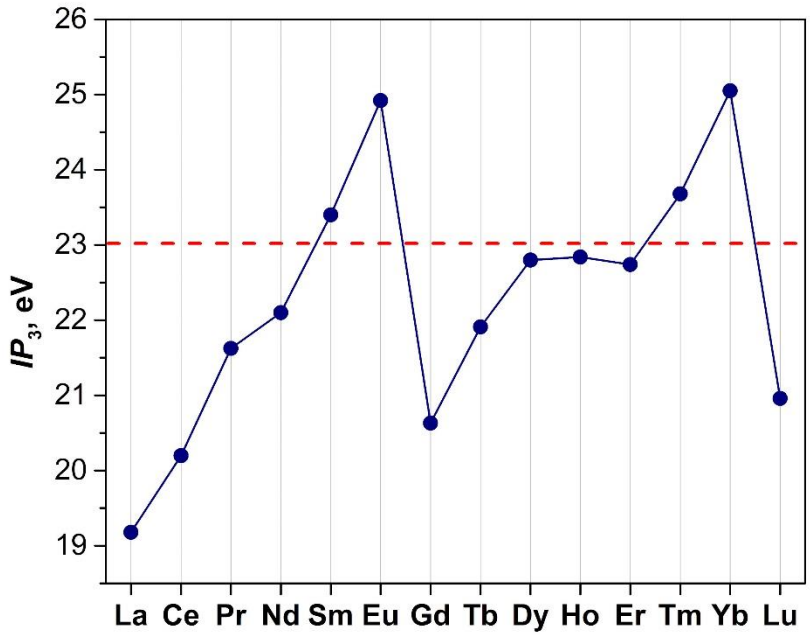

Figure S2. Third ionization potentials (IP_3) of lanthanides. Dashed red line marks the border at 23 eV between divalent and trivalent lanthanide in EMFs.

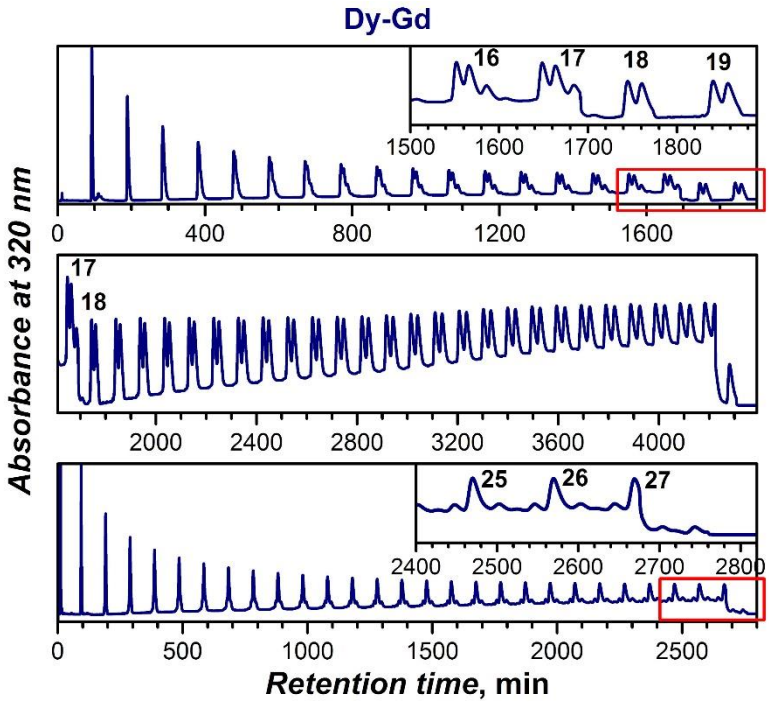

Figure S3. Recycling HPLC chromatograms of $Dy_xGd_{3-x}N@C_{80}$ mixture (x = 0–3) (semipreparative BuckyPrep column, toluene as eluent, 25 °C, flow rate1.0 mL/min). Insets show enlarged fragment of the chromatograms highlighted with red rectangles. $Gd_3N@C_{80}$ and $DyGd_2N@C_{80}$ are collected at the 17th cycle (top panel). The mixture of $Dy_2GdN@C_{80}$ and $Dy_3N@C_{80}$ was processed for additional 26 cycles, which allowed the separation of pure components (middle panel). The mixture of $Gd_3N@C_{80}$ and $DyGd_2N@C_{80}$ was processed with recycling HPLC as well, giving pure $DyGd_2N@C_{80}$ after 27 cycles (bottom).

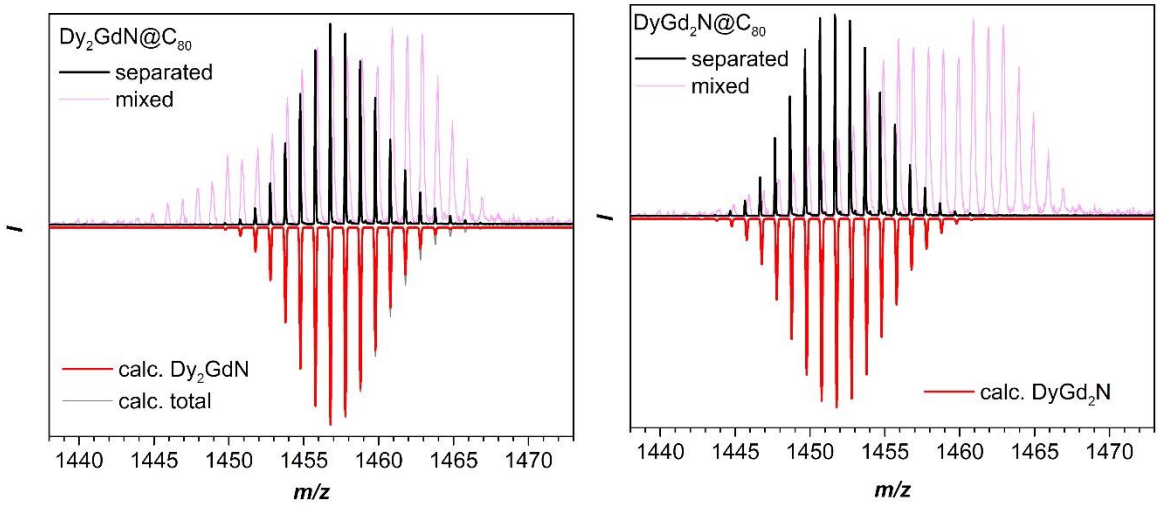

Figure S4. Experimental (black) and calculated (red) LDI mass-spectra of purified $Dy_2GdN@C_{80}$ (left) and $DyGd_2N@C_{80}$ (right). Also shown are mass-spectra of the whole $Dy_xGd_{3-x}N@C_{80}$ fraction (x = 0–3, light magenta lines) before separation by recycling HPLC. Gray line in the left panel show calculated spectrum of $Dy_2GdN@C_{80}$ with 5% admixture of $Dy_3N@C_{80}$.

