Electronic Supplementary Information for Dalton Transactions

Selective binding of benzenediol derivatives by simultaneous non-covalent interactions in bis-Pt(II) aza-aromatic host-guest system

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Supporting information

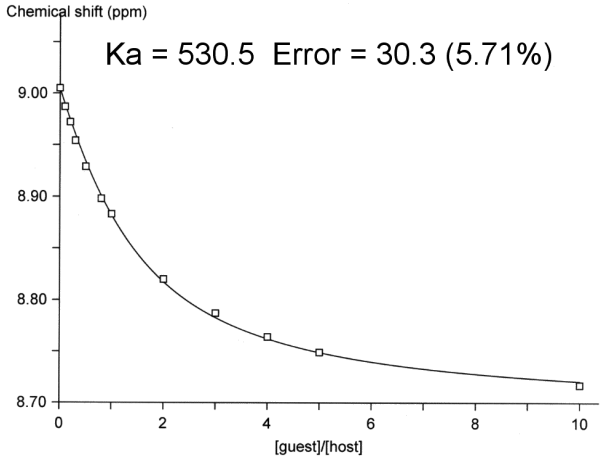

Fig. S1 Fit plot for the ^{1}H NMR titration of **1**·BF_4 with benzene-1,4-diol. [**1**·BF_4] = 2 mM, DMSO-d_6, 25 °C.

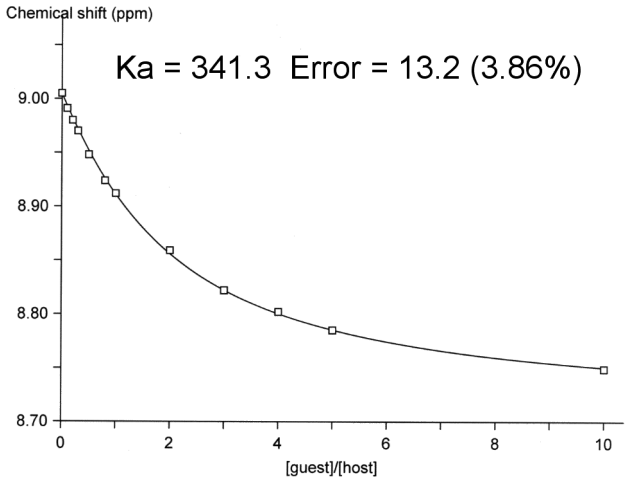

Fig. S2 Fit plot for the ^{1}H NMR titration of **1**·BF_4 with benzene-1,3-diol. [**1**·BF_4] = 2 mM, DMSO-d_6, 25 °C.

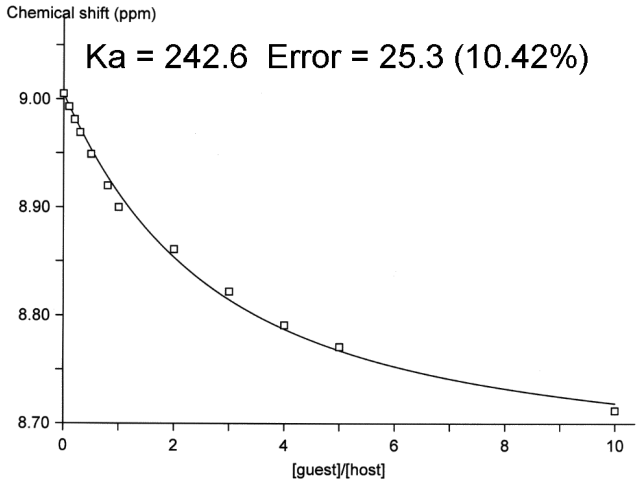

Fig. S3 Fit plot for the ^{1}H NMR titration of **1**·BF_4 with benzene-1,2-diol. [**1**·BF_4] = 2 mM, DMSO-d_6, 25 °C.

