

*Supporting Information*

# Highly Selective Binding of Nitric Oxide by $\text{Co}^{\text{III}}$ and $\text{Fe}^{\text{III}}$ Complexes

*Zizheng Zhang, Tatsuya Suwabe, Mai Ishikawa, Tomohiko Inomata, Tomohiro Ozawa and  
Hideki Masuda\**

Department of Frontier Materials, Graduate School of Engineering

Nagoya Institute of Technology, Showa, Nagoya 466-8555, Japan

To whom correspondence should be addressed. E-mail: [masuda.hideki@nitech.ac.jp](mailto:masuda.hideki@nitech.ac.jp)

## Contents

Figure S1. Cyclic voltammograms of  $[\text{Co}^{\text{III}}(\text{L1})]$  (**1**) and  $\text{Na}[\text{Co}^{\text{III}}(\text{L2})]$  (**2**) in DMF.

Figure S2. Cyclic voltammograms of  $[\text{Fe}^{\text{III}}(\text{L1})]$  (**3**) and  $(\text{PPh}_4)[\text{Fe}^{\text{III}}(\text{L2})]$  (**4**) in DMF.

Figure S3a-d. FT-IR spectra of the reaction products of  $[\text{Co}^{\text{III}}(\text{L1})]$  (**1**),  $\text{Na}[\text{Co}^{\text{III}}(\text{L2})]$  (**2**),  $[\text{Fe}^{\text{III}}(\text{L1})]$  (**3**) and  $(\text{PPh}_4)[\text{Fe}^{\text{III}}(\text{L2})]$  (**4**) with NO in DMF.

Figure S4a-d. Cyclic voltammograms of  $[\text{Co}^{\text{III}}(\text{L1})]$  (**1**),  $\text{Na}[\text{Co}^{\text{III}}(\text{L2})]$  (**2**),  $[\text{Fe}^{\text{III}}(\text{L1})]$  (**3**) and  $(\text{PPh}_4)[\text{Fe}^{\text{III}}(\text{L2})]$  (**4**) before and after introduction of NO in DMF, respectively.

Figure S5a-d. Electronic absorption spectra of  $[\text{Co}^{\text{III}}(\text{L1})]$  (**1**),  $\text{Na}[\text{Co}^{\text{III}}(\text{L2})]$  (**2**),  $[\text{Fe}^{\text{III}}(\text{L1})]$  (**3**), and  $(\text{PPh}_4)[\text{Fe}^{\text{III}}(\text{L2})]$  (**4**) before (blue line) and after (red line) addition of CO, respectively.

Figure S6a-d. Electronic absorption spectra of  $[\text{Co}^{\text{III}}(\text{L1})]$  (**1**),  $\text{Na}[\text{Co}^{\text{III}}(\text{L2})]$  (**2**),  $[\text{Fe}^{\text{III}}(\text{L1})]$  (**3**), and  $(\text{PPh}_4)[\text{Fe}^{\text{III}}(\text{L2})]$  (**4**) before (black line) and after (red line) exposed by air, respectively.

Figure S7a-d. Electronic absorption spectra of  $[\text{Co}^{\text{III}}(\text{L1})]$  (**1**),  $\text{Na}[\text{Co}^{\text{III}}(\text{L2})]$  (**2**),  $[\text{Fe}^{\text{III}}(\text{L1})]$  (**3**), and  $(\text{PPh}_4)[\text{Fe}^{\text{III}}(\text{L2})]$  (**4**) before (blue line) and after introduction of  $\text{NaNO}_2$ , 10 eq (green line), 100 eq (red line) and excess amount (pink line), respectively.

Figure S8a-b. Electronic absorption spectra of  $[\text{Fe}^{\text{III}}(\text{L1})]$  (**3**) and  $(\text{PPh}_4)[\text{Fe}^{\text{III}}(\text{L2})]$  (**4**) before (blue line) and after introduction of  $\text{NaNO}_3$ , 1 eq (green line), 10 eq (red line), 100 eq (pink line) and excess amount (black line), respectively.

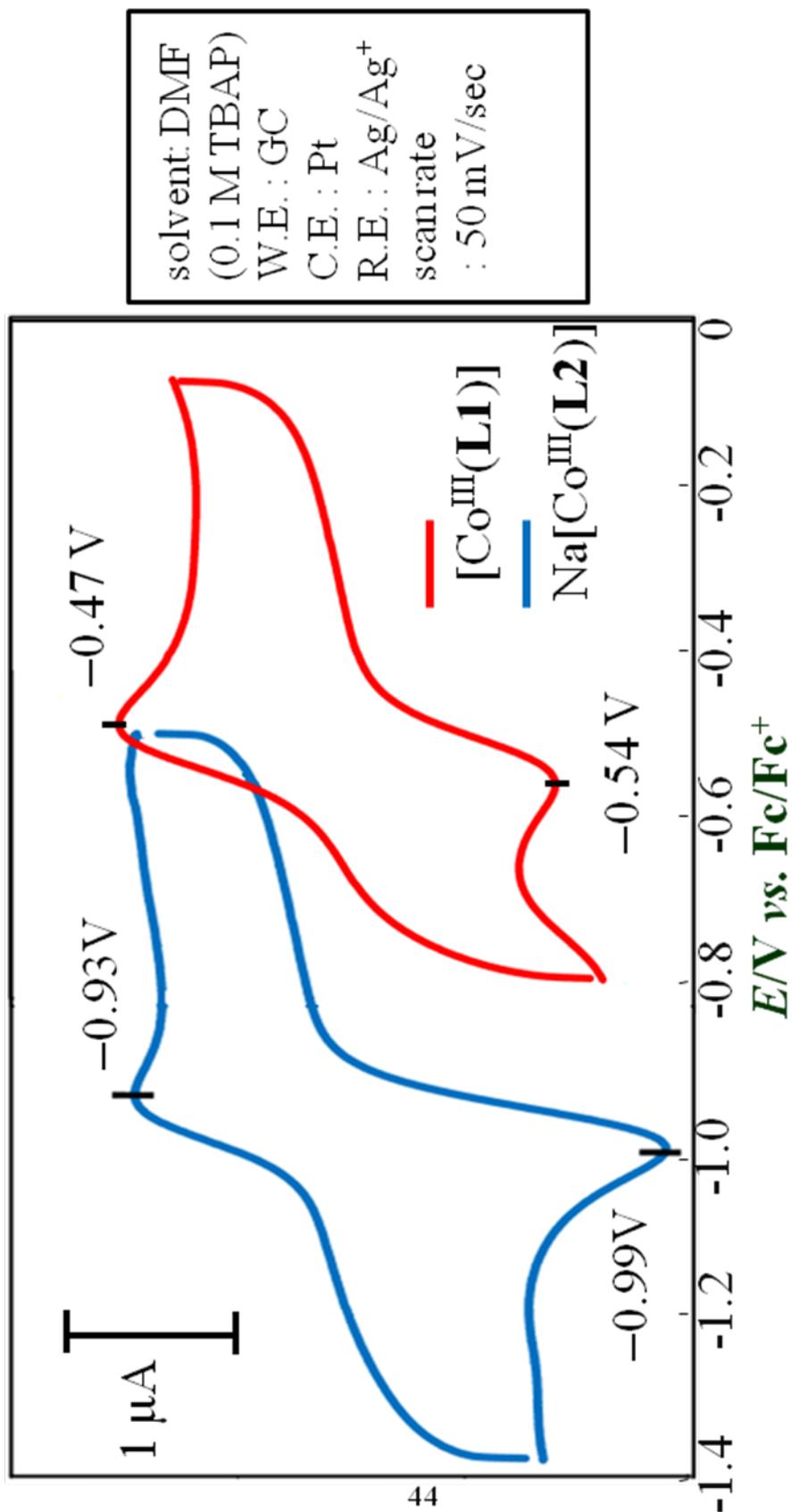


Figure S1. Cyclic voltammograms of [Co<sup>III</sup>(L1)] (1) and Na[Co<sup>III</sup>(L2)] (2) in DMF.

