Supplementary Materials

for

Effects of temperature, axial ligand, and photoexcitation on the structure and spin-state of nickel(II) complexes with water-soluble 5,10,15,20-tetrakis(1-methylpyridinium-4-yl)porphyrin

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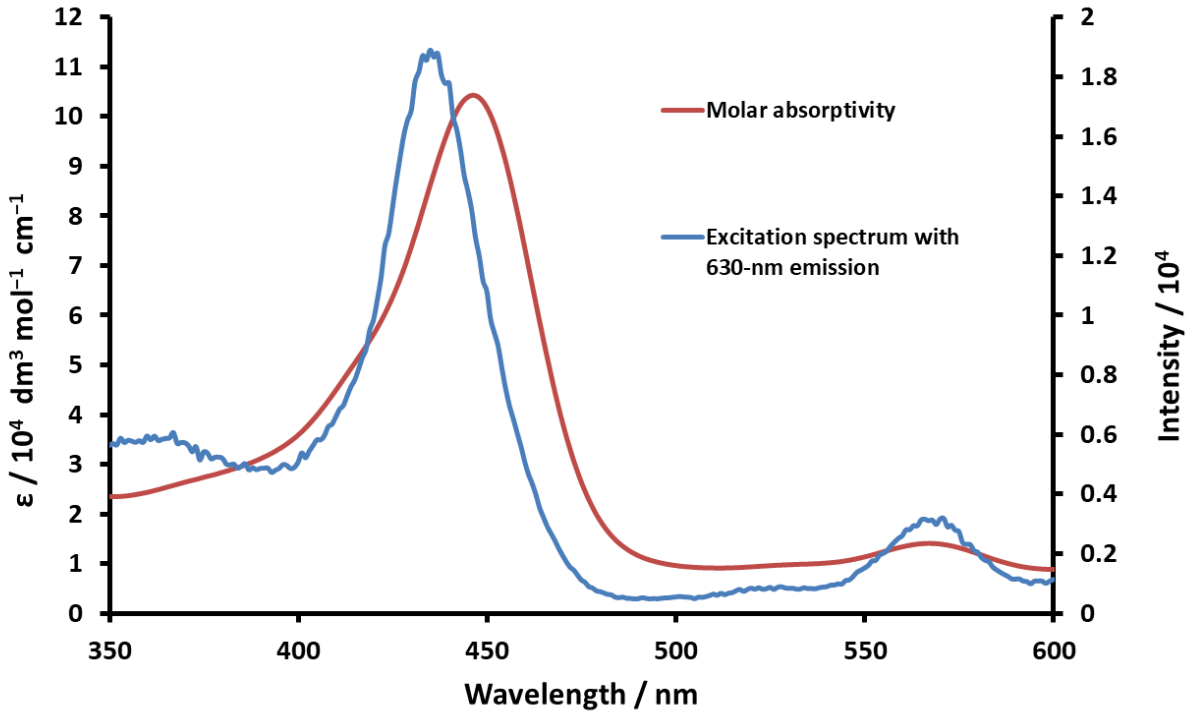


Figure S1. Excitation and absorption spectra of the high-spin complex (in NH_3 solution).

