Electronic Supplementary Material (ESI) for ChemComm.

Planar Rings in Nano-Saturns and Related Complexes

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Computational Methods

All structures were optimized in the gas phase using B3LYP/6-31G(d)[1] with the Becke-Johnson[2] variation of the D3[3] dispersion correction. All structures were confirmed to be local energy minima using analytical frequency analysis, except for the **10** and **11** complexes. The binding energy of **7** was also computed with the M05-2x,[4] M06-2x,[5] ωB97X-D[6] and TPSS-D3[7] functionals using the 6-31G(d) and 6-311+G(d,p) basis sets using the B3LYP-D3/6-31G(d) geometries. The unscaled zero-point vibrational frequencies were used to compute the enthalpy and free energies employing the quasiharmonic approximation[8] whereby frequencies less than 100 cm^{-1} were raised to 100 cm^{-1} for the vibrational partition functions. The corrected enthalpies and free energies were evaluated at 298 K. All computations were done using the *Gaussian-16* suite.[9]

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[1] a) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648-5650; b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789; c) S. H. Vosko, L. Wilk, M. Nusair, *Can. J. Phys.* **1980**, *58*, 1200-1211; d) P. J. Stephens, F. J. Devlin, C. F. Chabalowski, M. J. Frisch, *J. Phys. Chem.* **1994**, *98*, 11623-11627.

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Table S1. Binding energy (kcal mol^{-1}) of **7** with different functionals and basis sets.[a]

Method	Binding energy
B3LYP-D3/6-31G(d)	-30.5
B3LYP-D3/6-311+G(d,p)	-28.9
M06-2x/6-31G(d)	-14.3
M06-2x/6-311+G(d,p)	-16.8
M05-2x/6-31G(d)	-13.5
M05-2x/6-311+G(d,p)	-17.7
ωB97X-D/6-31G(d)	-29.2
ωB97X-D/6-311+G(d,p)	-30.5
TPSS-D3/6-31G(d)	-28.6
TPSS-D3/6-311+G(d,p)	-29.8

[a]All computations employed the B3LYP-D3/6-31G(d) optimized geometries.

Table S2. Computed binding enthalpy (B3LYP-D3/6-31G(d), kcal mol^{-1}) of the complexes.

Complex	Δ*H*
4	-60.4
8-N1	-57.9
8-N2	-58.7
8-N3	-57.2
7	-28.7
7-N1	-28.1
7-N2	-27.5
7-N3	-27.2
7-N4	-27.5
9	-81.7
9-N1	-85.1
9-N2	-85.2
9-N3	-85.9
10	-53.1[a]
10-N1	-45.7[a]
10-N2	-45.5[a]
10-N3	-44.3[a]
10-N4	-45.3[a]
11	-178.2[a]

[a]Computed bonding energy (Δ*E*).