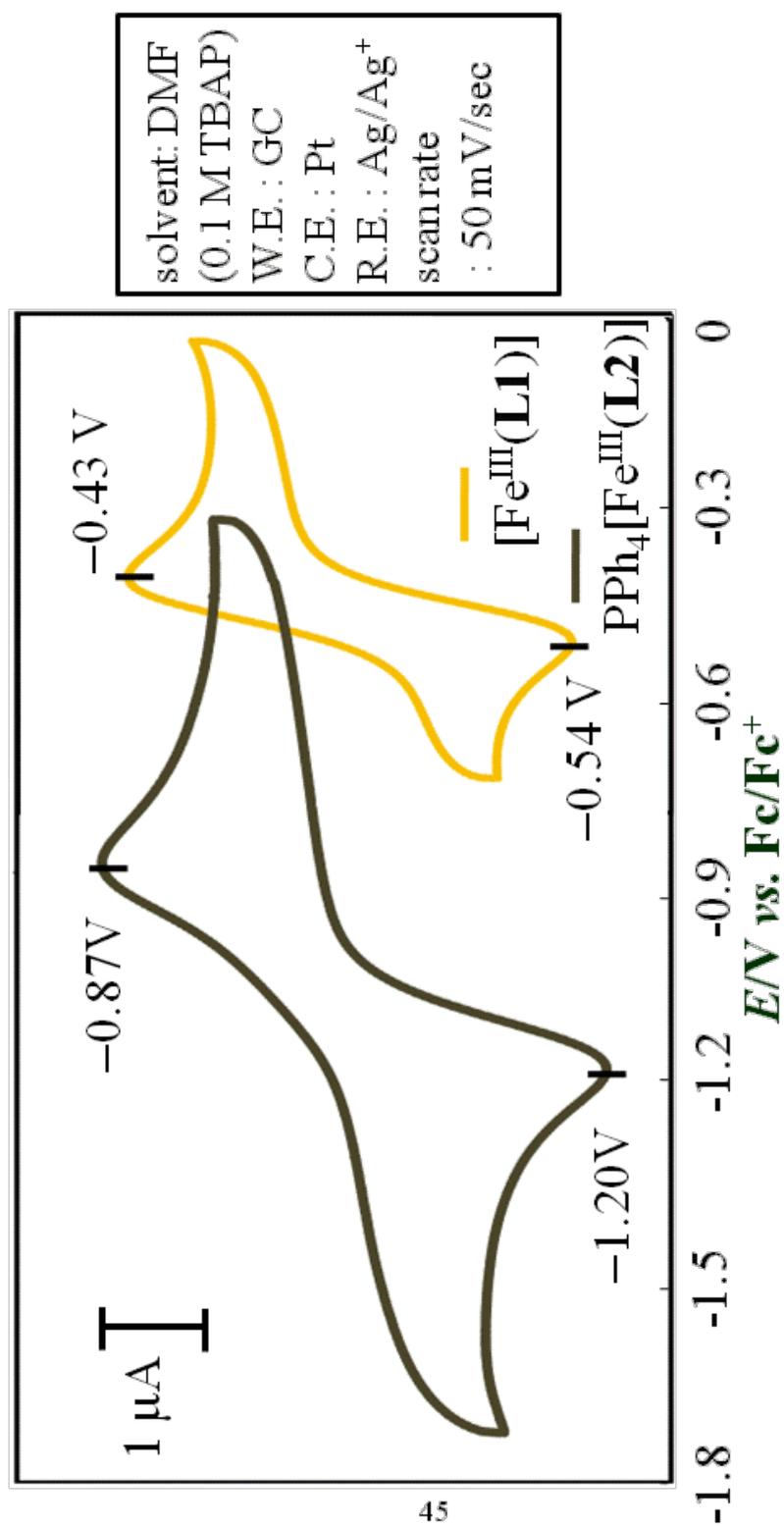


Figure S2. Cyclic voltammograms of [Fe<sup>III</sup>(L1)] (3) and (PPh<sub>4</sub>)[Fe<sup>III</sup>(L2)] (4) in DMF.

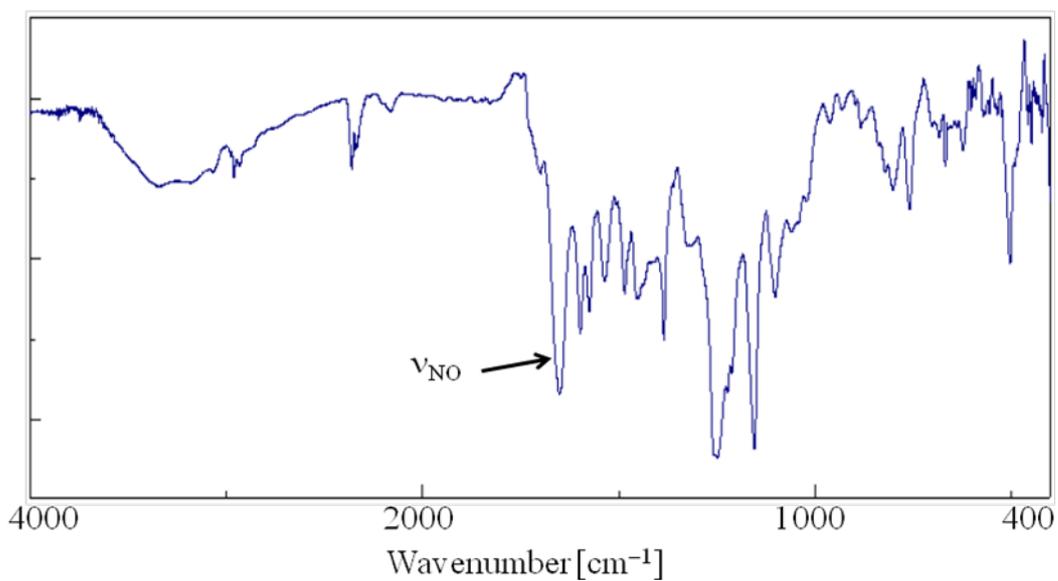


Figure S3a. FT-IR spectrum of the reaction product of [Co<sup>III</sup>(L1)] (1) with NO in DMF.

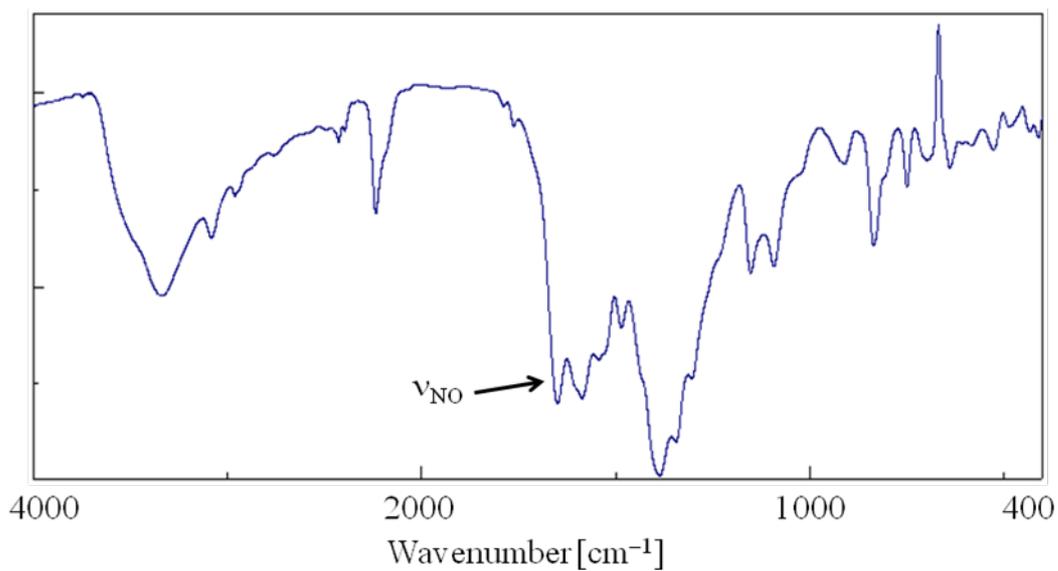


Figure S3b. FT-IR spectrum of the reaction product of Na[Co<sup>III</sup>(L2)] (2) with NO in DMF.