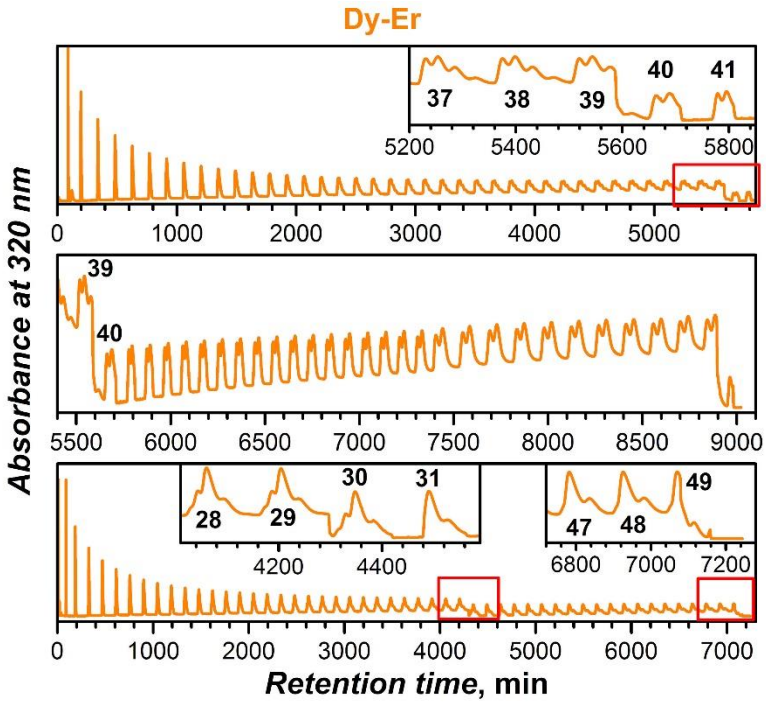

Figure S5. Recycling HPLC chromatograms of $Dy_xEr_{3-x}N@C_{80}$ mixture (x = 0–3) (semipreparative BuckyPrep column, toluene as eluent, 25 °C, flow rate1.0 mL/min). Insets show enlarged fragment of the chromatograms highlighted with red rectangles. $Dy_3N@C_{80}$ and $Dy_2ErN@C_{80}$ are collected at the 39th cycle (top). The mixture of $DyEr_2N@C_{80}$ and $Er_3N@C_{80}$ was processed for after additional 29 cycles, allowing isolation of pure compounds (middle). The mixture of $Dy_3N@C_{80}$ and $Dy_2ErN@C_{80}$ was processed with recycling HPLC as well, allowing isolation of $Dy_2ErN@C_{80}$ after 49 cycles (bottom).

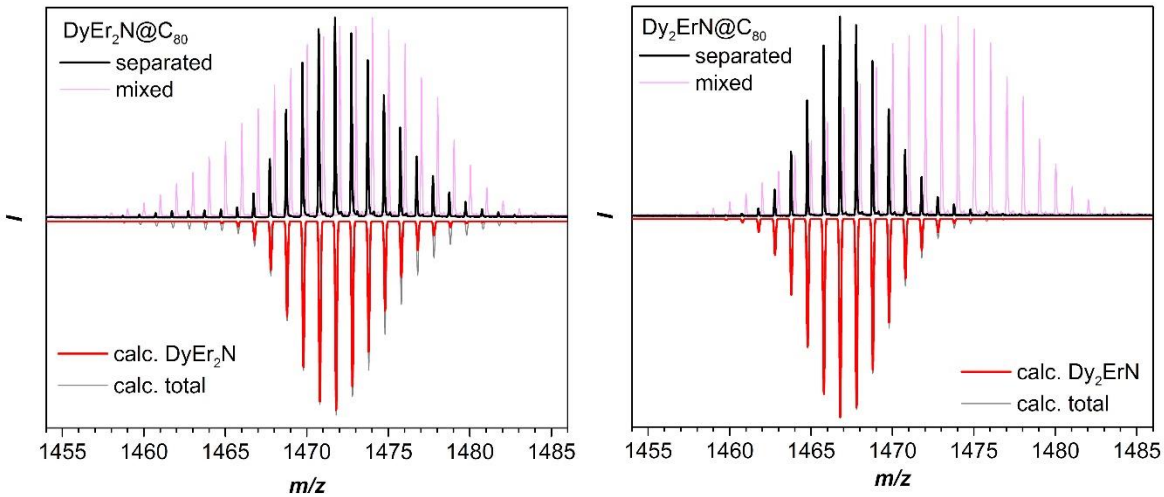

Figure S6. Experimental (black) and calculated (red) LDI mass-spectra of purified $DyEr_2N@C_{80}$ (left) and $Dy_2ErN@C_{80}$ (right). Also shown are mass-spectra of the whole $Dy_xEr_{3-x}N@C_{80}$ fraction (x = 0–3, light magenta lines) before separation by recycling HPLC. Gray lines show calculated spectra of $DyEr_2N@C_{80}$ with 10% admixture of $Er_3N@C_{80}$ (left) and $Dy_2ErN@C_{80}$ with 4% admixture of $DyEr_2N@C_{80}$ (right).