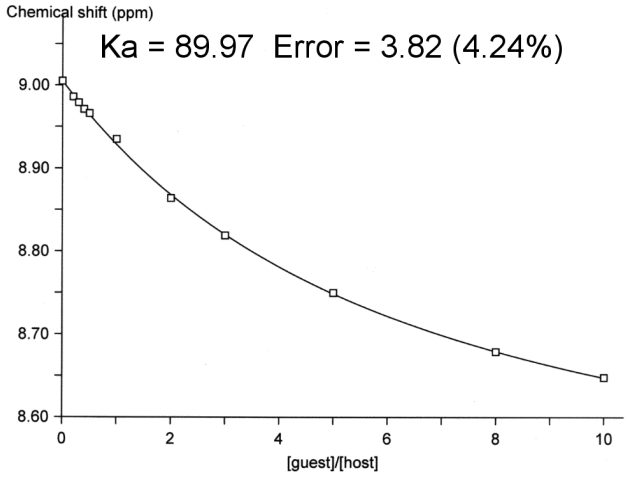

Fig. S4 Fit plot for the ^{1}H NMR titration of **1**·BF_4 with 2-chloronaphthalene. [**1**·BF_4] = 2 mM, DMSO-d_6, 25 °C.

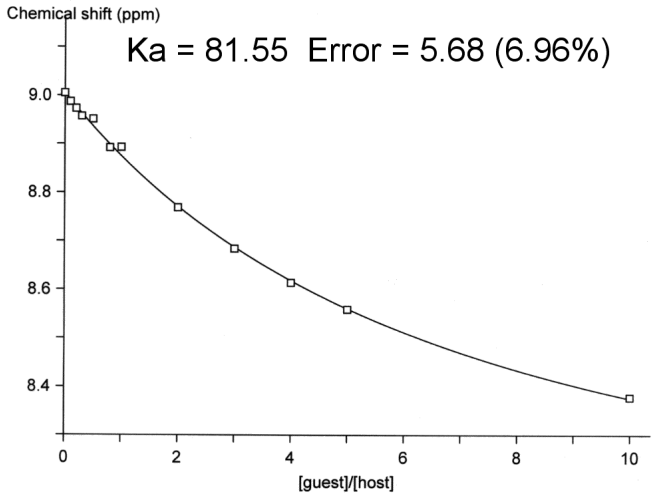

Fig. S5 Fit plot for the ^{1}H NMR titration of **1**·BF_4 with pyrene. [**1**·BF_4] = 2 mM, DMSO-d_6, 25 °C.

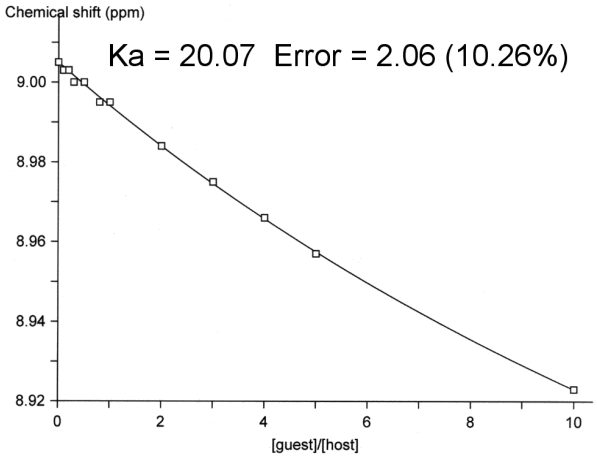

Fig. S6 Fit plot for the ^{1}H NMR titration of **1**·BF_4 with 1,4-dichlorobenzene. [**1**·BF_4] = 2 mM, DMSO-d_6, 25 °C.