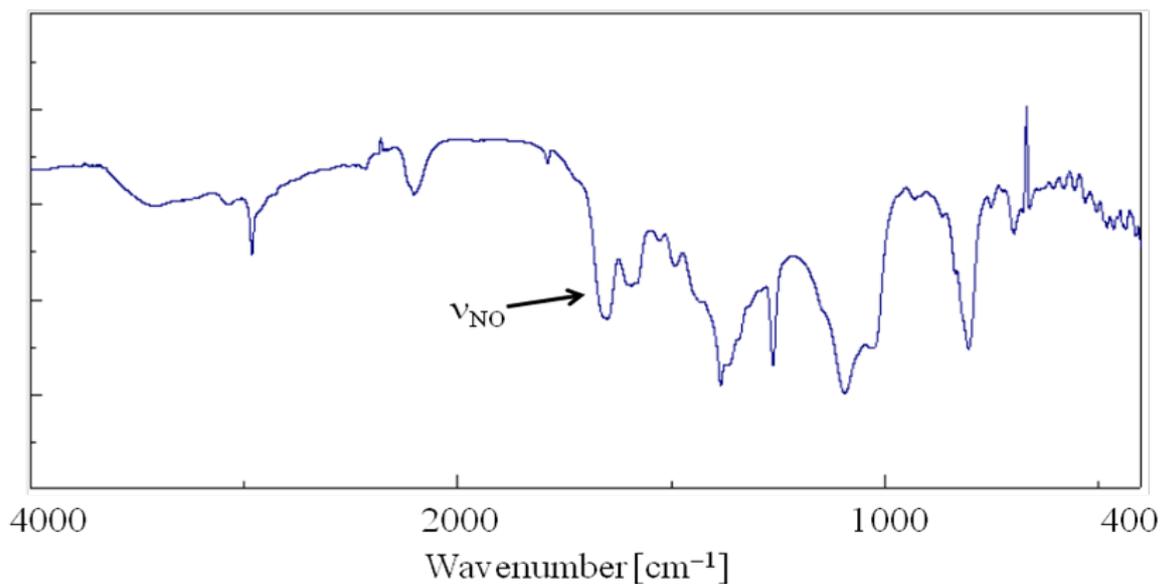


Figure S3c. FT-IR spectrum of the reaction product of [Fe<sup>III</sup>(L1)] (3) with NO in DMF.

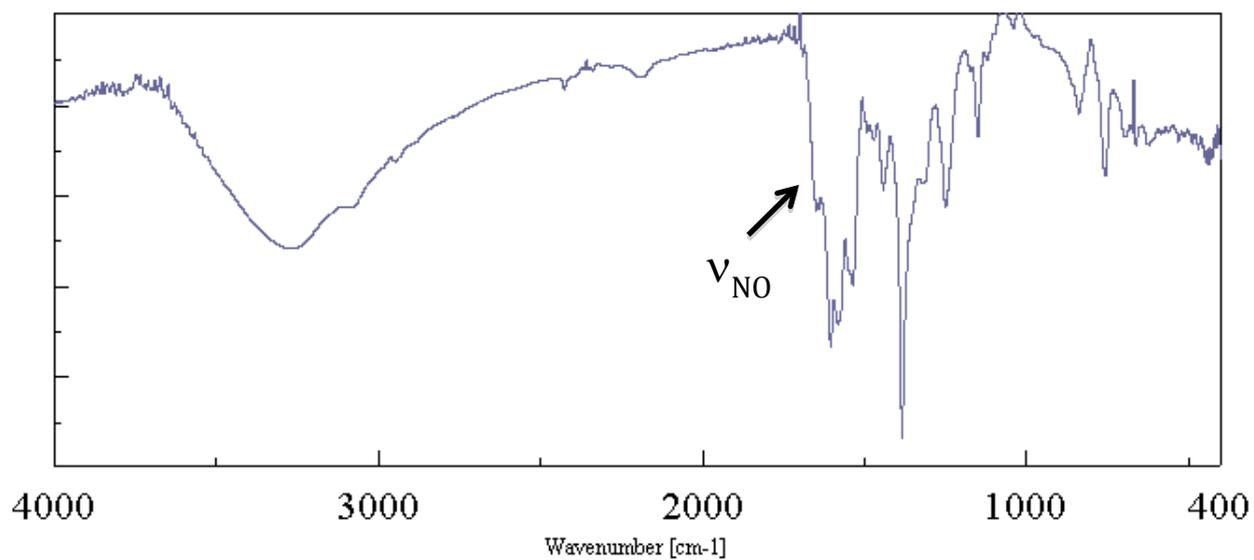


Figure S3d. FT-IR spectrum of the reaction product of (PPh<sub>4</sub>)[Fe<sup>III</sup>(L2)] (4) with NO in DMF.

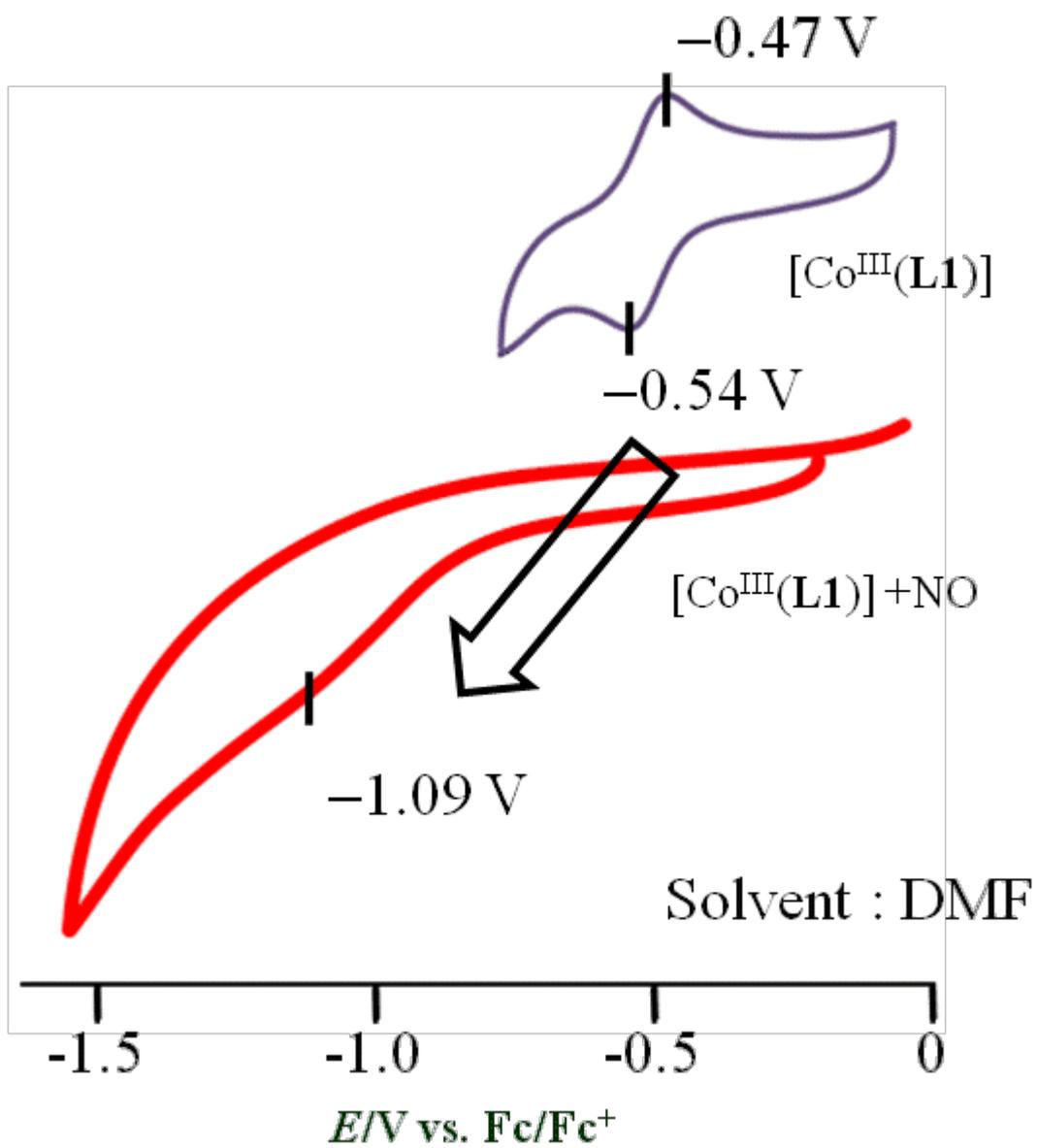


Figure S4a. Cyclic voltammograms of  $[\text{Co}^{\text{III}}(\text{L1})]$  (**1**) before (purple line) and after introduction of NO (red line) in DMF.