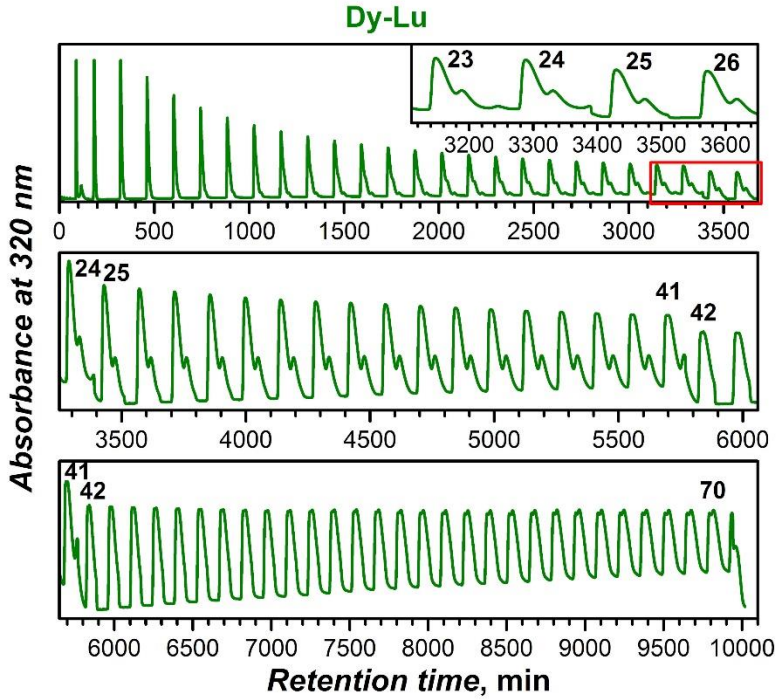

Figure S7. Recycling HPLC chromatograms of $Dy_xLu_{3-x}N@C_{80}$ mixture (x = 0–3) (semipreparative BuckyPrep column, toluene as eluent, 25 °C, flow rate1.0 mL/min). Insets show enlarged fragment of the chromatograms highlighted with red rectangles. $Dy_3N@C_{80}$ was collected at the 24th cycle (top). $Dy_2LuN@C_{80}$ was collected at the 42nd cycle (middle). The mixture of remaining $DyLu_2N@C_{80}$ and $Lu_3N@C_{80}$ still shows no sufficient resolution of peaks after 70 cycles.

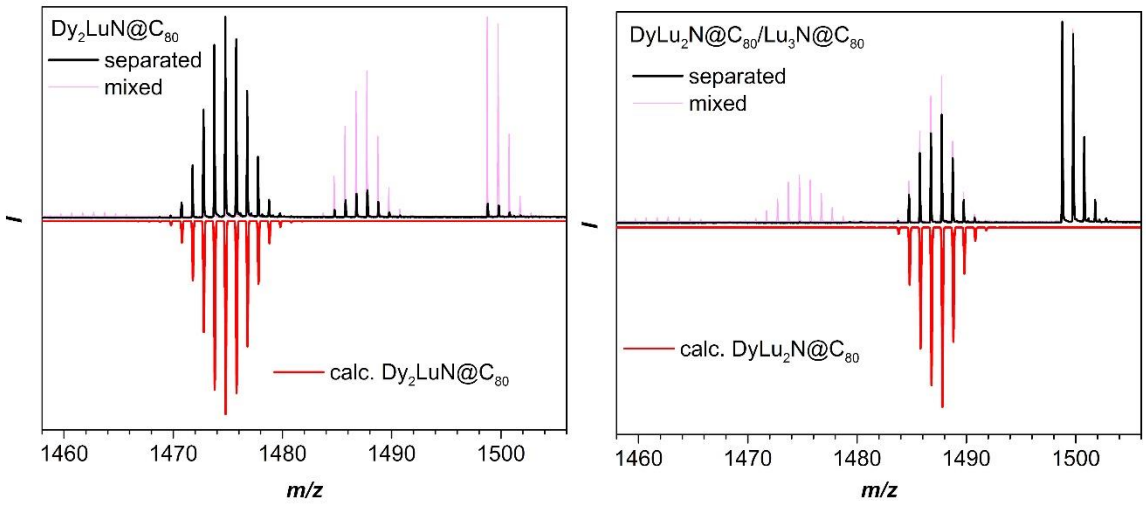

Figure S8. Experimental (black) and calculated (red) LDI mass-spectra of isolated $Dy_2LuN@C_{80}$ (left) and $DyLu_2N@C_{80}/Lu_3N@C_{80}$ mixture (right). Light magenta lines shows mass-spectrum of the whole $Dy_xLu_{3-x}N@C_{80}$ fraction (x = 0–3) before separation by recycling HPLC. The sample of $Dy_2LuN@C_{80}$ still contains ca 10% $DyLu_2N@C_{80}$ and 3% $Lu_3N@C_{80}$. The molar ratio of $DyLu_2N@C_{80}$ and $Lu_3N@C_{80}$ is estimated to be 1:1.35.

Single-crystal X-ray diffraction

Single crystals of $DyEr_2N@C_{80}$ and $DyGd_2N@C_{80}$ were grown by co-crystallization with Ni^{II}(OEP) (OEP = octaethylporphyrin), by layering benzene solution of Ni^{II}(OEP) over a benzene solution of $DyEr_2N@C_{80}$ or $DyGd_2N@C_{80}$. Black blocks of crystals formed after the fullerene and Ni^{II}(OEP) solutions diffused together over a period of ca. one month. X-ray diffraction data collection for the crystal was carried out at 100 K at the BESSY storage ring (BL14.3, Berlin-Adlershof, Germany)[1] using a MAR225 CCD detector, λ = 0.89429 Å. Processing diffraction data was done with XDSAPP2.0 suite.[2] The structure was solved by direct methods and refined using all data (based on F^2) by SHELX 2018.[3] Hydrogen atoms were located in a difference map, added geometrically, and refined with a riding model. The crystal data and collection parameters are presented in Table S2. The data can be obtained free of charge from the Cambridge Crystallographic Data Centre with CCDC Nos. 1874408 and 1874409.