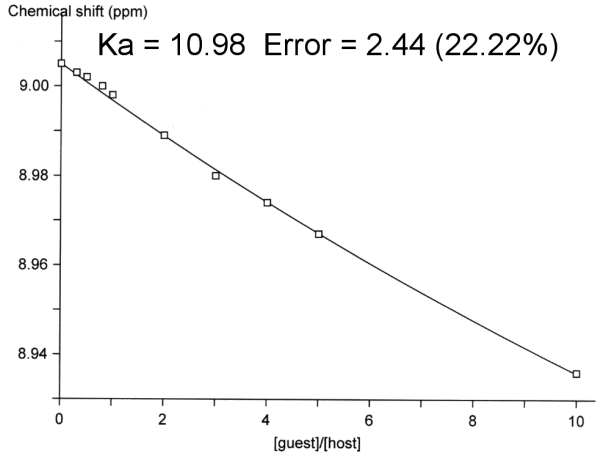

Fig. S7 Fit plot for the ^{1}H NMR titration of **1**·BF_4 with 1,2-dichlorobenzene. [**1**·BF_4] = 2 mM, DMSO-d_6, 25 °C.

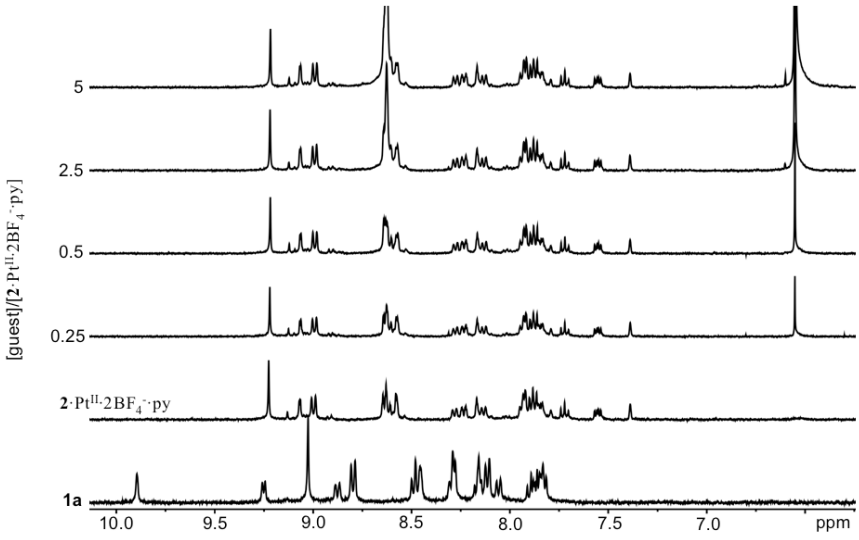

Fig. S8 Titration of **2**·Pt^{II}·$2BF_4^-$·py with benzene-1,4-diol ([**2**·Pt^{II}·$2BF_4^-$·py] = 2 mM, DMSO-d_6/(0.75% pyridine-d_5), 25 °C.