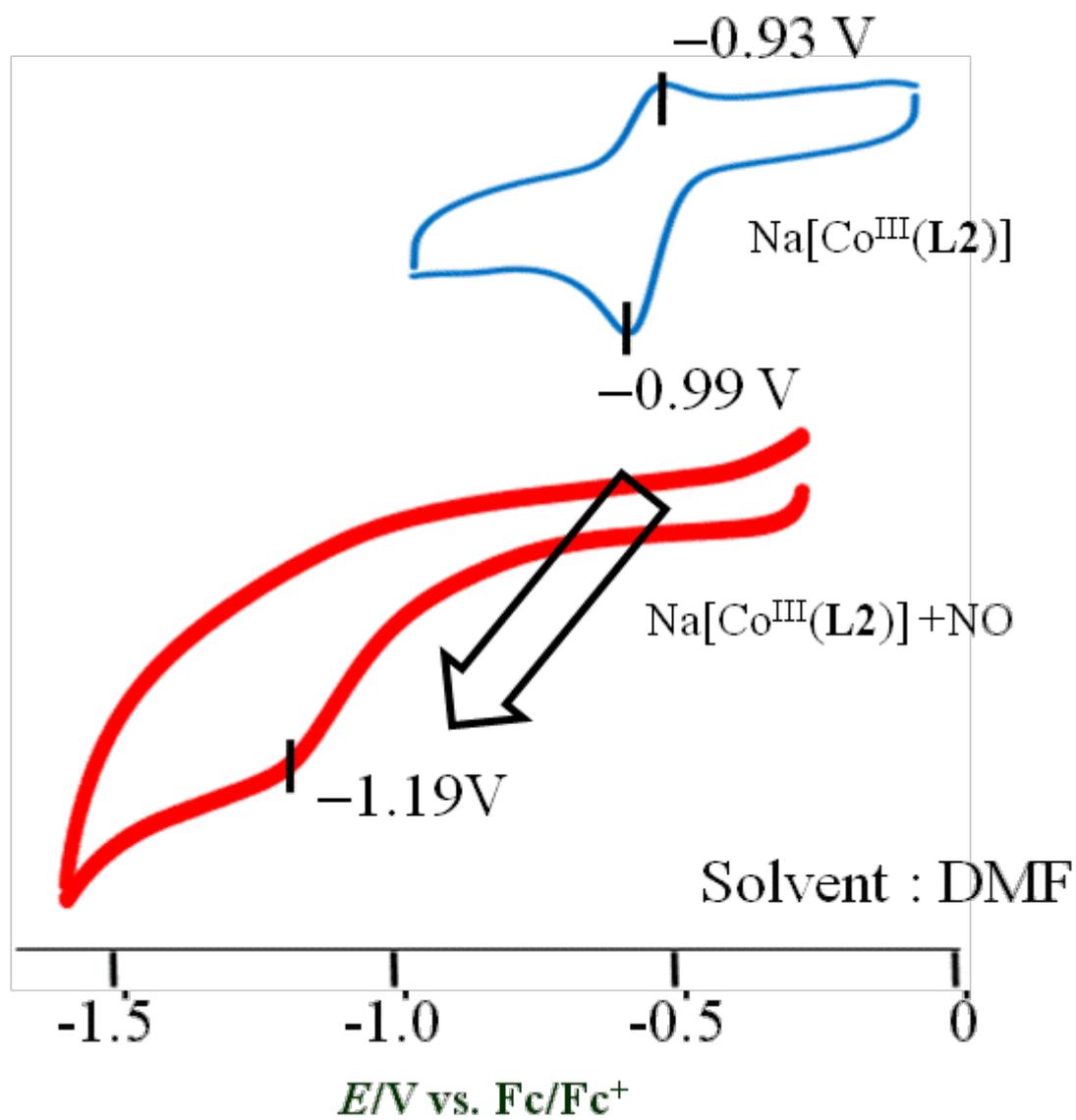


Figure S4b. Cyclic voltammograms of Na[Co<sup>III</sup>(L2)] (2) before (blue line) and after introduction of NO (red line) in DMF.

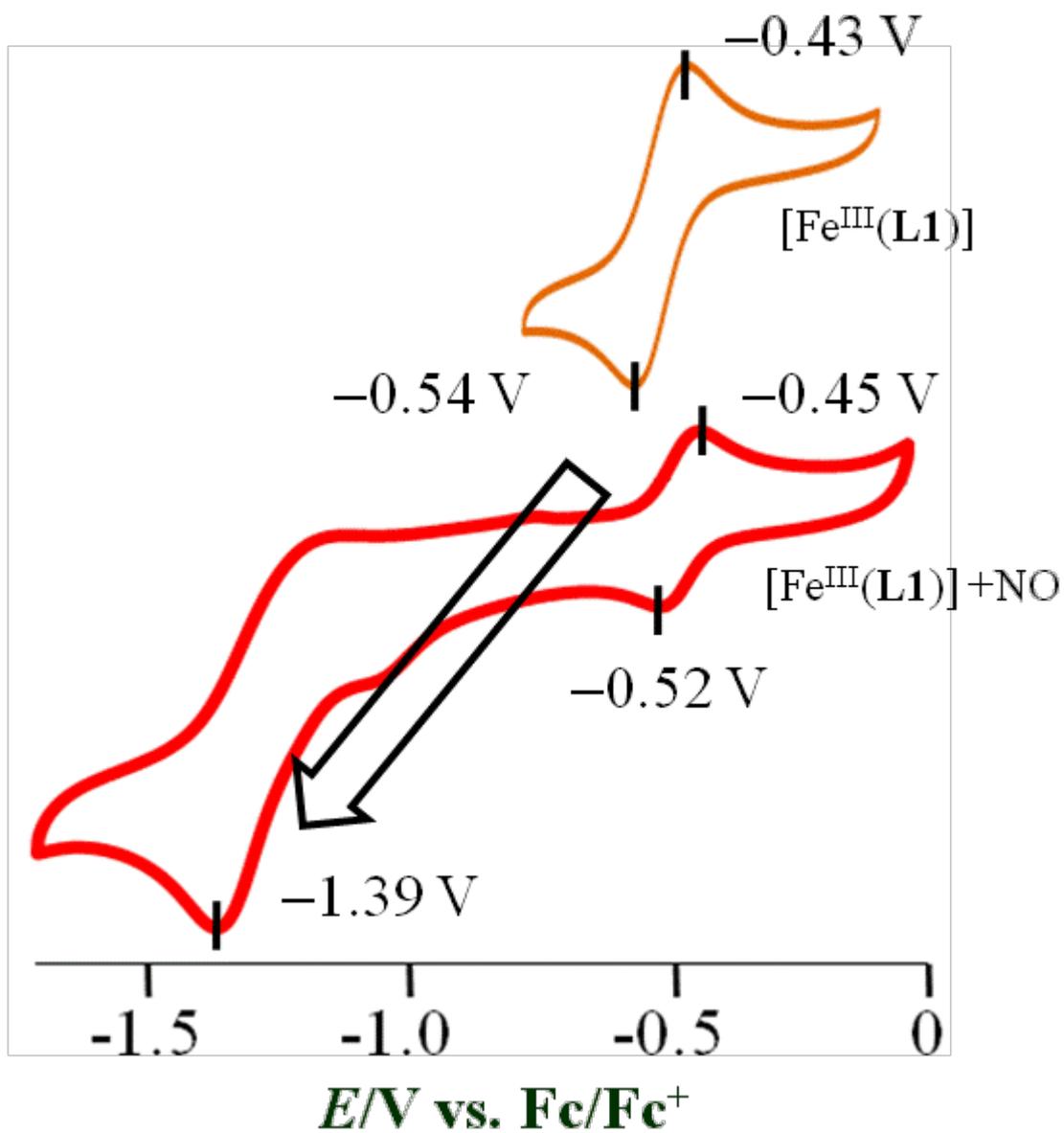


Figure S4c. Cyclic voltammograms of  $[\text{Fe}^{\text{III}}(\text{L1})]$  (**3**) before (orange line) and after introduction of NO (red line) in DMF.