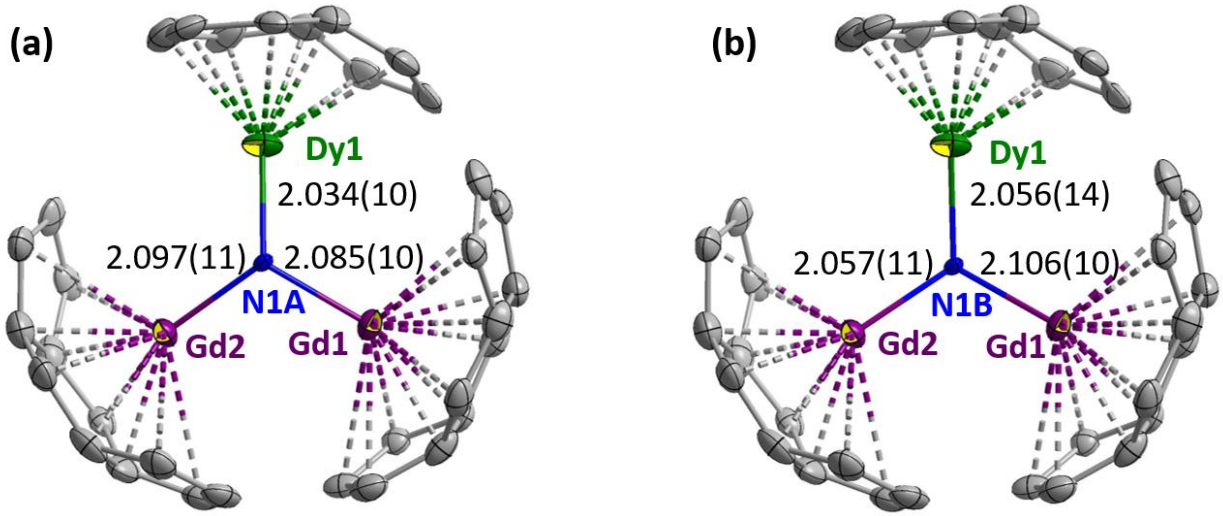

Figure S9. (a) The main $DyGd_2N$ site coordinated cage carbons and metal-nitrogen bond lengths (in Å). Bond angles: $\angle Dy1N1AGd1 = 116.8(5)°$, $\angle Dy1N1AGd2 = 118.0(5)°$, $\angle Gd1N1AGd2 = 111.1(5)°$, (b) The minor $DyGd_2N$ site coordinated cage carbons and metal-nitrogen bond lengths (in Å). Bond angles: $\angle Dy1N1BGd1 = 115.0(5)°$, $\angle Dy1N1BGd2 = 118.9(5)°$, $\angle Gd1N1BGd2 = 111.9(5)°$.The displacement parameters are shown at the 30% probability level.

Table S2. Crystal data

	$DyGd_2N@I_h(7)\text{-}C_{80}\cdot Ni^{II}(OEP)\cdot 2(C_6H_6)$	$DyEr_2N@I_h(7)\text{-}C_{80}\cdot Ni^{II}(OEP)\cdot 2(C_6H_6)$
Formula	C128 H56 Dy Gd2 N5 Ni	C128 H56 Dy Er2 N5 Ni
Formula weight	2199.48	2219.50
Color, habit	Black, block	Black, block
Crystal system	monoclinic	monoclinic
Space group	*C2/c*	*C2/c*
***a*, Å**	25.230(5)	25.170(5)
***b*, Å**	15.050(3)	15.030(3)
***c*, Å**	39.410(8)	39.410(8)
***α*, deg**	90	90
***β*, deg**	95.27(3)	95.16(3)
***γ*, deg**	90	90
Volume, Å^3	14901(5)	14849(5)
Z	8	8
***T*, K**	100	100
Radiation (λ, Å)	Synchrotron Radiation (0.89429)	Synchrotron Radiation (0.89429)
Unique data (R_{int})	16935 (0.0574)	13710 (0.1252)
Parameters	1253	1262
Restraints	6	1224
Observed data	10331	9685
R_1^a (observed data)	0.0659	0.1104
wR_2^b (all data)	0.2057	0.2825
CCDC NO.	1874409	1874408

[a]For data with $I > 2\sigma(I)$, $R_1 = \frac{\sum||F_o|-|F_c||}{\sum|F_o|}$. [b]For all data, $wR_2 = \sqrt{\frac{\sum\left[w\left(F_o^2-F_c^2\right)^2\right]}{\sum\left[w\left(F_o^2\right)^2\right]}}$.

DFT-optimized coordinates

$DyEr_2N@C_{80}$

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N	0.000000000	0.000000000	0.000000000
Dy	-0.897930000	1.863980000	0.058501000
Er	2.042670000	-0.149801000	0.060398000
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$Dy_2ErN@C_{80}$

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C	3.862889000	0.971981000	-1.294559000
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C	1.314501000	-0.537026000	3.928087000
C	1.464672000	-1.874524000	3.431403000
C	0.318713000	-2.673877000	3.123486000
C	0.019866000	0.027746000	4.146497000
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C	-2.960536000	-1.271985000	2.600706000
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C	-0.969175000	-2.145250000	3.416575000
C	-1.116219000	-0.811076000	3.928316000
N	0.000000000	0.000000000	0.000000000
Dy	-0.888873000	1.861380000	0.082952000
Dy	2.057333000	-0.135712000	0.090228000
Er	-1.153281000	-1.685241000	0.086124000

$Dy_3N@C_{80}$

C	0.983880000	2.168670000	-3.118700000
C	2.123617000	2.448664000	-2.289188000
C	2.996536000	1.289857000	-2.290345000
C	1.134884000	0.836364000	-3.636329000
C	2.366685000	0.296452000	-3.130744000
C	-0.000773000	-0.000032000	-3.851009000
C	-1.292777000	0.565526000	-3.635933000
C	-0.308053000	2.704501000	-2.823449000
C	-1.440933000	1.902217000	-3.130156000
C	-0.436781000	3.623047000	-1.712130000
C	1.995117000	3.264524000	-1.139807000
C	0.704106000	3.862263000	-0.873120000
C	2.835333000	2.951513000	-0.030699000
C	3.849929000	0.946829000	-1.180253000
C	3.752790000	1.822677000	-0.034229000
C	4.129228000	-0.471984000	-0.930269000
C	2.495021000	-1.085741000	-2.823672000
C	3.355639000	-1.433137000	-1.712959000
C	0.155497000	-1.401679000	-3.635443000
C	1.384967000	-1.936887000	-3.118140000
C	-0.927681000	-2.198359000	-3.129124000
C	-2.370772000	-0.231493000	-3.117453000
C	-2.188783000	-1.618329000	-2.822217000
C	-2.615734000	1.950927000	-2.289031000
C	-3.182453000	0.615420000	-2.287363000
C	-1.655616000	3.812380000	-0.928896000
C	-2.745014000	2.861440000	-1.178747000
C	0.229722000	4.147821000	0.456710000
C	-1.240748000	4.168325000	0.459502000
C	2.352712000	3.151776000	1.302446000
C	1.048198000	3.700708000	1.566001000
C	3.829250000	1.307944000	1.332042000
C	2.930335000	2.128526000	2.132886000
C	4.230627000	-1.008915000	0.458196000
C	4.029005000	-0.107403000	1.610920000
C	2.993034000	-2.540812000	-0.873563000
C	3.477858000	-2.272160000	0.455934000
C	1.058125000	-3.063543000	-2.288078000
C	-0.381763000	-3.240325000	-2.288885000
C	1.829610000	-3.359987000	-1.139002000
C	-1.104901000	-3.807933000	-1.178431000
C	-2.919164000	-2.189410000	-1.710586000
C	-2.473124000	-3.339745000	-0.927765000