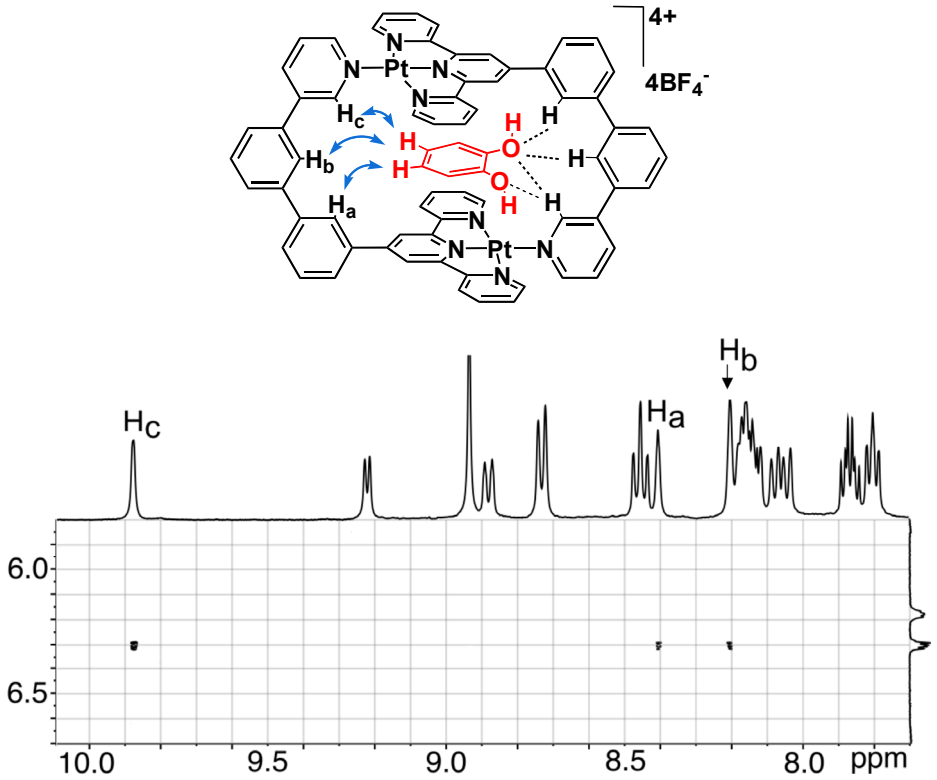

Fig. S9 Portion of the ^{1}H NOESY spectrum of a mixture of **1**·BF_4 with benzene-1,2-diol ([**1**·BF_4] = 9 mM, [benzene-1,2-diol] = 3 mM in DMSO-d_6, at 25 °C with a mixing time of 2.0 sec. The assignment and illustration of observed intermolecular NOE cross peaks are also reported.

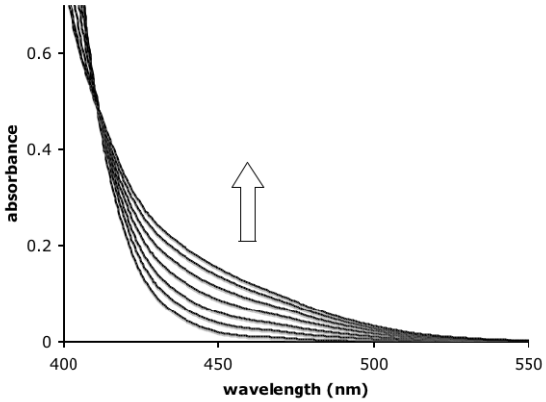

Fig. S10 Portion of the UV-vis titration of **1**·BF_4 ([**1**·BF_4] = 2 mM) by addition of various concentrations of benzene-1,3-diol (0-100 mM) in DMSO at 25 °C.

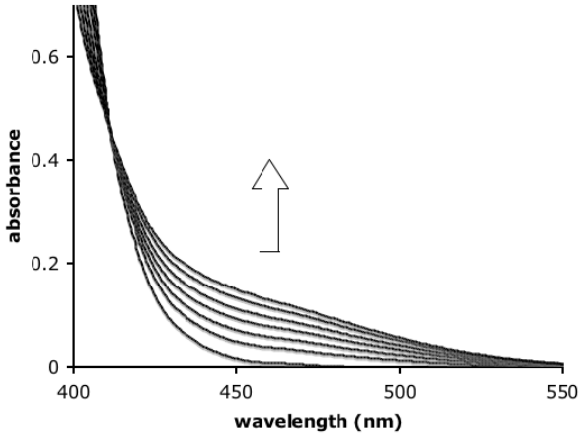

Fig. S11 Portion of the UV-vis titration of **1**·BF_4 ([**1**·BF_4] = 2 mM) by addition of various concentrations of benzene-1,2-diol (0-100 mM) in DMSO at 25 °C.

