Supporting M3aterials

Portable Nitric Oxide (NO) Generator Based on Electrochemical Reduction of Nitrite for Potential Applications in Inhaled NO Therapy and Cardiopulmonary Bypass Surgery

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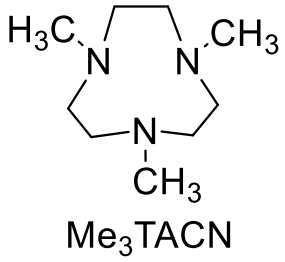
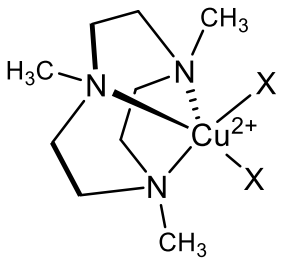
Physical Methods

UV-Vis absorbance spectra were measured using an Analytical Jena Specord 600 instrument at room temperature in 10 mm path length quartz cuvettes. FT-IR spectra where recorded on a Nicolet iS50 FT-IR equipped with a ZnSe Attenuated Total Reflectance (ATR) accessory. Electron paramagnetic resonance (EPR) spectra were recorded on a Bruker X-band EMX spectrometer equipped with a Varian liquid nitrogen cryostat set to 110K using a Bruker N_2 temperature controller. All EPR spectra were obtained of frozen samples in H_2O solutions containing 30% glycerol, at 20.51 mW microwave power, 9.297 GHz microwave frequency and 100 kHz field modulation with the amplitude set to 3 G.



Me$_3$TACN



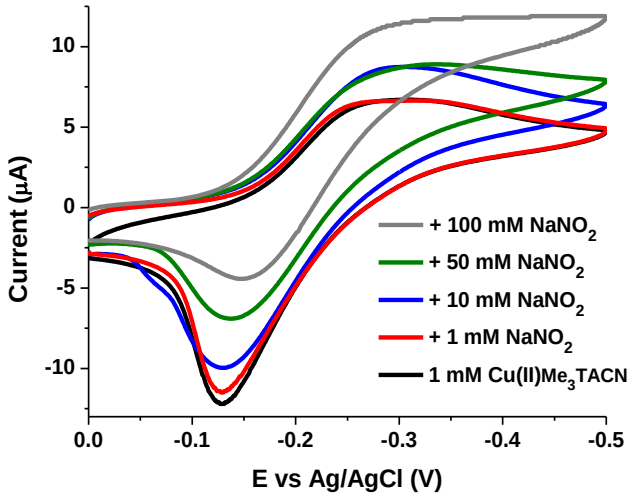


Figure S1. Upper: chemical structure of Me_3TACN ligand and $Cu(II)Me_3TACN(X)_2$ (X = H_2O, SO_4, or NO_2^-); lower: Cyclic voltamogram of 1 mM $Cu(II)Me_3TACN$ in 0.1 M HEPES buffer (pH 7.3) and 0.1 M NaCl in the presence of different concentrations of $NaNO_2$ by using a 2 mm diameter Pt disk working electrode.

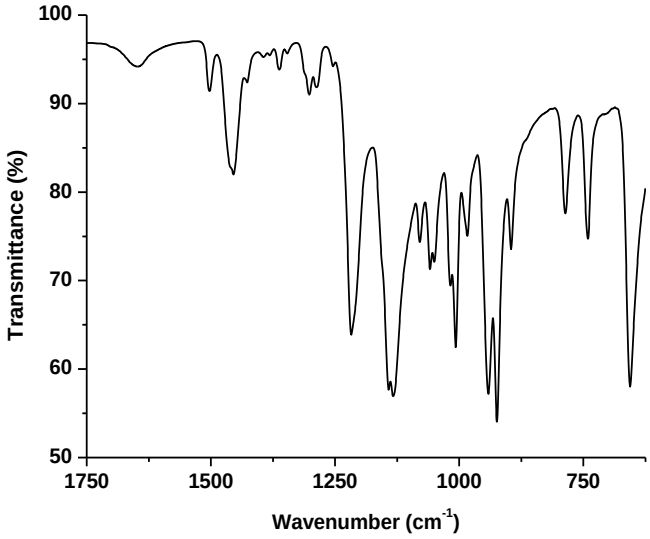


Figure S2. FT-IR (ATR) spectrum of the isolated $Cu(II)Me_3TACN$ solid.

Note: The isolated solid was treated as $[Cu(II)Me_3TACN(SO_4)]$ for concentration calculations, however it is suspected to exist as the dehydrate complex $[Cu(Me_3TACN)(H_2O)_2](SO_4)$ in aqueous media due to the similarity of the UV-Vis spectrum of the previously reported complex $[Cu(Me_3TACN)(H_2O)_2](ClO_4)_2$.[1]