C	-3.824347000	0.095924000	-1.137868000
C	-3.696441000	-1.321123000	-0.871274000
C	-3.454071000	2.338899000	-0.032432000
C	-3.973150000	0.979915000	-0.028666000
C	-1.919997000	3.542593000	1.612600000
C	-3.045826000	2.661994000	1.333808000
C	0.365019000	3.232784000	2.716615000
C	-1.083214000	3.097719000	2.705719000
C	2.192750000	1.609756000	3.239240000
C	0.926942000	2.202891000	3.547014000
C	3.225369000	-0.609177000	2.704320000
C	2.378934000	0.229941000	3.532205000
C	2.681950000	-2.757036000	1.565644000
C	2.618212000	-1.930662000	2.715780000
C	1.139065000	-3.931181000	-0.029498000
C	-0.297450000	-4.161749000	-0.032770000
C	1.554092000	-3.612467000	1.303097000
C	-0.781276000	-3.969766000	1.333656000
C	0.379188000	-3.600853000	2.133855000
C	-2.988699000	-3.158962000	0.460588000
C	-3.705961000	-1.875113000	0.458302000
C	-2.106809000	-3.435240000	1.613286000
C	-3.904313000	0.461307000	1.304186000
C	-3.306490000	1.473012000	2.134450000
C	-3.727441000	-0.942795000	1.567615000
C	-1.386172000	1.944765000	3.533142000
C	-0.156600000	1.404116000	4.043452000
C	-2.487822000	1.093346000	3.240107000
C	1.296003000	-0.564296000	4.042954000
C	1.445676000	-1.901931000	3.546544000
C	0.299178000	-2.702046000	3.239632000
C	0.001646000	0.000565000	4.261183000
C	-2.139036000	-2.487721000	2.706449000
C	-2.979830000	-1.300900000	2.717649000
C	-2.368128000	-0.299502000	3.547658000
C	-0.988713000	-2.173643000	3.533351000
C	-1.134702000	-0.838428000	4.043633000
N	0.000000000	0.000000000	0.000000000
Dy	-0.907100000	1.841178000	0.202814000
Dy	2.048221000	-0.134534000	0.202385000
Dy	-1.140292000	-1.706456000	0.204740000

$Dy_2GdN@C_{80}$

C	0.965393000	2.137505000	-3.010293000
C	2.105439000	2.418209000	-2.181719000
C	2.979807000	1.259651000	-2.182825000
C	1.116508000	0.805394000	-3.527680000
C	2.348749000	0.266052000	-3.023585000
C	-0.019782000	-0.030904000	-3.741405000
C	-1.311537000	0.535119000	-3.527364000
C	-0.326786000	2.673371000	-2.715299000
C	-1.460135000	1.872264000	-3.022986000
C	-0.454537000	3.591031000	-1.603457000
C	1.977655000	3.234386000	-1.032653000
C	0.686367000	3.832041000	-0.765254000
C	2.819231000	2.920878000	0.075988000
C	3.838570000	0.919008000	-1.075059000
C	3.742973000	1.795797000	0.072864000
C	4.112209000	-0.501712000	-0.823479000
C	2.475537000	-1.116132000	-2.716100000
C	3.335364000	-1.462347000	-1.605088000
C	0.135512000	-1.432819000	-3.526182000
C	1.365112000	-1.967837000	-3.010104000
C	-0.947675000	-2.230032000	-3.019972000
C	-2.389476000	-0.262028000	-3.009033000
C	-2.208367000	-1.649159000	-2.713343000
C	-2.634724000	1.920638000	-2.181645000
C	-3.200996000	0.585103000	-2.179215000
C	-1.673119000	3.780222000	-0.819583000
C	-2.762482000	2.829480000	-1.069899000
C	0.211561000	4.119795000	0.564346000
C	-1.259924000	4.140730000	0.568177000
C	2.334210000	3.119799000	1.408268000
C	1.029614000	3.670216000	1.672560000
C	3.818333000	1.280655000	1.440964000
C	2.913428000	2.097610000	2.239163000
C	4.209211000	-1.037503000	0.566070000
C	4.012602000	-0.136591000	1.719823000
C	2.969813000	-2.568310000	-0.764932000
C	3.453036000	-2.297848000	0.563726000
C	1.037772000	-3.094738000	-2.180340000
C	-0.402519000	-3.273514000	-2.180096000
C	1.807568000	-3.388767000	-1.030494000
C	-1.126279000	-3.846488000	-1.071111000
C	-2.938259000	-2.219854000	-1.601748000
C	-2.490917000	-3.369767000	-0.817823000