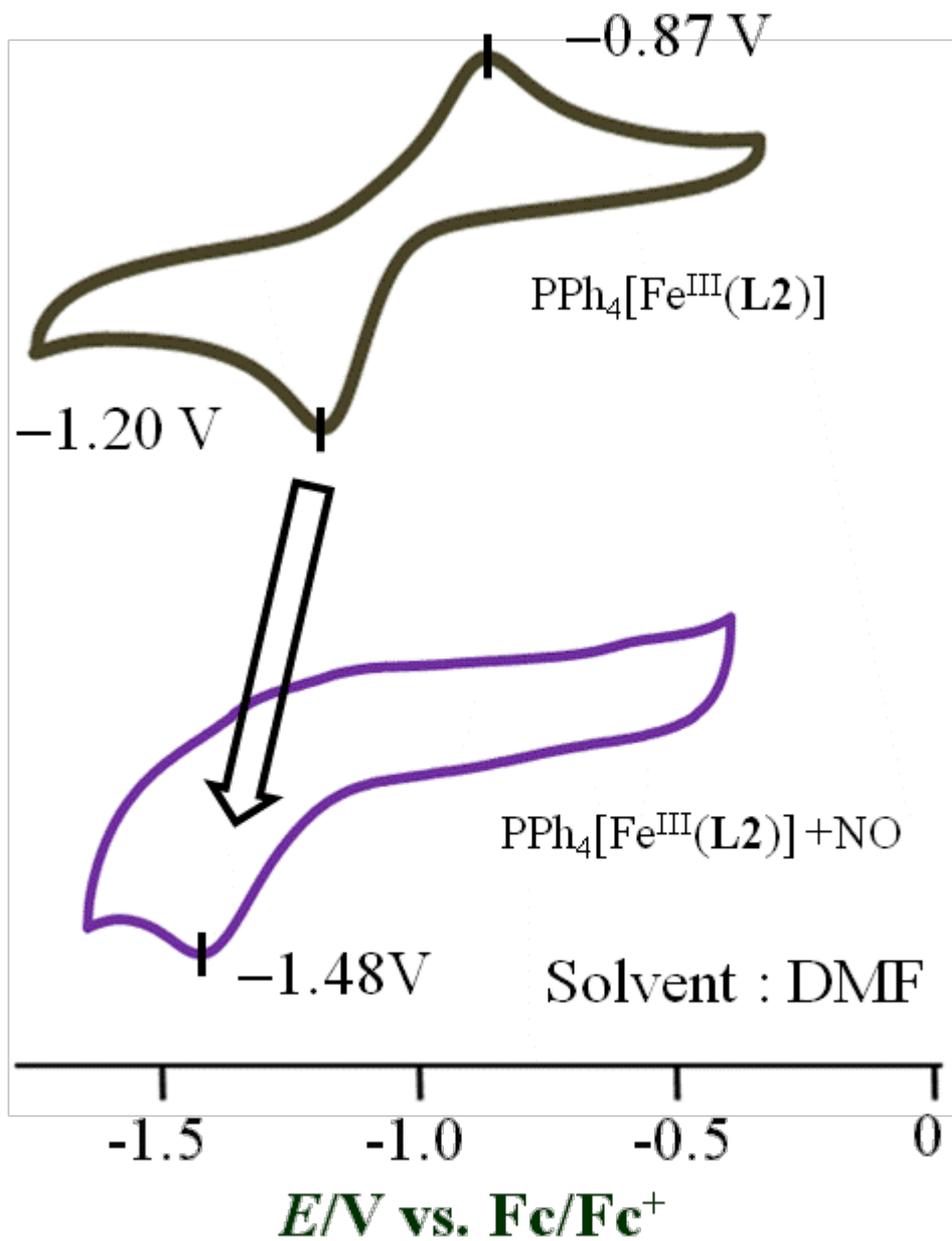


Figure S4d. Cyclic voltammograms of  $(\text{PPh}_4)[\text{Fe}^{\text{III}}(\text{L}2)]$  (**4**) before (black line) and after introduction of NO (purple line) in DMF.

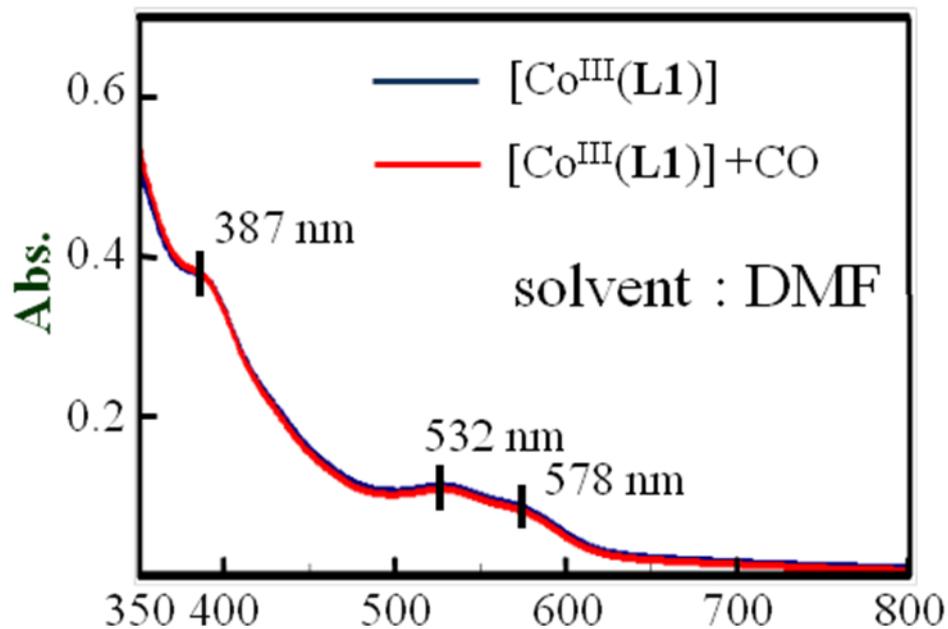


Figure S5a. Electronic absorption spectra of  $[\text{Co}^{\text{III}}(\text{L1})]$  (1) before (blue line) and after (red line) addition of CO in DMF.

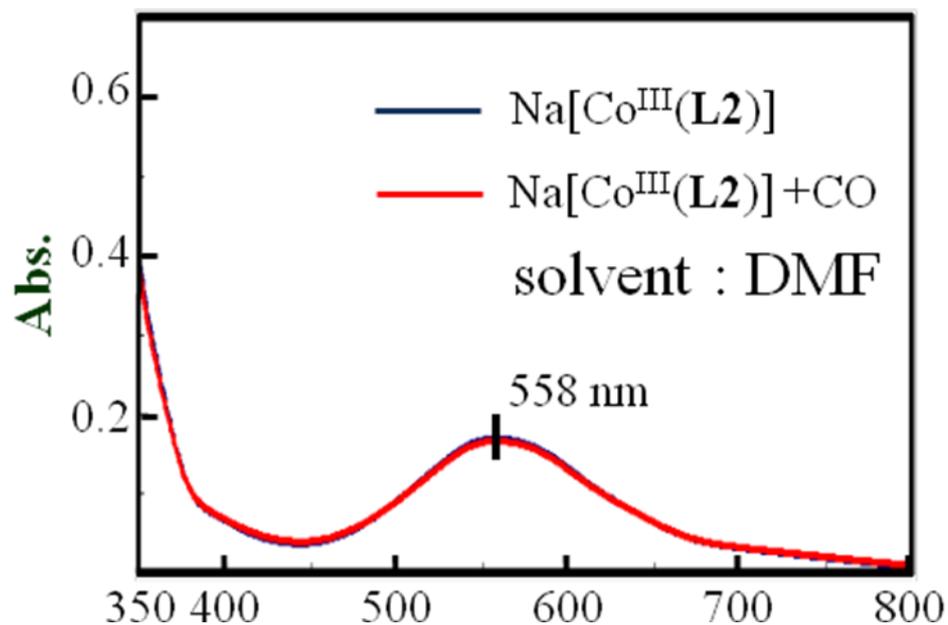


Figure S5b. Electronic absorption spectra of  $\text{Na}[\text{Co}^{\text{III}}(\text{L2})]$  (2) before (blue line) and after (red line) addition of CO in DMF.

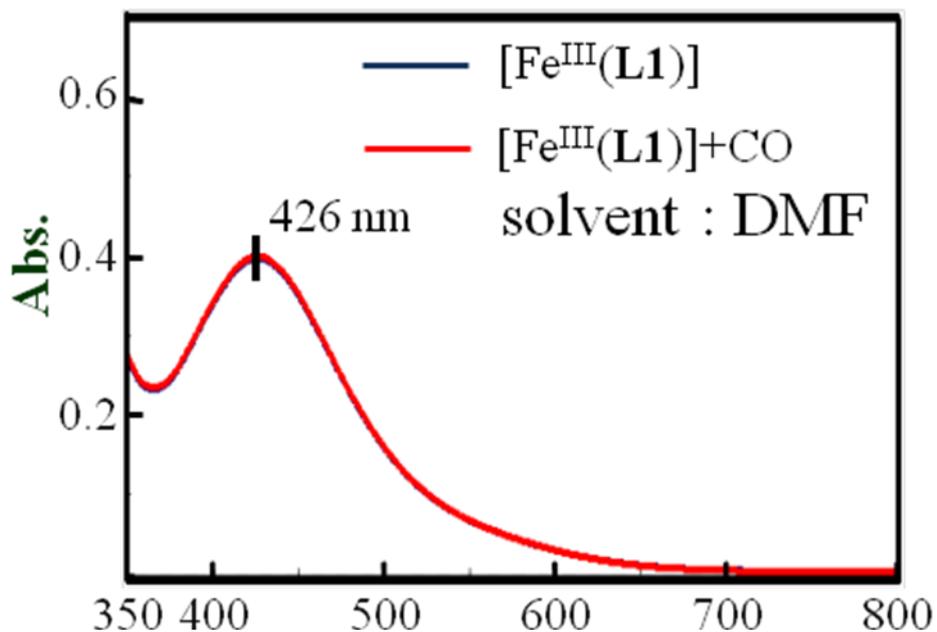


Figure S5c. Electronic absorption spectra of  $[\text{Fe}^{\text{III}}(\text{L1})]$  (**3**) before (blue line) and after (red line) addition of CO in DMF.

