Electronic Supplementary Information for

A Symmetric Organic - Based Nonaqueous Redox Flow Battery and Its State of Charge Diagnostics by FTIR

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**Figure S1.** PTIO solubility measurements in MeCN: (a) photographs of a series of PTIO solutions in MeCN at different concentrations of 1 mM, 3 mM, 10 mM, 100 mM, 500 mM, 1.0 M, 2.0 M, and oversaturated; (b) photographic comparison of the 1000-fold diluted supernatant from the oversaturated PTIO solution with other PTIO solutions, with the former closest to the 3 mM one; (c) the UV-vis spectrum of the 5 mM PTIO solution in MeCN showing that PTIO has strong absorption, which explains the similarly deep-blue solution color at ≥0.1 M PTIO.
Figure S2. Expanded view of the redox peaks in the repeated CV scans of PTIO (Figure 1a), showing respective CV curves of the 5\textsuperscript{th}, 100\textsuperscript{th}, 300\textsuperscript{th} and 500\textsuperscript{th} cycles.

Figure S3. The voltage curves of the PTIO flow cells using (a) 0.1 M PTIO; and (b) 0.5 M PTIO; (c) cycling efficiency and capacity of the 0.1 M PTIO flow cell for 100 cycles. The supporting electrolyte was 1.0 M TBAPF\textsubscript{6} in MeCN. The current density was 20 mA cm\textsuperscript{-2}. 
Figure S4. Full range FTIR spectra of the PTIO electrolyte systems: (a) MeCN, 1.0 M TBAPF$_6$/MeCN, and 0.5 M PTIO in 1.0 M TBAPF$_6$/MeCN; (b) 0.5 M PTIO and charge species (PTIO$^+$ and PTIO$^-$) in 1.0 M TBAPF$_6$/MeCN.

Figure S5. The FTIR spectra of the TBAPF$_6$ salt (charge carrier) at 0, 0.5 M, and 1.0 M concentrations in the range of 1400-1000 cm$^{-1}$. Dark yellow: MeCN; Blue: 0.5 M TBAPF$_6$/MeCN; Red: 1.0 M TBAPF$_6$/MeCN.
Figure S6. The FTIR spectra of the samples #0-4: (a) from the catholyte side; and (b) from the anolyte side.
**Scheme S1. Derivation of the linear relationship between the transmittance (T) and [PTIO].**

The real transmittance ($T_{\text{real}}$) and the concentration ([PTIO]) of PTIO satisfy the Beer-Lambert Law (Equation S1):

$$-\log(T_{\text{real}}) = \varepsilon b[PTIO]$$ (S1)

where $\varepsilon$ is the absorptivity coefficient and $b$ is the path length. Because the supporting electrolyte of 1.0 M TBAPF$_6$/MeCN is the spectral background, the $T_{\text{real}}$ of PTIO can be calculated by the nominal transmittance ($T$) divided by the electrolyte background transmittance ($T_0$) in the FTIR spectra (Equation S2).

$$T_{\text{real}} = \frac{T}{T_0}$$ (S2)

Thus, from Equations S1 and S2, we can derive Equation 1 in the main text:

$$-\log^{\text{nom}}(T) = \varepsilon b[PTIO] - \log^{\text{nom}}(T_0)$$ (1)