C	-3.842250000	0.065087000	-1.029475000
C	-3.715526000	-1.351753000	-0.763137000
C	-3.472639000	2.308842000	0.076371000
C	-3.990420000	0.949596000	0.079749000
C	-1.941520000	3.517479000	1.722630000
C	-3.066419000	2.634770000	1.443071000
C	0.346213000	3.203203000	2.823299000
C	-1.102964000	3.069906000	2.813888000
C	2.174486000	1.579649000	3.345725000
C	0.908574000	2.172909000	3.653078000
C	3.206960000	-0.638552000	2.811638000
C	2.360046000	0.200050000	3.639109000
C	2.659016000	-2.783845000	1.672822000
C	2.598873000	-1.960120000	2.823922000
C	1.115110000	-3.960724000	0.078711000
C	-0.320097000	-4.204465000	0.076365000
C	1.529843000	-3.638379000	1.409902000
C	-0.804585000	-4.013631000	1.445553000
C	0.356009000	-3.632889000	2.241877000
C	-3.005065000	-3.188025000	0.570279000
C	-3.721763000	-1.904415000	0.566757000
C	-2.129387000	-3.472914000	1.725264000
C	-3.921344000	0.431180000	1.412367000
C	-3.325229000	1.444068000	2.242657000
C	-3.745353000	-0.973343000	1.676007000
C	-1.404731000	1.915206000	3.640016000
C	-0.175071000	1.374287000	4.149665000
C	-2.506562000	1.063163000	3.347820000
C	1.276707000	-0.594248000	4.150092000
C	1.426047000	-1.932114000	3.654120000
C	0.278745000	-2.732514000	3.347837000
C	-0.017435000	-0.029366000	4.367484000
C	-2.160334000	-2.521811000	2.816643000
C	-2.999554000	-1.333127000	2.826425000
C	-2.387466000	-0.330172000	3.655342000
C	-1.009058000	-2.204839000	3.642302000
C	-1.154170000	-0.868741000	4.151523000
N	0.000000000	0.000000000	0.000000000
Dy	-0.922960000	1.816760000	0.318866000
Dy	2.037617000	-0.132154000	0.298614000
Gd	-1.117102000	-1.736420000	0.316992000

$DyGd_2N@C_{80}$

C	1.003130000	2.135453000	-2.924621000
C	2.143720000	2.415689000	-2.096520000
C	3.020050000	1.257709000	-2.096891000
C	1.154312000	0.803233000	-3.440837000
C	2.387076000	0.263893000	-2.936869000
C	0.017201000	-0.032220000	-3.654258000
C	-1.274727000	0.534457000	-3.440819000
C	-0.289689000	2.671334000	-2.629829000
C	-1.423766000	1.871749000	-2.937604000
C	-0.417889000	3.587402000	-1.517386000
C	2.014879000	3.229143000	-0.946588000
C	0.723086000	3.824741000	-0.678700000
C	2.858499000	2.914462000	0.161532000
C	3.884154000	0.919052000	-0.990828000
C	3.792927000	1.797053000	0.158940000
C	4.148167000	-0.502887000	-0.736496000
C	2.512951000	-1.118330000	-2.629900000
C	3.372514000	-1.464579000	-1.519122000
C	0.172004000	-1.434158000	-3.439913000
C	1.401729000	-1.969365000	-2.924152000
C	-0.911449000	-2.231705000	-2.934659000
C	-2.352604000	-0.262569000	-2.922624000
C	-2.171376000	-1.649903000	-2.627281000
C	-2.599029000	1.921065000	-2.095664000
C	-3.164588000	0.584534000	-2.093395000
C	-1.637383000	3.779624000	-0.734312000
C	-2.731171000	2.833075000	-0.985943000
C	0.247901000	4.109807000	0.650259000
C	-1.222627000	4.135425000	0.654470000
C	2.370544000	3.110875000	1.492579000
C	1.066297000	3.662837000	1.757715000
C	3.868832000	1.281258000	1.529687000
C	2.954410000	2.092511000	2.324517000
C	4.242785000	-1.037843000	0.652700000
C	4.056433000	-0.138320000	1.808359000
C	3.006984000	-2.570438000	-0.679575000
C	3.487160000	-2.297796000	0.649461000
C	1.074104000	-3.096104000	-2.094599000
C	-0.366177000	-3.275117000	-2.094552000
C	1.844063000	-3.389463000	-0.944571000
C	-1.089622000	-3.847711000	-0.985017000
C	-2.900842000	-2.219622000	-1.515249000
C	-2.453612000	-3.369674000	-0.731097000

C	-3.805889000	0.065045000	-0.943812000
C	-3.678483000	-1.351802000	-0.676948000
C	-3.443333000	2.313763000	0.162297000
C	-3.954292000	0.950815000	0.165226000
C	-1.906206000	3.517320000	1.810201000
C	-3.035990000	2.638948000	1.531068000
C	0.383641000	3.200149000	2.909594000
C	-1.066122000	3.067844000	2.899647000
C	2.213105000	1.576036000	3.431610000
C	0.946663000	2.169985000	3.738750000
C	3.248045000	-0.640931000	2.899167000
C	2.398883000	0.197007000	3.726027000
C	2.695385000	-2.784776000	1.758589000
C	2.637669000	-1.961987000	2.910123000
C	1.150628000	-3.961154000	0.164557000
C	-0.284111000	-4.207514000	0.162704000
C	1.565349000	-3.638588000	1.495552000
C	-0.769220000	-4.018942000	1.532710000
C	0.391661000	-3.635382000	2.327884000
C	-2.968717000	-3.189617000	0.656819000
C	-3.684912000	-1.905172000	0.652696000
C	-2.094452000	-3.477824000	1.812746000
C	-3.882794000	0.431031000	1.497077000
C	-3.288384000	1.444659000	2.327828000
C	-3.707582000	-0.974007000	1.761215000
C	-1.367201000	1.913140000	3.725640000
C	-0.137384000	1.371825000	4.235417000
C	-2.469370000	1.061979000	3.433056000
C	1.314487000	-0.596923000	4.236406000
C	1.463688000	-1.934390000	3.739797000
C	0.315644000	-2.734404000	3.433570000
C	0.019979000	-0.031765000	4.452728000
C	-2.124281000	-2.524690000	2.902763000
C	-2.962680000	-1.334711000	2.911741000
C	-2.350404000	-0.331510000	3.740244000
C	-0.972465000	-2.206651000	3.727661000
C	-1.117274000	-0.870426000	4.236593000
N	0.000000000	0.000000000	0.000000000
Dy	-0.919420000	1.804736000	0.395497000
Gd	2.051683000	-0.098225000	0.386535000
Gd	-1.079916000	-1.741603000	0.406488000