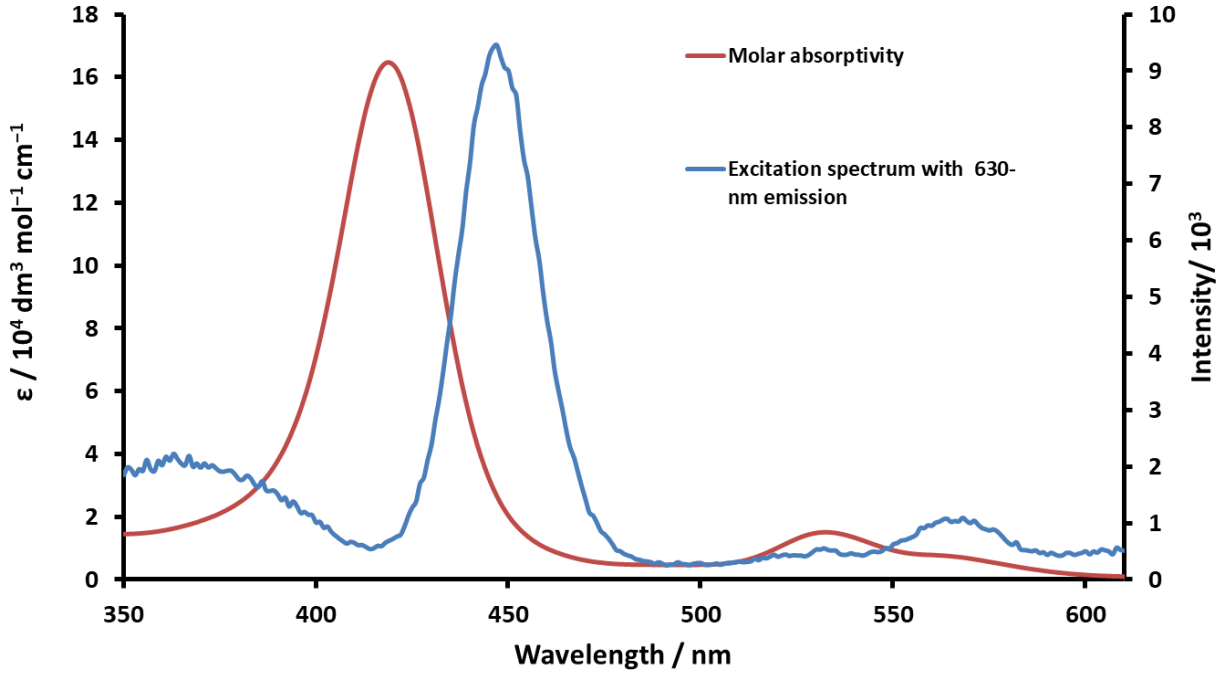


Figure S2. Excitation and absorption spectra of the low-spin complex (in n-propanol system).

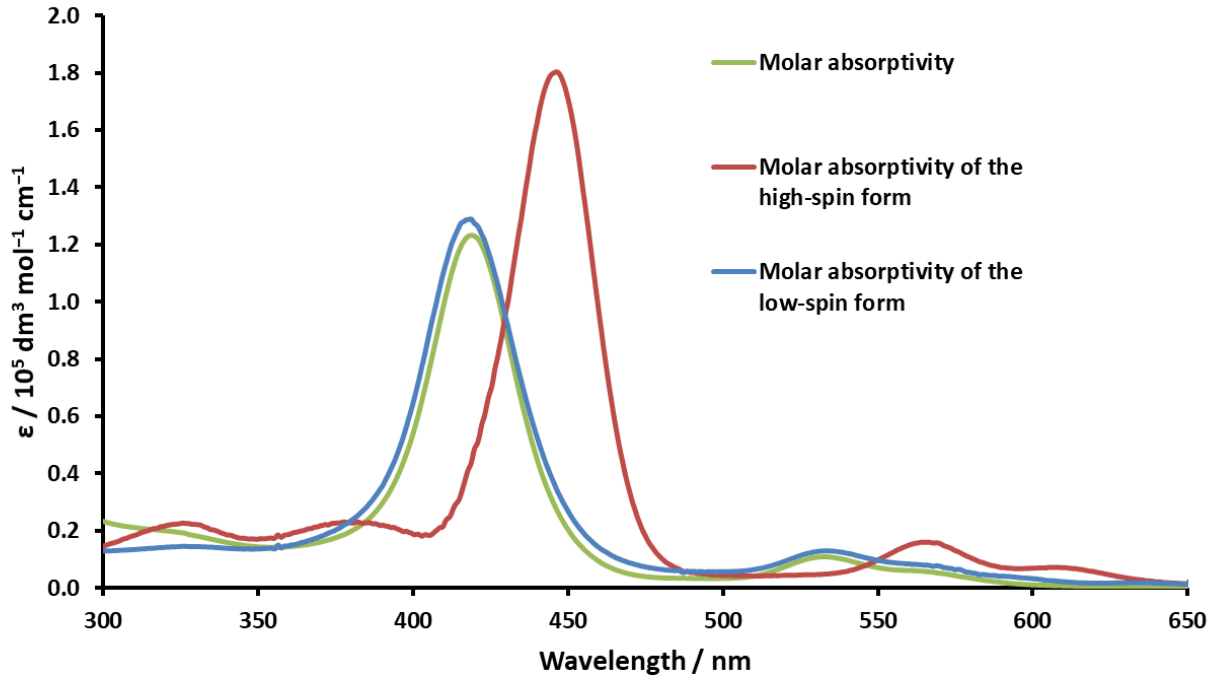


Figure S3. Molar absorptivity spectra estimated for calculating the TEOA—Ni(II)-$TMPyP^{4+}$ interaction.

Text S1

Formulas used for evaluations

1) Equation for the Gaussian curve (band):

$$A(\bar{\nu}) = \frac{A_{max}(\overline{\nu_0})}{exp\frac{(\bar{\nu} - \overline{\nu_0})^2}{2\sigma^2}} \quad (1)$$

where A(ν) is the absorbance (or intensity in the case of an emission spectrum) at the given wavenumber (ν) and its maximum (ν_0), respectively.

2) Oscillator strength:

$$f = (4.32 \times 10^{-9}\ \ Mcm^2)F \int \varepsilon(\omega)d\omega \quad (2)$$

where f is the oscillator strength, F=9n/(n^2+2)^2 is a factor dependent on the refractive index (n_{water} =1.33), $\varepsilon(\omega)$ is the molar absorptivity ($M^{-1}cm^{-1}$) at ω wavenumber.

3) Half-width (of a band):

$$w\,1/2 = \Delta\ = 2 \times 1.18\ \ \sigma \quad (3)$$

where σ is the standard deviation parameter of the Gaussian curve, and $\omega_{1/2}$ is its half-width.