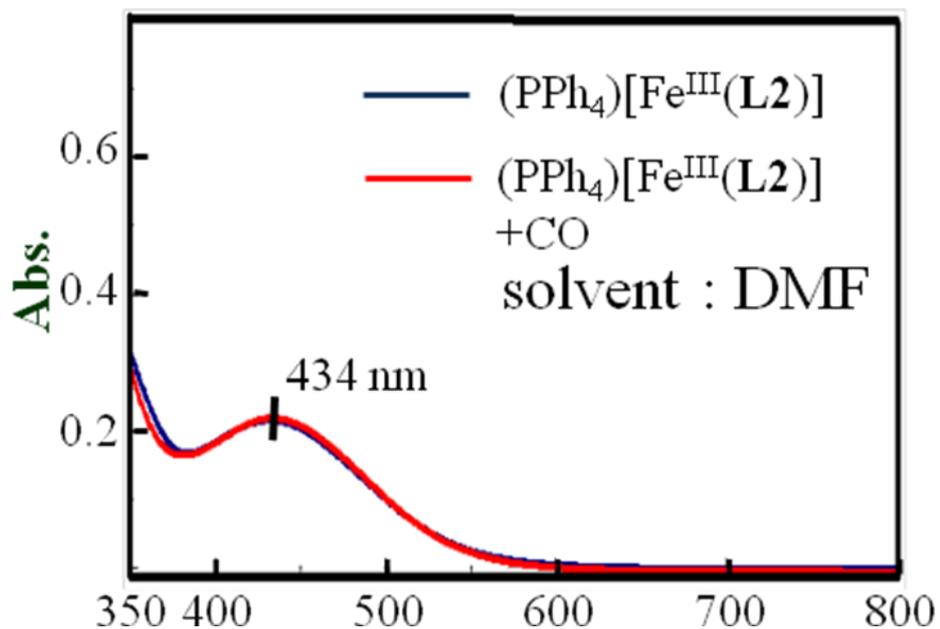


Figure S5d. Electronic absorption spectra of  $(\text{PPh}_4)[\text{Fe}^{\text{III}}(\text{L2})]$  (**4**) before (blue line) and after (red line) addition of CO in DMF.

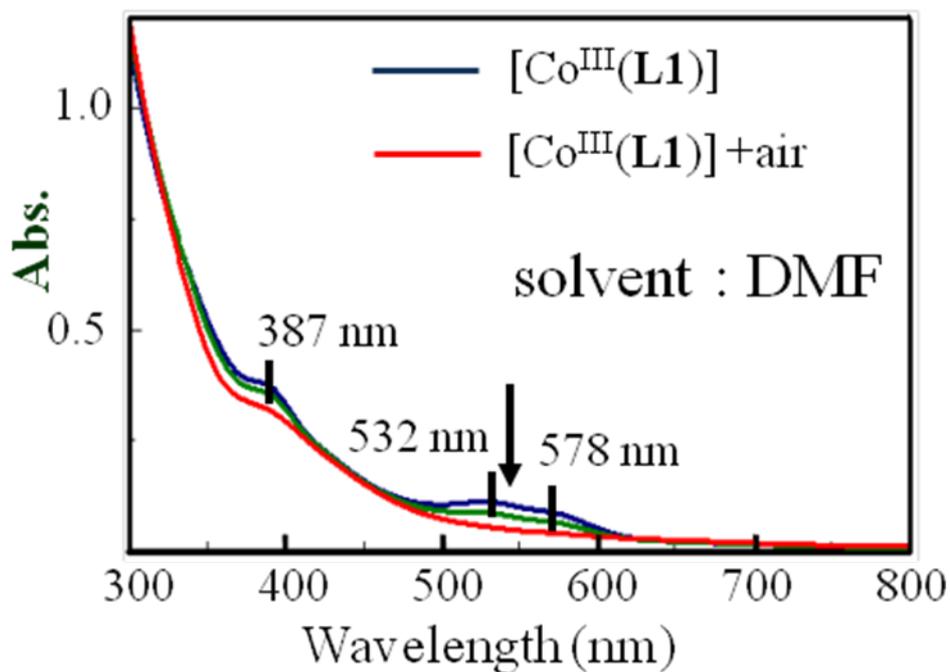


Figure S6a. Electronic absorption spectra of  $[\text{Co}^{\text{III}}(\text{L1})]$  (1) before (black line) and after (red line) exposed by air in DMF.

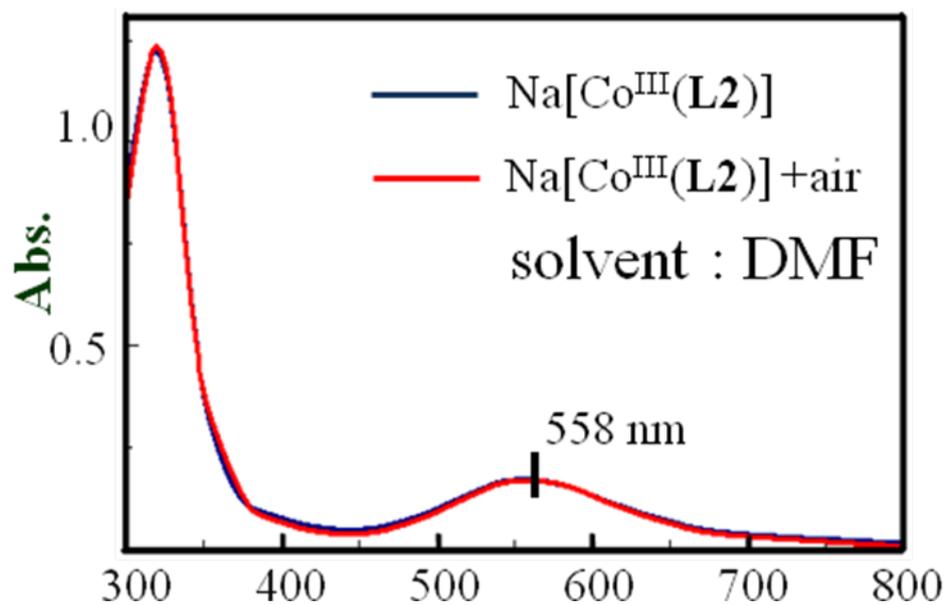


Figure S6b. Electronic absorption spectra of  $\text{Na}[\text{Co}^{\text{III}}(\text{L2})]$  (2) before (black line) and after (red line) exposed by air in DMF.

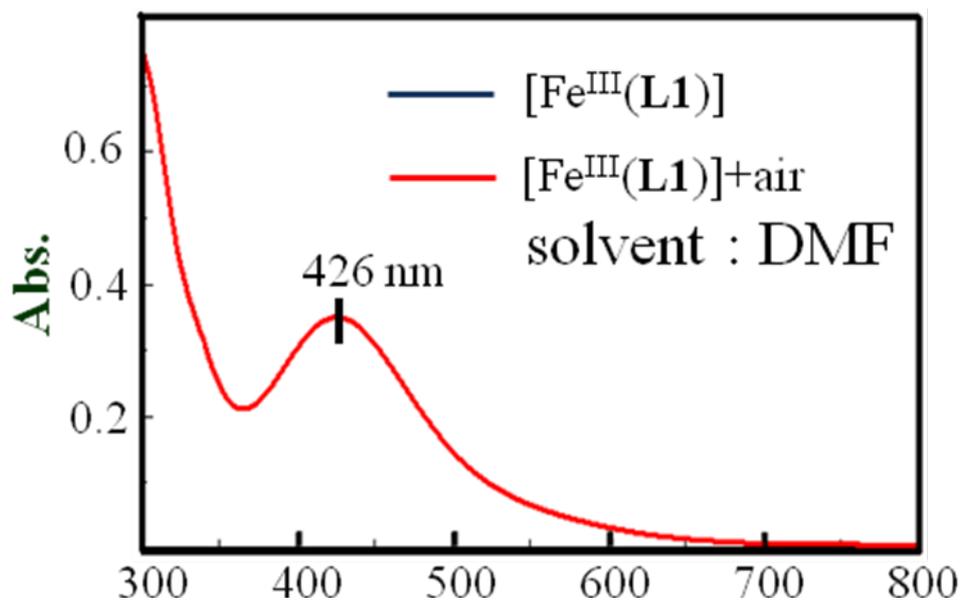


Figure S6c. Electronic absorption spectra of [Fe<sup>III</sup>(L1)] (**3**) before (black line) and after (red line) exposed by air in DMF.