$Gd_3N@C_{80}$

C	0.985662000	2.166013000	-2.849424000
C	2.126318000	2.445812000	-2.021405000
C	3.003003000	1.288078000	-2.021595000
C	1.136496000	0.833463000	-3.365009000
C	2.369719000	0.294122000	-2.861875000
C	-0.001217000	-0.001314000	-3.577585000
C	-1.292794000	0.566718000	-3.364075000
C	-0.306906000	2.702966000	-2.554045000
C	-1.441752000	1.904335000	-2.860893000
C	-0.435132000	3.618346000	-1.441952000
C	1.996700000	3.258429000	-0.871067000
C	0.705753000	3.854331000	-0.603614000
C	2.840855000	2.943090000	0.237206000
C	3.867702000	0.950442000	-0.915290000
C	3.779496000	1.829184000	0.235173000
C	4.127845000	-0.471754000	-0.659700000
C	2.493928000	-1.087779000	-2.553916000
C	3.351932000	-1.433548000	-1.442459000
C	0.152744000	-1.403748000	-3.363513000
C	1.382368000	-1.938973000	-2.848009000
C	-0.930755000	-2.201524000	-2.859047000
C	-2.371004000	-0.230013000	-2.847010000
C	-2.189536000	-1.617881000	-2.551382000
C	-2.618245000	1.955936000	-2.019293000
C	-3.182549000	0.617953000	-2.018153000
C	-1.655168000	3.809596000	-0.658080000
C	-2.756864000	2.873281000	-0.912650000
C	0.230224000	4.133588000	0.725652000
C	-1.238932000	4.159692000	0.730628000
C	2.352699000	3.139492000	1.568065000
C	1.048558000	3.692124000	1.833461000
C	3.857526000	1.314016000	1.607567000
C	2.939148000	2.123252000	2.400697000
C	4.222779000	-1.006081000	0.729512000
C	4.042060000	-0.106551000	1.886393000
C	2.986320000	-2.539034000	-0.602961000
C	3.466048000	-2.265350000	0.725781000
C	1.054819000	-3.065662000	-2.018636000
C	-0.386102000	-3.246096000	-2.018134000
C	1.824177000	-3.358792000	-0.868519000
C	-1.110076000	-3.825133000	-0.910920000
C	-2.917001000	-2.186779000	-1.438607000
C	-2.471623000	-3.338981000	-0.655173000

C	-3.820589000	0.099280000	-0.867262000
C	-3.691153000	-1.316785000	-0.599838000
C	-3.472806000	2.357829000	0.238360000
C	-3.968528000	0.987959000	0.241069000
C	-1.926669000	3.553697000	1.888618000
C	-3.064739000	2.683118000	1.610618000
C	0.365635000	3.233699000	2.986241000
C	-1.084755000	3.103251000	2.977164000
C	2.195901000	1.607943000	3.507776000
C	0.929540000	2.202966000	3.815012000
C	3.231407000	-0.609091000	2.975843000
C	2.381335000	0.228794000	3.802285000
C	2.675130000	-2.751913000	1.834476000
C	2.619524000	-1.930047000	2.986323000
C	1.129698000	-3.931140000	0.240573000
C	-0.304466000	-4.187220000	0.239154000
C	1.544317000	-3.605187000	1.570718000
C	-0.789130000	-3.996187000	1.611625000
C	0.371283000	-3.604321000	2.403813000
C	-2.981608000	-3.153338000	0.733801000
C	-3.693853000	-1.868244000	0.729265000
C	-2.111760000	-3.445985000	1.890765000
C	-3.893191000	0.466854000	1.571752000
C	-3.305326000	1.482916000	2.403662000
C	-3.719514000	-0.938681000	1.837019000
C	-1.384432000	1.947790000	3.803407000
C	-0.154315000	1.405451000	4.312877000
C	-2.486152000	1.097151000	3.509630000
C	1.296727000	-0.564726000	4.312776000
C	1.445348000	-1.902310000	3.815690000
C	0.296937000	-2.702088000	3.509873000
C	0.002674000	0.001492000	4.529501000
C	-2.141278000	-2.491388000	2.979374000
C	-2.979355000	-1.300789000	2.988866000
C	-2.367567000	-0.297039000	3.816803000
C	-0.990162000	-2.173180000	3.804587000
C	-1.134758000	-0.836651000	4.313722000
N	0.000000000	0.000000000	0.000000000
Gd	-0.970761000	1.790634000	0.469269000
Gd	2.036894000	-0.053563000	0.465964000
Gd	-1.064256000	-1.736530000	0.470065000

$Er_3N@C_{80}$

C	0.983094000	2.170093000	-3.304176000
C	2.121918000	2.449150000	-2.472343000
C	2.991357000	1.289573000	-2.473763000
C	1.133460000	0.837967000	-3.823831000
C	2.363773000	0.297102000	-3.315775000
C	-0.001935000	0.000797000	-4.039183000
C	-1.294497000	0.565629000	-3.822767000
C	-0.308383000	2.703916000	-3.006668000
C	-1.440889000	1.901191000	-3.313649000
C	-0.436109000	3.619618000	-1.892967000
C	1.994995000	3.264190000	-1.321507000
C	0.704363000	3.858803000	-1.053596000
C	2.832411000	2.953414000	-0.210839000
C	3.837018000	0.944070000	-1.360315000
C	3.737422000	1.817624000	-0.215725000
C	4.121361000	-0.471753000	-1.112670000
C	2.493052000	-1.084975000	-3.008878000
C	3.351281000	-1.432121000	-1.896081000
C	0.155366000	-1.400941000	-3.823477000
C	1.384845000	-1.936717000	-3.305258000
C	-0.927642000	-2.195803000	-3.314066000
C	-2.372730000	-0.230915000	-3.303002000
C	-2.188934000	-1.616488000	-3.006254000
C	-2.613609000	1.947821000	-2.470843000
C	-3.183037000	0.615051000	-2.469939000
C	-1.652580000	3.806158000	-1.108910000
C	-2.736847000	2.852345000	-1.356814000
C	0.231562000	4.143837000	0.276912000
C	-1.236947000	4.159850000	0.278375000
C	2.353783000	3.155574000	1.124406000
C	1.049609000	3.700024000	1.388211000
C	3.811024000	1.302826000	1.147609000
C	2.925920000	2.129281000	1.954222000
C	4.221528000	-1.008404000	0.274450000
C	4.012381000	-0.109021000	1.424892000
C	2.989578000	-2.539623000	-1.056334000
C	3.473894000	-2.272374000	0.273569000
C	1.058080000	-3.062312000	-2.472774000
C	-0.380824000	-3.235425000	-2.472696000
C	1.828716000	-3.359910000	-1.322600000
C	-1.101568000	-3.794922000	-1.358480000
C	-2.916946000	-2.185634000	-1.892417000
C	-2.469504000	-3.332651000	-1.109317000