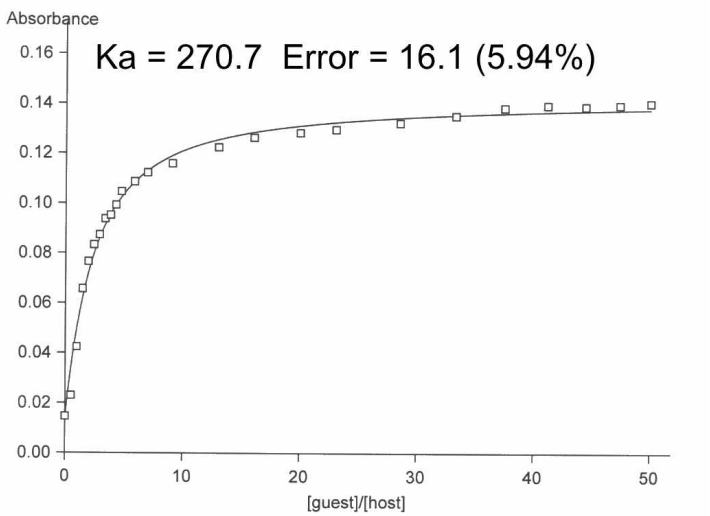

Fig. S12 Fit plot for the UV-vis titration of **1**·BF_4 with benzene-1,4-diol. [**1**·BF_4] = 2 mM, DMSO, 25 °C.

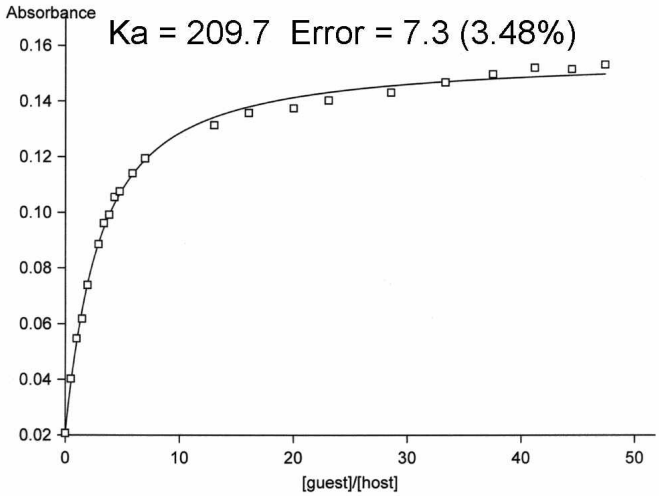

Fig. S13 Fit plot for the UV-vis titration of **1**·BF_4 with benzene-1,3-diol. [**1**·BF_4] = 2 mM, DMSO, 25 °C.

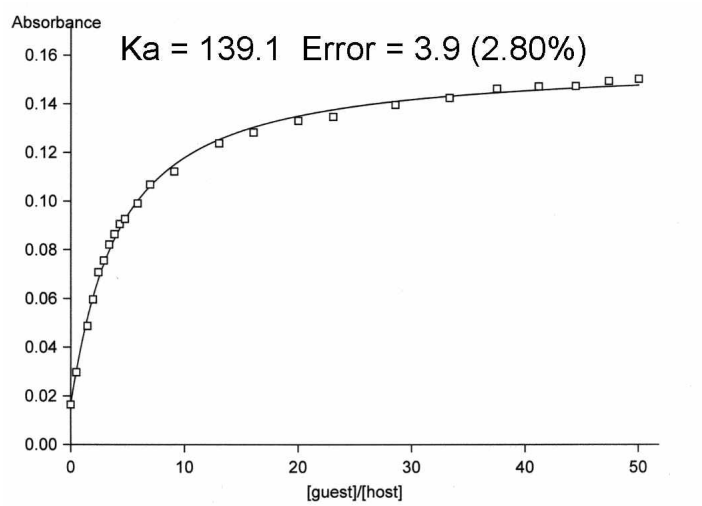

Fig. S14 Fit plot for the UV-vis titration of **1**·BF_4 with benzene-1,2-diol. [**1**·BF_4] = 2 mM, DMSO, 25 °C.

Calculation of Electrostatic Potential Surfaces

The structure of **1**·BF_4 was entered into *Spartan '04* by using the crystal structure data of **1**·BF_4·benzene-1,3-diol (**1**·**meta**·BF_4) saved in pdb format.
Electrostatic Potential Surfaces were calculated using the following settings:

Properties: total charge – 4+; multiplicity – singlet;
Calculations: calculate – single point energy; at – ground state; with – Density Functional – B3LYP – 6-31G* – pseudopotential; start from – initial geometry.