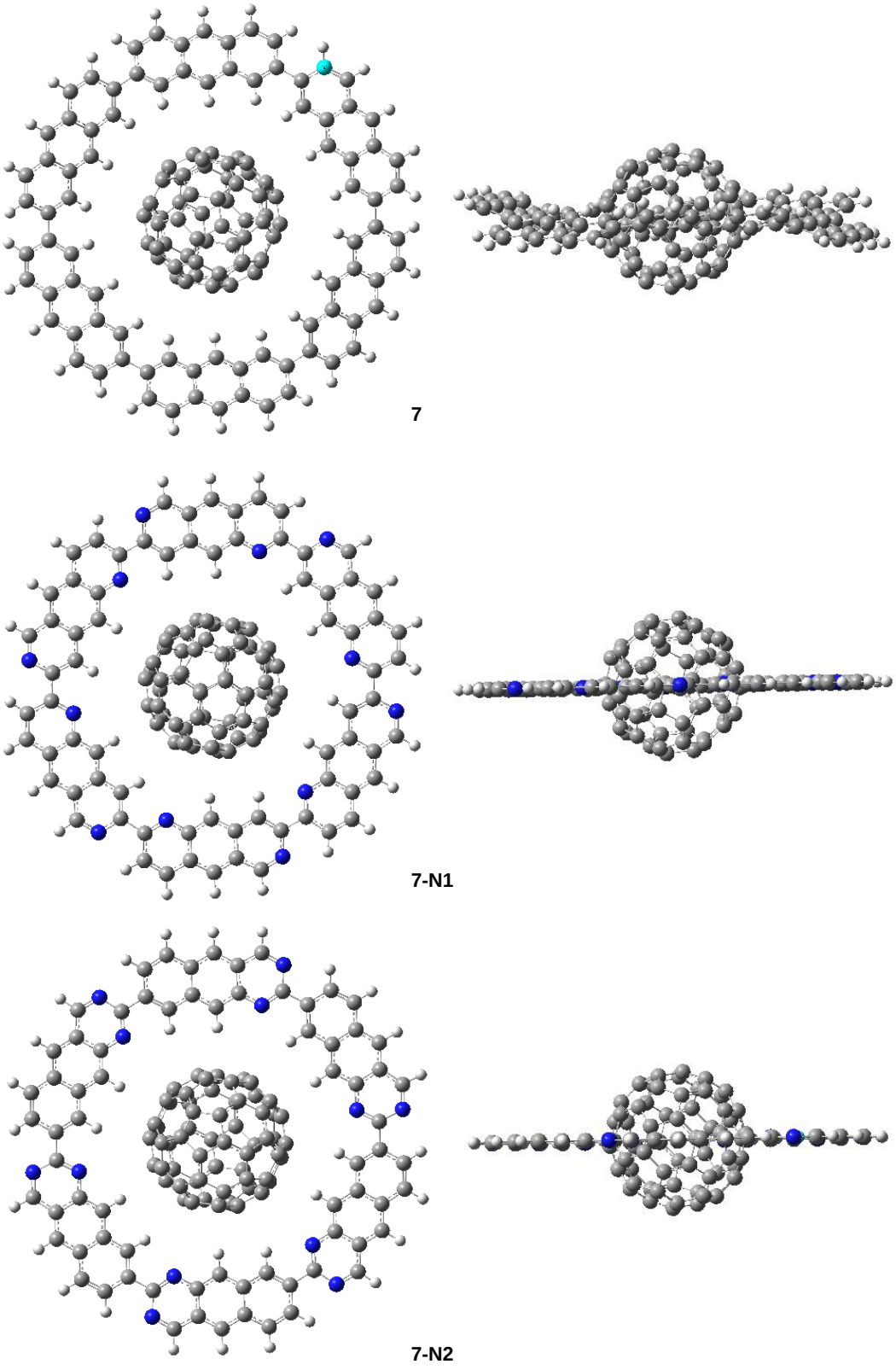
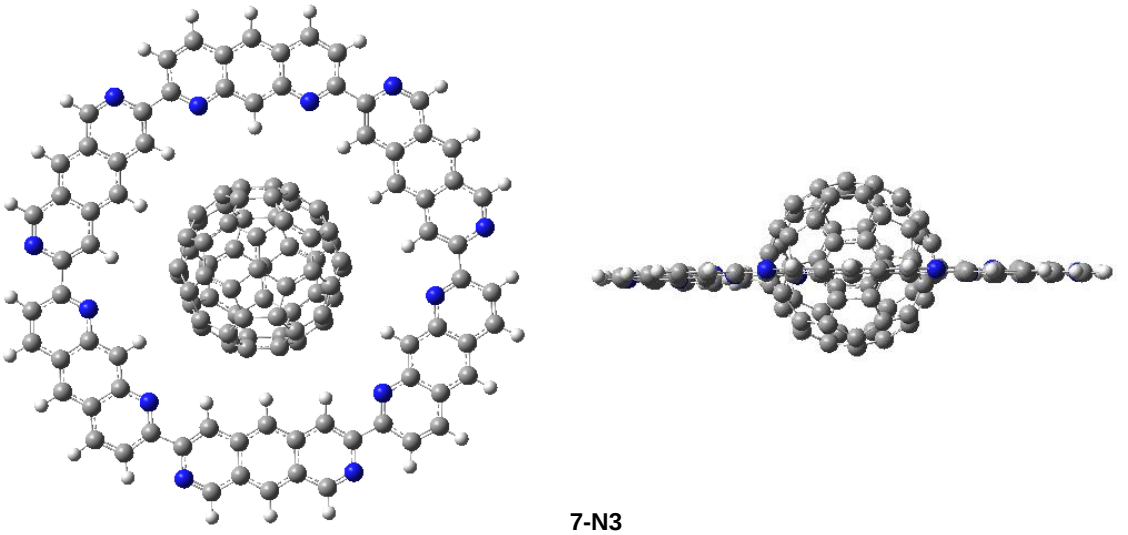
