Supporting Information

Molecular Inclusion of Organometallic Sandwich Complexes within Hybrid Cavitand-resorcin[4]arene Receptors

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Figure S1. Structure of substrates and the receptors 2a-b.
Fluorescence titrations

**Figure S2.** Fluorescence titration of $6^+$ (8.25 × 10^{-6} M) in MeOH upon addition of incremental amounts of $2a$. 

$2a$ 
$6^+$ 
$2a \cdot 6^+$ 

R= CH$_2$CH$_3$ 

$y = (0.8 \times 10^4) x + 0.9642$

$K_c = 1 \pm 0.2 \times 10^4 \text{M}^{-1}$
Figure S3. Fluorescence titrations of $6^+$ (0.24 mM) in MeOH in the presence of $2a$ (0.15 mM) and upon addition of incremental amounts of $1a^+$. 

$^1$H NMR titrations

Figure S4. NMR titration of $2a$ ([2a] = 4.48 mM) with $4^+$ in MeOH-$d_4$. 

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Figure S5. NMR titration of 2b ([2b] = 2.80 mM) with 4+ in acetone-d$_6$.

Figure S6. NMR titration of 2b ([2b] = 2.64 mM) with 7+ in acetone-d$_6$.

Figure S7. NMR titration of 2b ([2b] = 4.20 mM) with 8+ in acetone-d$_6$. 

$K_a = 1.7 \pm 0.2 \times 10^7$ M$^{-1}$

$K_a = 2.3 \pm 0.7 \times 10^2$ M$^{-1}$

$K_a = 1.4 \pm 0.2 \times 10^2$ M$^{-1}$
Figure S8. NMR spectra of 2a ([2a] = 2.50 mM) and 2a with 3 equivalents of 9a in MeOH-$d_4$.

Figure S9. NMR spectra of 2b ([2b] = 4.50 mM) and 2b with 3 equivalents of 9a in acetone-$d_6$. 
**ITC titration.**

**Figure S10:** Calorimetric titration between the receptor or 2b ([2b] = 10 mM in acetone) and 1a$^+$ seven times more concentrated than the corresponding receptor.
Cyclic voltammetry

**Scheme S1**: Coupled electrochemical and chemical equilibria for the cobaltocenium $1a^+$ forming supramolecular complexes with non-electroactive hosts $2a$ or $2b$.

**Figure S11**: Cyclic voltammetric behavior on glass carbon (0.071 cm$^2$) of 1.0 mM $2b$ in acetone also containing 0.1 M tetraoctylammonium bromide (a) and after each addition (b) 0.5 (c) 1.5 (d) 4.0 eq) of cobaltocenium $1a^-$. Scan rate 100 mV/s.
Diffusion coefficients

**Figure S12**: Representation of $I$ vs $v^{1/2}$ of a 1.0 mM solution of 1a$^+$.  

\[ y = 26.988x \]
\[ R^2 = 0.9938 \]
\[ D = 1.43 \times 10^{-6} \text{ cm}^2/\text{s} \]

**Figure S13**: Representation of $I$ vs $v^{1/2}$ of a 1.0 mM solution of 1a$^+$ with 2 equivalents of 2a.  

\[ y = 5.7768x \]
\[ R^2 = 0.9789 \]
\[ D = 3.52 \times 10^{-7} \text{ cm}^2/\text{s} \]