Supporting Informations


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Figure S1  Job’s plots of the interaction between benzo[6]uril 1 and a) guest 3; b) guest 4; c) guest 5; d) guest 6; e) guest 8. The total concentration was maintained at $1.0 \times 10^{-5}$ mol·L$^{-1}$, and fluorescence intensities were recorded at $\lambda_{em} = 326$ nm, $\lambda_{ex} = 300$ nm.
Figure S2 Fluorescence spectra of benzo[6]uril 1 (1.0 × 10^{-5} mol·L^{-1} in DMSO) in the absence (blue solid) and presence of 1 eq. guest 7 (red dash).
Figure S3 Fluorescence titration spectra of benzo[6]uril 1 with guest 8. The host concentration was fixed at $1.0 \times 10^{-5}$ mol·L$^{-1}$ in DMSO. Insets: nonlinear fitting of the changes in fluorescence intensity upon addition of the guest ($\lambda_{em} = 326$ nm, $\lambda_{ex} = 300$ nm)
Figure S4 $^1$H NMR spectra of benzo[6]uril 1 at a) 50 and b) 25 °C
Figure S5 $^1$H NMR spectra (400 MHz, [D$_6$]DMSO) of a) free guest 3($1.0 \times 10^{-3}$ mol·L$^{-1}$), and in the presence of b) 0.5 equiv.; c) 1.0 equiv.; d) 2.0 equiv.; e) 3.0 equiv. of benzo[6]uril 1, and f) free benzo[6]uril 1.
Figure S6 $^1$H NMR spectra (400 MHz, [D$_6$]DMSO) of a) free benzo[6]uril 1 ($2.0 \times 10^{-3}$ mol·L$^{-1}$), and in the presence of b) 0.5 equiv.; c) 1.0 equiv.; d) 2.0 equiv.; e) 3.0 equiv. of guest 4, and f) free guest 4.
Figure S7 $^1$H NMR spectra (400 MHz, $[D_6]$DMSO) of a) free benzo[6]uril 1 ($2.0 \times 10^{-3}$ mol·L$^{-1}$), and in the presence of b) 0.5 equiv.; c) 1.0 equiv.; d) 2.0 equiv.; e) 3.0 equiv. of guest 5, and f) free guest 5.
Figure S8 $^1$H NMR spectra (400 MHz, D$_6$DMSO) of a) free benzo[6]uril 1 (2.0 × 10$^{-3}$ mol·L$^{-1}$), and in the presence of b) 0.5 equiv.; c) 1.0 equiv.; d) 2.0 equiv.; e) 3.0 equiv. of guest 6, and f) free guest 6.
Figure S9 \(^1\)H NMR spectra (400 MHz, [D\(_6\)]DMSO) of a) free benzo[6]uril 1 (2.0 \(\times\) 10\(^{-3}\) mol·L\(^{-1}\)), and in the presence of b) 2.0 equiv.; c) 4.0 equiv.; d) 6.0 equiv. of guest \(8\).
Figure S10 Job’s plots of the interaction between benzo[6]uril 2 and a) guest 3; b) guest 4; c) guest 5; d) guest 8. The total concentration was maintained at $1.0 \times 10^{-5}$ mol·L$^{-1}$, and fluorescence intensities were recorded at $\lambda_{em} = 327$ nm, $\lambda_{ex} = 304$ nm for host 2 system.
Figure S11 Fluorescence spectra of benzo[6]uril 2 (1.0 × 10^{-5} mol·L^{-1} in CH_2Cl_2/CH_3OH, 5:1, v/v) in the absence (blue solid) and presence of 1 eq. guest 7 (red dash).
Figure S12 $^1$H NMR spectra (400 MHz, CDCl$_3$/CD$_3$OD, 5:1, v/v) of a) benzo[6]uril 2 ($2.0 \times 10^{-3}$ mol·L$^{-1}$), and in the presence of b) 0.5 equiv.; c) 1.0 equiv.; d) 2.0 equiv.; and e) 3.0 equiv. of guest 4, and f) free guest 4.
Figure S13 $^1$H NMR spectra (400 MHz, CDCl$_3$/CD$_3$OD, 5:1, v/v) of a) benzo[6]uril 2 (2.0 × 10$^{-3}$ mol·L$^{-1}$), and in the presence of b) 0.5 equiv.; c) 1.0 equiv.; d) 2.0 equiv.; and e) 3.0 equiv. of guest 5, and f) free guest 5.
Figure S14 $^1$H NMR spectra (400 MHz, CDCl$_3$/CD$_3$OD, 5:1, v/v) of a) benzo[6]uril 2 (2.0 × 10$^{-3}$ mol·L$^{-1}$), and in the presence of b) 0.2 equiv.; c) 0.4 equiv.; and d) 0.6 equiv. of guest 8.
Figure S15 UV-vis spectra of benzo[6]uril 1 in DMSO (1.0 × 10^{-5} mol·L^{-1}, solid line) and benzo[6]uril 2 in CH\textsubscript{2}Cl\textsubscript{2}/CH\textsubscript{3}OH (v/v, 5:1; 1.5 × 10^{-5} mol·L^{-1}, dash line).
Figure S16 $^{13}$CNMR spectrum of benzo[6]uril 1.
Figure S17 gCOSY NMR spectrum of benzo[6]uril 1.
Figure S18 NOESY NMR spectrum of benzo[6]uril 1.
Figure S19 gHSQC (Heteronuclear Single Quantum Correlation) NMR spectrum of benzo[6]uril 1.
Figure S20 gHMBC (Heteronuclear Multiple Bond Correlation) NMR spectrum of benzo[6]uril 1.
Figure S21 High resolution MS of benzo[6]uril 1.
Figure S22 $^{13}$CNMR spectrum of benzo[6]uril 2.
Figure S23 gCOSY NMR spectrum of benzo[6]uril 2.
Figure S24 NOESY NMR spectrum of benzo[6]uril 2.
Figure S25 gHSQC (Heteronuclear Single Quantum Correlation) NMR spectrum of benzo[6]uril 2.
Figure S26 gHMBC (Heteronuclear Multiple Bond Correlation) NMR spectrum of benzo[6]uril 2.
Figure S27 High resolution MS of benzo[6]uril 2.