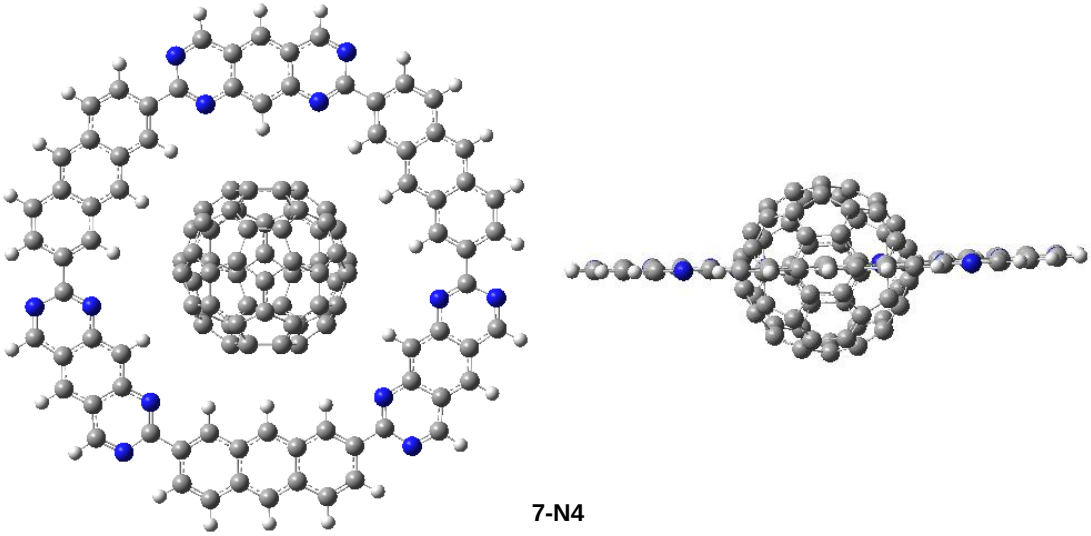