C	-3.824933000	0.096603000	-1.319180000
C	-3.694354000	-1.318736000	-1.052173000
C	-3.442600000	2.328050000	-0.212165000
C	-3.974045000	0.976305000	-0.207707000
C	-1.910320000	3.527842000	1.428711000
C	-3.032592000	2.648043000	1.151106000
C	0.367577000	3.229311000	2.538895000
C	-1.078567000	3.090254000	2.526240000
C	2.192536000	1.609044000	3.061937000
C	0.927869000	2.201698000	3.372289000
C	3.218107000	-0.610455000	2.522895000
C	2.377553000	0.229051000	3.354514000
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C	2.615405000	-1.932133000	2.536070000
C	1.142068000	-3.929889000	-0.211157000
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C	1.557394000	-3.616002000	1.123426000
C	-0.775980000	-3.952066000	1.148610000
C	0.383178000	-3.598265000	1.954026000
C	-2.983711000	-3.151650000	0.277832000
C	-3.704178000	-1.871888000	0.277695000
C	-2.099464000	-3.420926000	1.427547000
C	-3.908680000	0.459587000	1.126980000
C	-3.305295000	1.467612000	1.956993000
C	-3.728235000	-0.942224000	1.389543000
C	-1.384842000	1.941968000	3.356784000
C	-0.155827000	1.402825000	3.869260000
C	-2.487295000	1.091505000	3.063672000
C	1.296525000	-0.565795000	3.867894000
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C	0.300310000	-2.702542000	3.061471000
C	0.002333000	-0.000751000	4.087304000
C	-2.135320000	-2.481812000	2.525463000
C	-2.978484000	-1.298640000	2.539245000
C	-2.367890000	-0.300273000	3.372668000
C	-0.987068000	-2.173110000	3.355540000
C	-1.134065000	-0.839719000	3.868895000
N	0.000000000	0.000000000	0.000000000
Er	-0.882416000	1.856182000	0.019169000
Er	2.048705000	-0.163796000	0.018372000
Er	-1.165971000	-1.692353000	0.022572000

$Lu_3N@C_{80}$

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C	2.119107000	2.449493000	-2.491351000
C	2.984102000	1.289506000	-2.493926000
C	1.132457000	0.838211000	-3.848186000
C	2.361987000	0.297603000	-3.338623000
C	-0.002605000	0.000045000	-4.064069000
C	-1.295844000	0.564042000	-3.847034000
C	-0.309104000	2.699981000	-3.026859000
C	-1.442090000	1.898855000	-3.336614000
C	-0.433189000	3.608706000	-1.907634000
C	1.995738000	3.264328000	-1.338948000
C	0.705862000	3.853589000	-1.068823000
C	2.827929000	2.957907000	-0.224659000
C	3.810330000	0.940441000	-1.370977000
C	3.712319000	1.811608000	-0.229572000
C	4.099595000	-0.469492000	-1.123134000
C	2.489778000	-1.083974000	-3.028533000
C	3.339978000	-1.430198000	-1.909985000
C	0.155984000	-1.401991000	-3.847764000
C	1.385104000	-1.937050000	-3.326265000
C	-0.926409000	-2.195985000	-3.336554000
C	-2.373511000	-0.232445000	-3.324155000
C	-2.186640000	-1.615489000	-3.025742000
C	-2.611490000	1.941292000	-2.490830000
C	-3.183462000	0.612137000	-2.488379000
C	-1.644349000	3.786174000	-1.119685000
C	-2.721363000	2.830921000	-1.367094000
C	0.234547000	4.139647000	0.262666000
C	-1.231307000	4.143985000	0.263205000
C	2.354289000	3.161979000	1.113345000
C	1.050382000	3.700490000	1.376879000
C	3.784653000	1.297292000	1.129717000
C	2.919395000	2.132539000	1.943334000
C	4.205025000	-1.005620000	0.259848000
C	3.989909000	-0.108943000	1.406549000
C	2.984030000	-2.539024000	-1.070498000
C	3.468827000	-2.273125000	0.260340000
C	1.059661000	-3.061268000	-2.490871000
C	-0.377354000	-3.230261000	-2.492136000
C	1.828473000	-3.361259000	-1.338909000
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C	-2.910067000	-2.178173000	-1.906109000
C	-2.457112000	-3.316064000	-1.119324000

C	-3.826404000	0.096865000	-1.335585000
C	-3.691405000	-1.315085000	-1.066332000
C	-3.425267000	2.309119000	-0.225355000
C	-3.976099000	0.970034000	-0.220638000
C	-1.899069000	3.508088000	1.410148000
C	-3.014855000	2.627801000	1.133763000
C	0.369196000	3.226930000	2.528429000
C	-1.074317000	3.082046000	2.513705000
C	2.191179000	1.611182000	3.053373000
C	0.928096000	2.203048000	3.366306000
C	3.208866000	-0.609576000	2.510774000
C	2.374654000	0.230781000	3.345512000
C	2.681737000	-2.759682000	1.375506000
C	2.612570000	-1.931874000	2.526486000
C	1.148253000	-3.928220000	-0.223655000
C	-0.286675000	-4.120416000	-0.227484000
C	1.563039000	-3.619606000	1.113698000
C	-0.767117000	-3.925862000	1.131999000
C	0.389367000	-3.593742000	1.944503000
C	-2.973012000	-3.138952000	0.263841000
C	-3.702432000	-1.867404000	0.264640000
C	-2.087445000	-3.400500000	1.409892000
C	-3.914759000	0.456742000	1.117002000
C	-3.304825000	1.460457000	1.946924000
C	-3.729185000	-0.941615000	1.379246000
C	-1.384442000	1.939072000	3.347946000
C	-0.155740000	1.403112000	3.863956000
C	-2.488247000	1.089972000	3.055830000
C	1.296558000	-0.565074000	3.862741000
C	1.446991000	-1.903354000	3.365354000
C	0.302830000	-2.701841000	3.053863000
C	0.002501000	-0.000185000	4.083705000
C	-2.129832000	-2.473314000	2.513683000
C	-2.976874000	-1.295652000	2.529914000
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C	-0.984353000	-2.170478000	3.346991000
C	-1.133830000	-0.838914000	3.863954000
N	0.000000000	0.000000000	0.000000000
Lu	-0.834876000	1.873844000	0.006041000
Lu	2.040573000	-0.214602000	0.006486000
Lu	-1.206478000	-1.659500000	0.008941000

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