The structure of host-guest complexes between dibenzo-18-crown-6 and water, ammonia, methanol, and acetylene - Evidence of molecular recognition on the complexation -

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Supporting Information

Calculated results (M05-2X/6-31+G*)

DB18C6 and DB18C6-H$_2$O

Optimized geometries S3
IR spectra S4
S$_1$-S$_0$ and S$_2$-S$_0$ transition energy S5

DB18C6-NH$_3$ built on II and IV conformations

Optimized geometries S6
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DB18C6-CH$_3$OH

Optimized geometries S8
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DB18C6-C$_2$H$_2$

Optimized geometries  S10

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boat-(NH$_3$)$_n$ ($n$=1-3) and boat-H$_2$O-NH$_3$

Optimized geometries  S12

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S$_1$-S$_0$ electronic transition energies of complexes  S14
**Fig. S1.** Optimized structures of (a) DB18C6 and (b) DB18C6-H$_2$O at higher energy.
Fig. S2. IR spectra of m1, m2 and a and calculated IR spectra of DB18C6 and DB18C6-H2O in the CH stretching energy region.
**Fig. S3.** (a) LIF spectrum of bare DB18C6 and DB18C6·H$_2$O. (b) Calculated S$_1$-S$_0$ and S$_2$-S$_0$ electronic transition energies of DB18C6 and DB18C6·H$_2$O.
Fig. S4. Optimized structures of DB18C6-NH$_3$ built on (a) II and (b) IV conformations.
**Fig. S5.** Calculated IR spectra of DB18C6-NH$_3$ built on II and IV conformations in the region of (a) CH and (b) NH stretching vibrations.
**Fig. S6.** Optimized structures of DB18C6-CH$_3$OH built on (a) II, (b) IV, and (c) boat conformations.
Fig. S7. Calculated IR spectra of DB18C6-CH₃OH in the region of (a) CH and (b) NH stretching vibrations.
Fig. S8. Optimized structures of DB18C6-C$_2$H$_2$ built on (a) II, (b) IV, and (c) boat conformations.
**Fig. S9.** Calculated IR spectra of DB18C6-C$_2$H$_2$ in the region of (a) methylene and (b) acetylene CH stretching vibrations.
Fig. S10. Optimized structures of boat-(NH₃)$_n$ with (a) $n=1$, (c) $n=2$, (d) $n=3$, and (b) boat-H$_2$O-NH$_3$.
Fig. S11. Calculated IR spectra of boat-(NH₃)ₙ with n=1-3 and boat-H₂O-NH₃ in the region of the (a) CH and (b)-(d) NH stretching vibrations.
Fig. S12. Calculated $S_1 - S_0$ electronic transition energies of DB18C6 complexes with (a) NH$_3$, (b) CH$_3$OH, and (c) C$_2$H$_2$. 