Figure 1. Optimized structure of **7** and its nitrogen analogues.

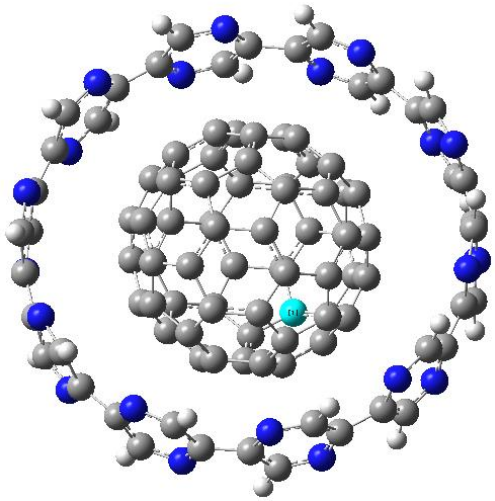


7-N3



7-N4

Figure 1. Optimized structure of **7** and its nitrogen analogues. (continued)



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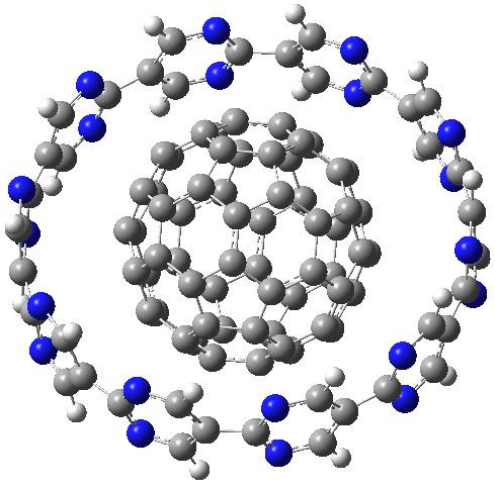
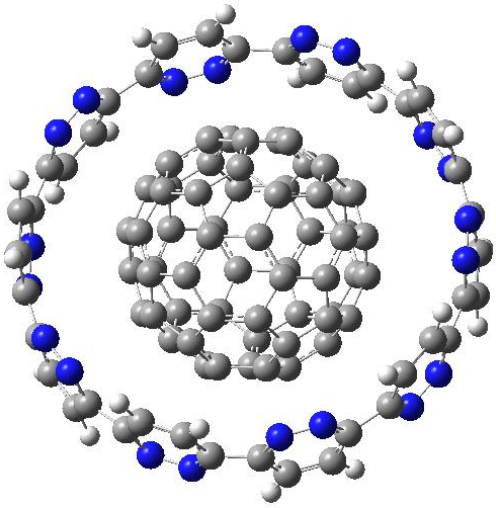
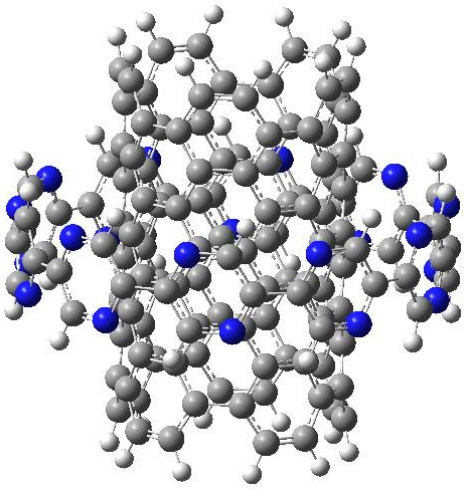


8-N2



8-N3

Figure S2. Optimized structures of **8-N1**, **8-N2**, and **8-N3**.



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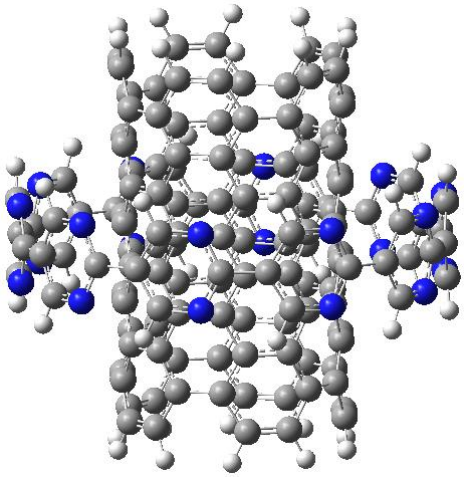

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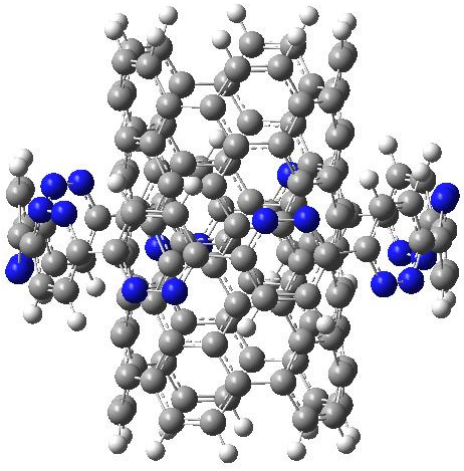
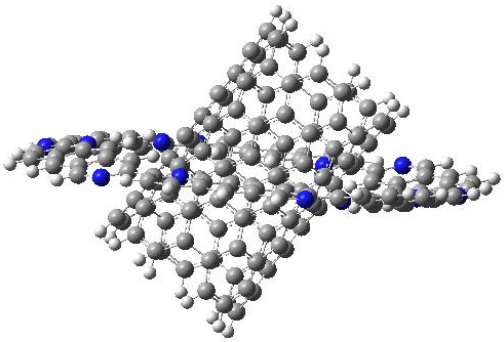


9-N3

Figure S3. Optimized structures of **9-N1**, **9-N2**, and **9-N3**.



