S1. Synthesis and isolation of DySc$_2$N@C$_{68}$ (1), LuSc$_2$N@C$_{68}$ (2) and Lu$_2$ScN@C$_{68}$ (3):

The three new nitride clusterfullerenes (NCFs) 1-3 are produced by a modified Krätschmer-Huffman DC-arc discharging method with the addition of NH$_3$ (20 mbar) as described before. Briefly, a mixture of Dy$_2$O$_3$ (Lu$_2$O$_3$) and Sc$_2$O$_3$ (99.9%, MaTeck GmbH, Germany) and graphite powder was used (molar ratio of Dy:Sc:C(or Lu:Sc:C)=1:1:15). After DC-arc discharging, the soot was pre-extracted by acetone and further Soxhlet-extracted by CS$_2$ for 20 h. The extracted fullerene mixture is distilled and dissolved in toluene. Fullerene isolation was performed by two-step HPLC. In the first step running in a Hewlett-Packard instrument (series 1050), a linear combination of two analytical 4.6 × 250 mm Buckyprep columns (Nacalai Tesque, Japan) was applied with toluene as the eluent. The second-step isolation is performed by recycling HPLC (Sunchrom, Germany) using a semi-preparative Buckyprep column (Nacalai Tesque, Japan) and toluene as the eluent. A UV detector set to 320 nm was used for fullerene detection for both steps.
**Fig. S1.** The first-step HPLC isolations of the Lu$_x$Sc$_{3-x}$N@C$_{80}$ and Dy$_x$Sc$_{3-x}$N@C$_{80}$ fullerene extract mixtures synthesized by the ‘‘reactive gas atmosphere’’ method (combination of two 4.6 x 250 mm Buckyprep columns; flow rate 1.6 ml/min; injection volume 100 µl; toluene as eluent (mobile phase); 40°C). The dominant peaks with the retention of 30-37 min are the major products M$_x$Sc$_{3-x}$N@C$_{80}$ (I, II) (M= Lu, Dy, x=0-3).

The typical chromatograms of a Lu$_x$Sc$_{3-x}$N@C$_{2n}$ and Dy$_x$Sc$_{3-x}$N@C$_{2n}$ fullerene extract mixtures obtained on two Buckyprep columns are shown in Fig. S1. Together with mass-spectroscopic (MS) analysis it shows that Dy$_x$Sc$_{3-x}$N@C$_{2n}$ (a) and Lu$_x$Sc$_{3-x}$N@C$_{2n}$ (b) NCFs (fractions A-D) (retention time 30 - 70 min) are the dominant products. This first step in HPLC results in isolation of fractions A and B, respectively, which are subject to the second-step isolation by recycling HPLC (Buckyprep column) and the corresponding chromatograms are illustrated in Fig. S2.
**Fig. S2.** The chromatograms of the isolated fractions A and B by the second-step recycling HPLC (10 x 250 mm Buckyprep-M column; flow rate 5.0 ml/min; injection volume 5 ml; toluene as eluent; 20°C). A1 and B1: Sc$_3$N@C$_{68}$, A2: LuSc$_2$N@C$_{68}$ (2), A3: Lu$_2$ScN@C$_{68}$ (3), B2: DySc$_2$N@C$_{68}$ (1).

Based on the integrated HPLC peak area, the relative yield of 1 (2) to Sc$_3$N@C$_{68}$ is estimated to be 1:2, while that of 3 to Sc$_3$N@C$_{68}$ is ca. 1:12 (i.e., the relative yield of 3:2:Sc$_3$N@C$_{68}$ = 1:6:12) (see Fig. S2).

Besides, for Lu$_x$Sc$_{3-x}$N@C$_{68}$ (fraction A), there are 3 isolable structures (x=0-2). However, for Dy$_x$Sc$_{3-x}$N@C$_{68}$ (fraction B), only Sc$_3$N@C$_{68}$ and DySc$_2$N@C$_{68}$ (1) formed. This indicates clearly the difference between Lu/Sc and Dy/Sc mixed NCFs.
S2. Comparison of the colors of 1-3 and Sc$_3$N@C$_{68}$ solutions (in toluene):

Owing to the same cage symmetries ($D_3$:6140) of 1-3 and Sc$_3$N@C$_{68}$, the electronic absorption properties of 1-3 are almost identical to that of Sc$_3$N@C$_{68}$ (see Fig. 2), as a result the colors of 1-3 dissolved in toluene are same to that of Sc$_3$N@C$_{68}$ (purple) as clearly shown in Fig. S3.

Fig. S3. Photographs of Sc$_3$N@C$_{68}$ (left) and DySc$_2$N@C$_{68}$ (1) (right) dissolved in toluene. The colors of LuSc$_2$N@C$_{68}$ (2) and Lu$_2$ScN@C$_{68}$ (3) are same to 1.