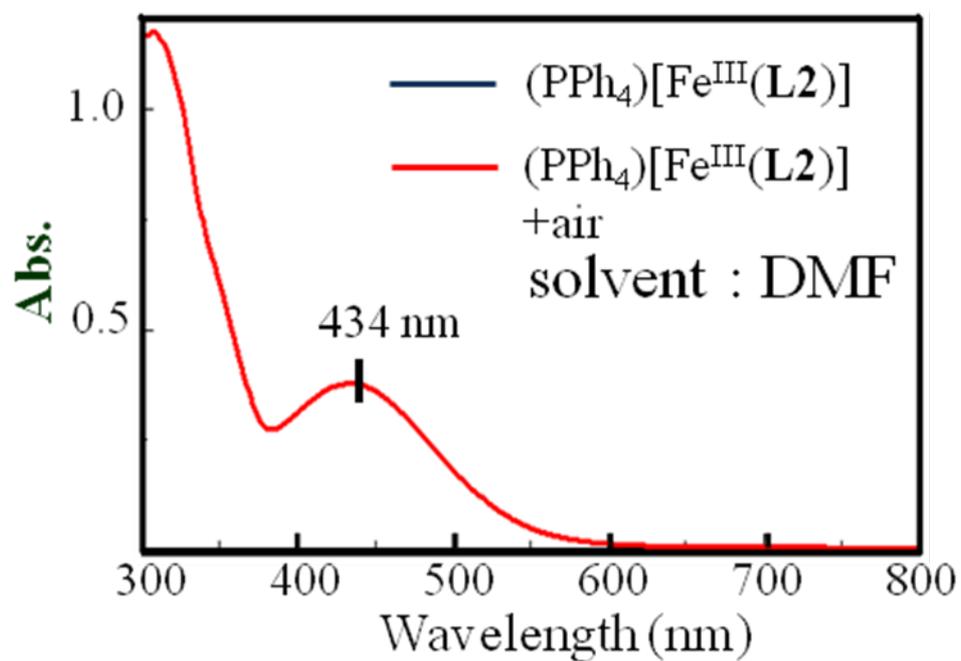


Figure S6d. Electronic absorption spectra of (PPh<sub>4</sub>)[Fe<sup>III</sup>(L2)] (**4**) before (black line) and after (red line) exposed by air in DMF.

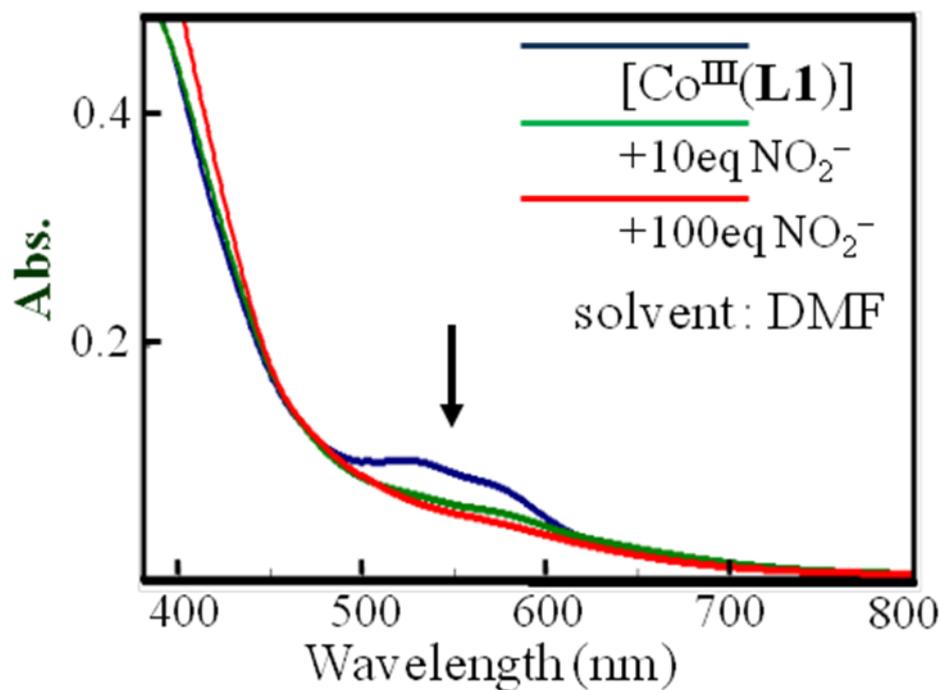


Figure S7a. Electronic absorption spectra of  $[\text{Co}^{\text{III}}(\text{L1})]$  (1) before (blue line) and after introduction of  $\text{NaNO}_2$ , 10 eq (green line) and 100 eq (red line), respectively in DMF.

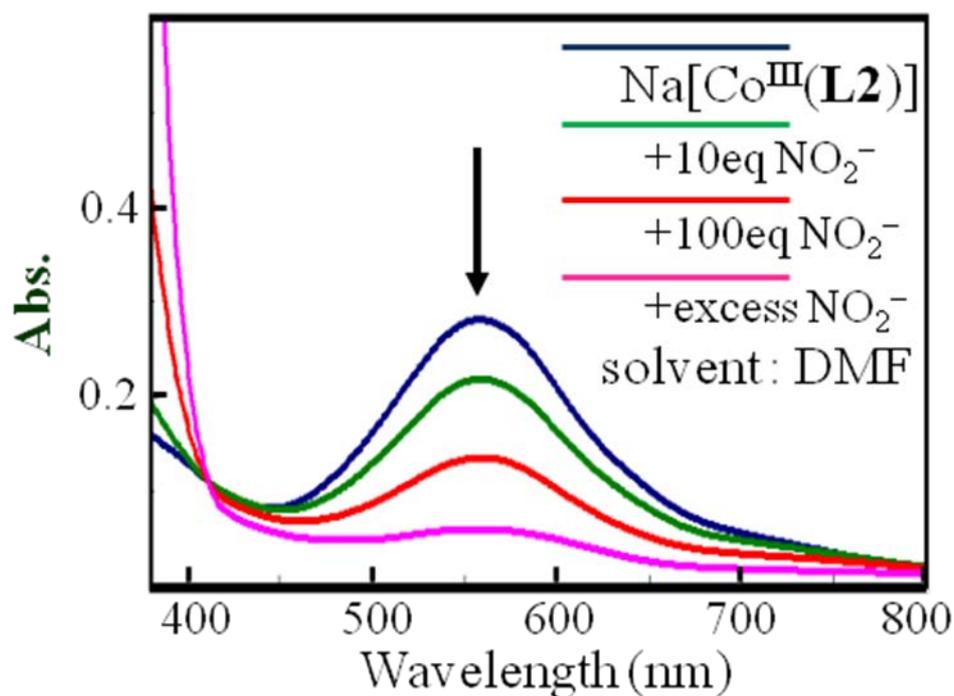


Figure S7b. Electronic absorption spectral of  $\text{Na}[\text{Co}^{\text{III}}(\text{L2})]$  (2) before (blue line) and after introduction of  $\text{NaNO}_2$ , 10 eq (green line), 100 eq (red line) and excess amount (pink line), respectively in DMF.