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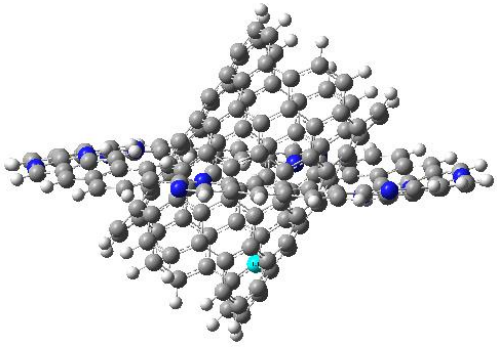
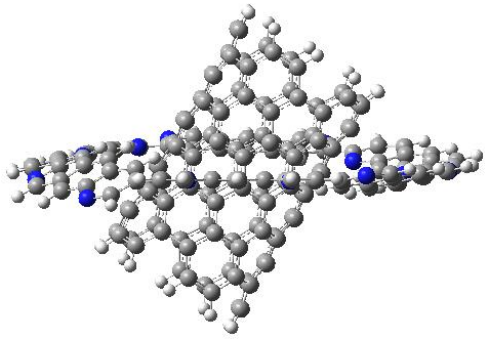
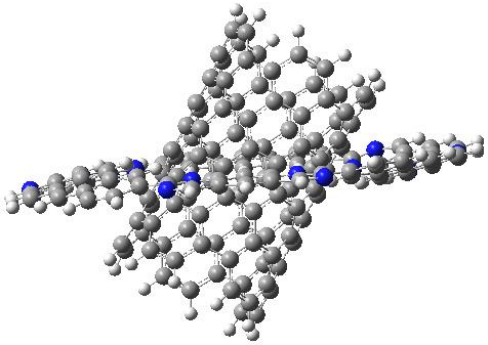


10-N2



10-N3



10-N4

Figure S4. Optimized geometry of **10-N1**, **10-N2**, **10-N3**, and **10-N4**.

Optimized coordinates and corrected enthalpies and free energies (in hartrees) computed at B3LYP-D3/6-31G(d).

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C	0.727519	-1.001344	3.329335
C	-0.727519	-1.001344	3.329335
C	-1.424978	-1.961315	2.595982
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C	0.697460	-2.962658	1.831024
C	1.424978	-1.961315	2.595982
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C	0.000000	1.237729	3.329335
C	-1.177150	0.382479	3.329335
C	-2.305664	0.749156	2.595982
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C	2.602129	-2.343794	0.593295
C	2.602129	-1.578835	1.831024
C	3.033182	-0.252188	1.831024
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C	3.482814	-0.366676	-0.593295
C	3.033182	-1.750499	-0.593295
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C	1.177150	-2.806797	-1.831024
C	-2.602129	-2.343794	0.593295
C	-1.177150	-0.382479	-3.329335
C	-2.305664	-0.749156	-2.595982
C	-3.033182	0.252188	-1.831024
C	-2.602129	1.578835	-1.831024
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C	-3.482814	0.366676	0.593295
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C	0.697460	2.962658	-1.831024
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C	-0.727519	3.425662	0.593295
C	-1.177150	2.806797	1.831024
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C	-3.033182	-1.750499	-0.593295
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ΔH = -2286.092083

ΔG = -2286.156511

[5,5]nanotube 2

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C	0.686026	3.458290	5.510946
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C	2.584050	2.323209	4.312355
C	3.077036	1.721120	5.510946
C	3.501023	0.416221	5.510946
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C	-0.724992	-3.398382	4.312355
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C	0.718732	3.356017	3.090378
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C	-0.707441	-3.345843	1.847326
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[10]CPP 3

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9-N1

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