

Electronic Supplementary Information

Paper Ref: C3CC41468J - Chemical Communications

A molecular probe for recognizing the size of hydrophobic cavities based on near-infrared absorbing diradical–Pt^{II} complexes

Kousaku Tamura, Atsuko Masuya, Hitoshi Hoshino and Nobuhiko Iki*

Graduate School of Environmental Studies, Tohoku University, 6-6-07, Aramaki-Aoba, Aoba-ku, Sendai, 980-8579, Japan

Contents

Experimental details

Supplementary data

Continuous variation plots Figures S1 and S3

Estimation of the size of the complexes Figure S2

Corresponding Author

*Fax: +81-22-795-7293; E-mail: iki@m.tohoku.ac.jp

Experimental Details

Material

Pt^{II}-DBA was synthesized according to a method as described in the literature¹. Human serum albumin (MW 66 kDa) and α -chymotrypsin, from bovine pancreas (MW 25 kDa) were purchased from Sigma-Aldrich. β - And γ -cyclodextrin (CD) were purchased from Wako Pure Chemical Co., Ltd (Osaka). All reagents were used without further purification.

Equipment

¹H NMR spectra were measured on a Bruker Biospin DPX-400 (400 MHz) using D₂O as solvents and (3-trimethylsilyl)propanesulfonic acid sodium salt (DSS) as an external standard. Absorption spectra were measured on a SHIMADZU UV-1800 spectrophotometer. The cyclic voltammetric measurements were performed with a Hokuto Denko HAB-151 potentiostat/galvanostat using a glassy carbon working electrode, an Ag/AgCl reference electrode, and a Pt counter electrode in aqueous solution containing 0.2 M Na₂HPO₄ as the supporting electrolyte and NaOH to adjust pH under N₂. pH of the solutions were measured by using a TOA-DKK HM-25R pH meter equipped with a GST-5731C combined electrode.

Supporting Data

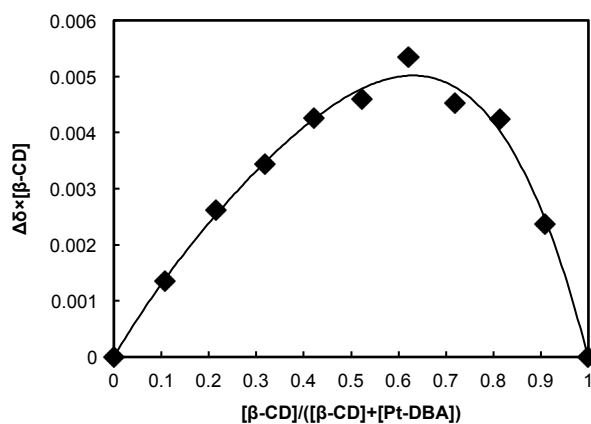
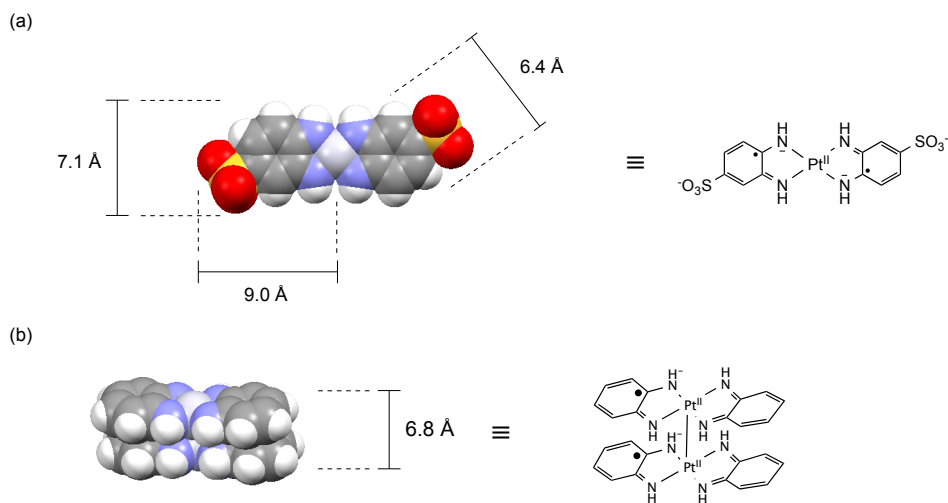


Fig. S1 Continuous variation plot of Pt^{II}-DBA/ β -CD system using ¹H NMR chemical shift of H3 as a probe. [Pt^{II}-DBA] + [β -CD] = 5.0 mM, pD 12.60.



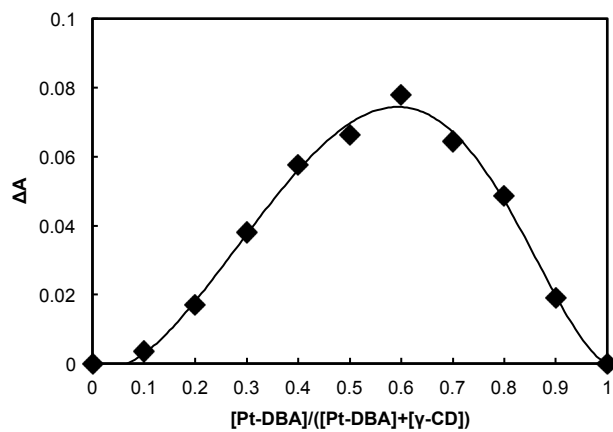


Fig. S3 Continuous variation plot of Pt^{II} -DBA/ γ -CD system using absorbance at 850 nm.
 $[\text{Pt}^{\text{II}}\text{-DBA}] + [\gamma\text{-CD}] = 1.0 \times 10^{-4} \text{ M}$, pH 12.25.

References

1. K. Tamura, A. Masuya, N. Iki, Y. Ohba, S. Yamauchi and H. Hoshino, *Inorg. Chim. Acta*, 2012, **378**, 81.
2. A. Masuya, N. Iki, C. Kabuto, Y. Ohba, S. Yamauchi and H. Hoshino, *Eur. J. Inorg. Chem.*, 2010, **22**, 3458.
3. Y. Konno and N. Matsushita, *Bull. Chem. Soc. Jpn.*, 2006, **79**, 1046.
4. Structure visualization program developed by the Cambridge Crystallographic Data Centre available at http://www.ccdc.cam.ac.uk/free_services/mercury/ .