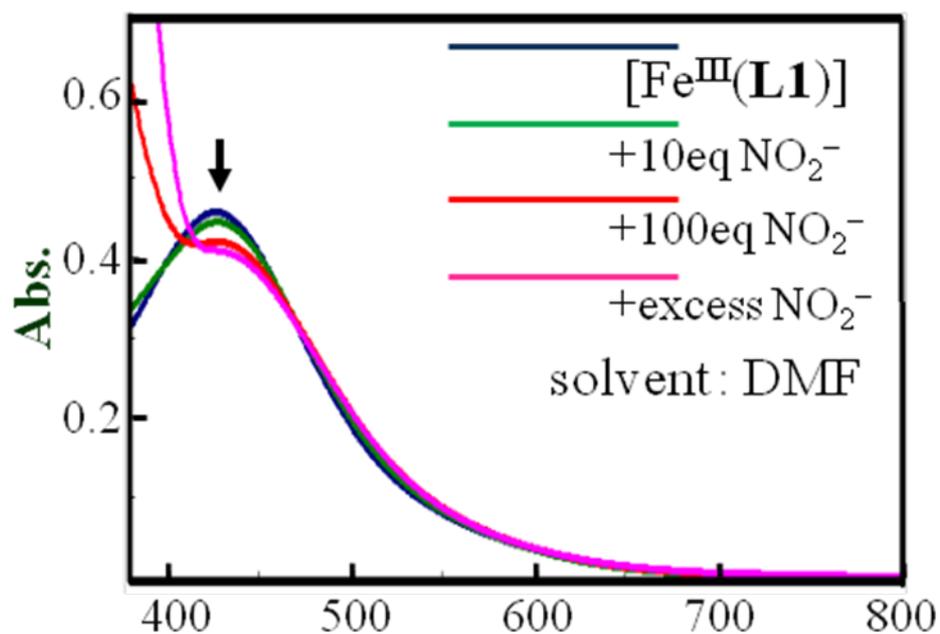


Figure S7c. Electronic absorption spectra of  $[\text{Fe}^{\text{III}}(\text{L1})]$  (3) before (blue line) and after introduction of  $\text{NaNO}_2$ , 10 eq (green line), 100 eq (red line) and excess amount (pink line), respectively in DMF.

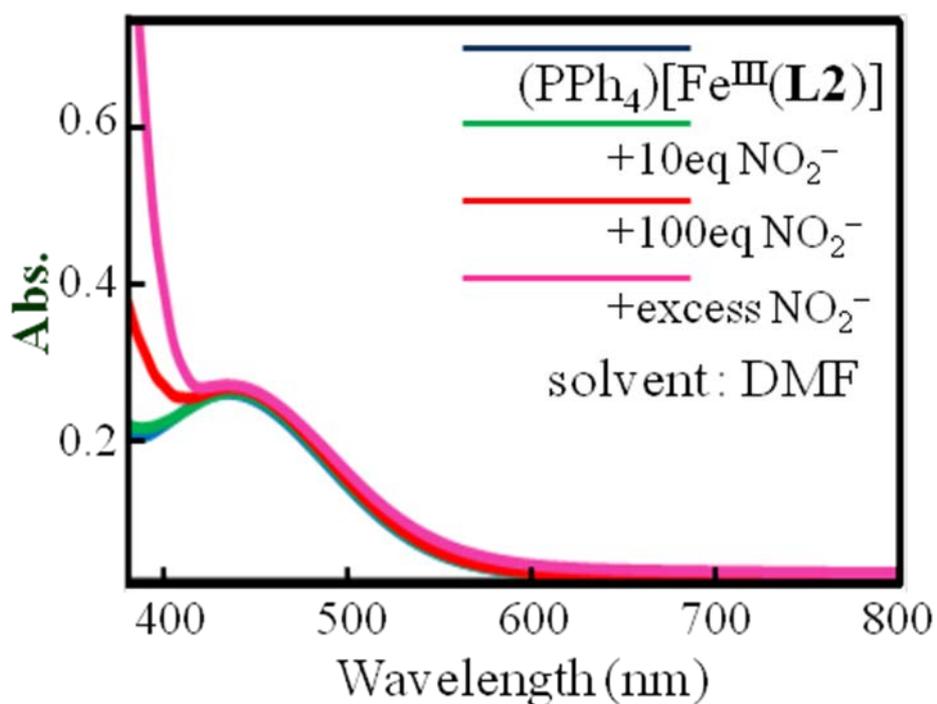


Figure S7d. Electronic absorption spectra of  $(\text{PPh}_4)[\text{Fe}^{\text{III}}(\text{L2})]$  (4) before (blue line) and after introduction of  $\text{NaNO}_2$ , 10 eq (green line), 100 eq (red line) and excess amount (pink line), respectively in DMF.

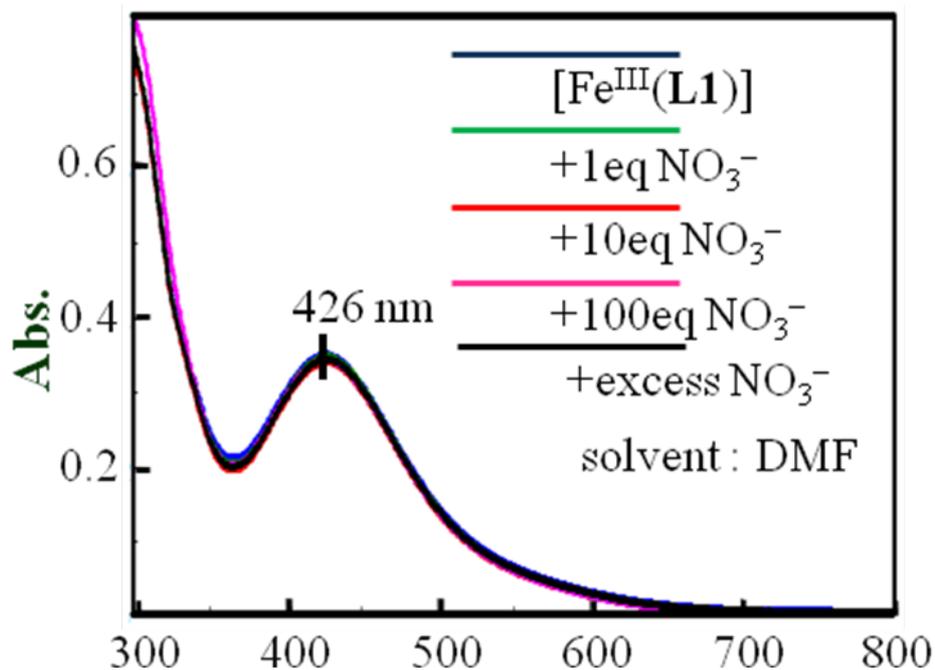


Figure S8a. Electronic absorption spectra of  $[\text{Fe}^{\text{III}}(\text{L1})]$  (**3**) before (blue line) and after introduction of  $\text{NaNO}_3$ , 1 eq (green line), 10 eq (red line), 100 eq (pink line) and excess amount (black line), respectively in DMF.

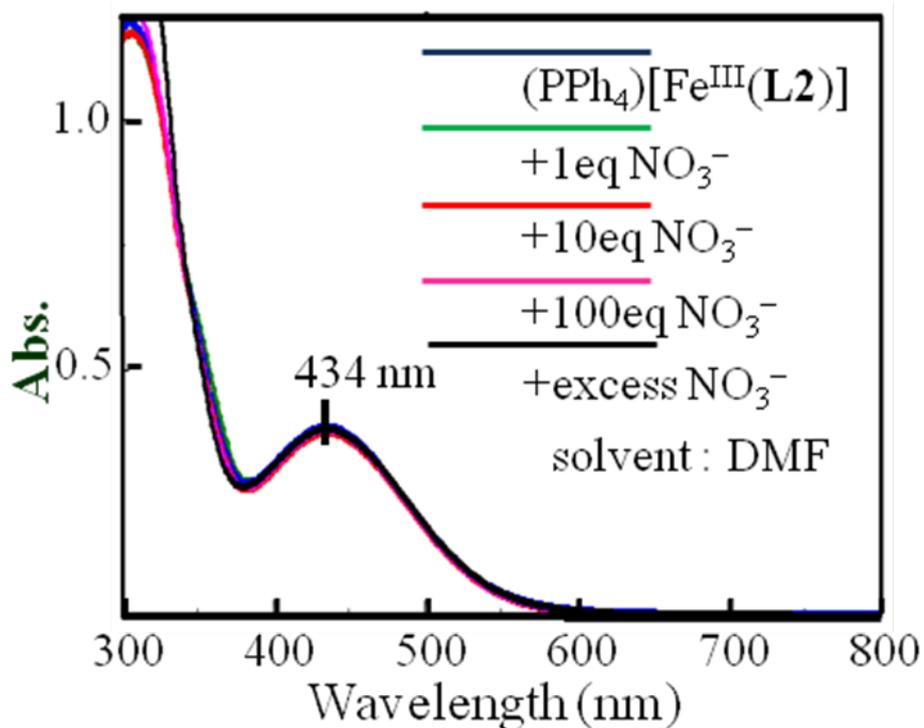


Figure S8b. Electronic absorption spectra of  $(\text{PPh}_4)[\text{Fe}^{\text{III}}(\text{L2})]$  (**4**) before (blue line) and after introduction of  $\text{NaNO}_3$ , 1 eq (green line), 10 eq (red line), 100 eq (pink line) and excess amount (black line), respectively in DMF.