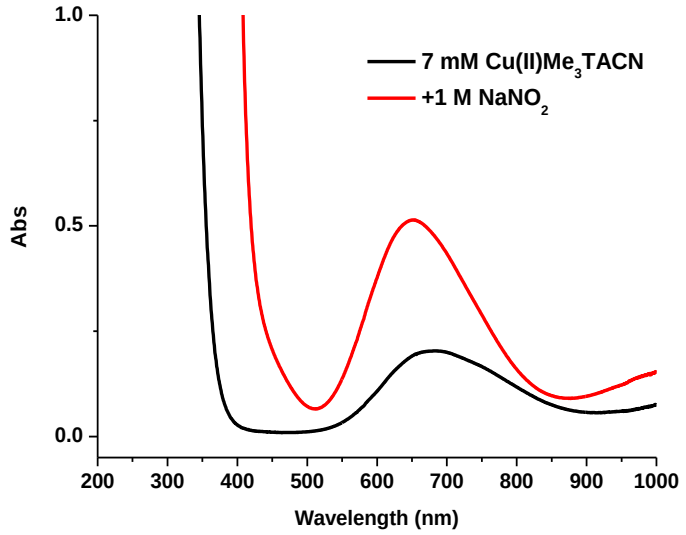


Figure S3. UV-Vis spectra of 7 mM Cu(II)Me_3TACN in H_2O (black), and 7 mM Cu(II)Me_3TACN + 1 M $NaNO_2$ (red).

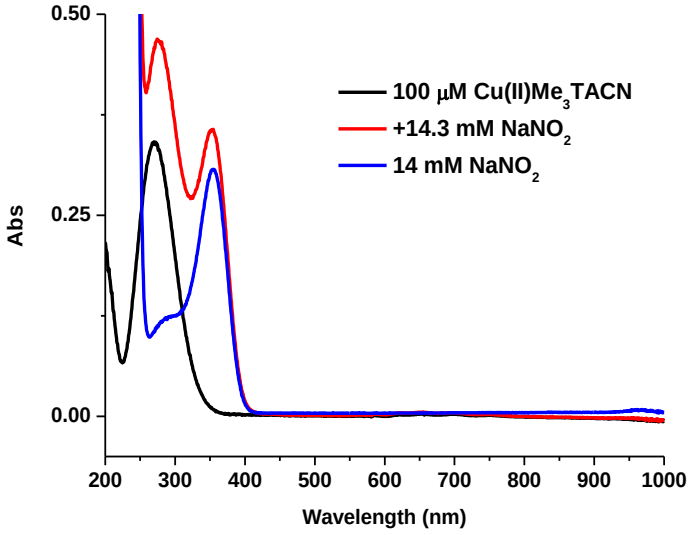


Figure S4. UV-Vis spectra of 100 μM Cu(II)Me_3TACN in H_2O (black), and 100 μM Cu(II)Me_3TACN + 14.3 mM $NaNO_2$ (red), and a solution of 14 mM $NaNO_2$ (blue).

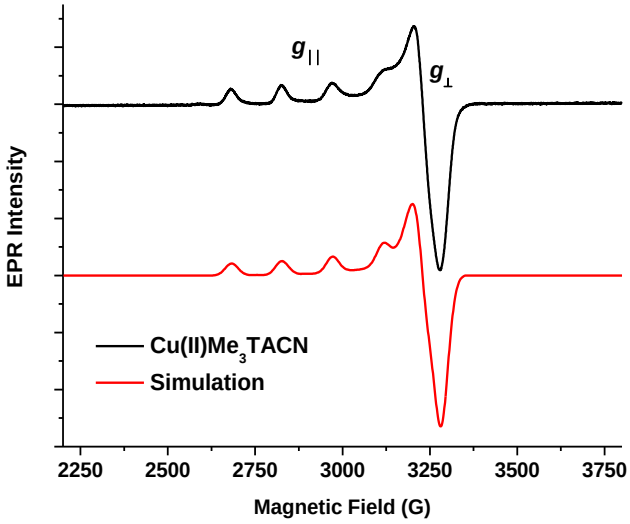


Figure S5. EPR spectrum of 1 mM Cu(II)Me_3TACN in a 30% glycerol/H_2O solution, recorded at 110 K (black). Simulation of the experimental spectrum (red) generated using SpinCount with the following parameters: $g_x = g_y = 2.055$, $g_z = 2.292$, $A_z = 463$ MHz, $sg_x = sg_y = 0.018$, $sg_z = 0.014$.

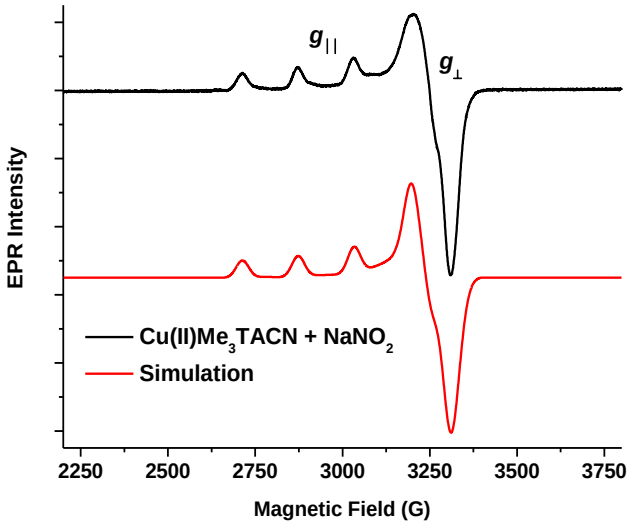


Figure S6. EPR spectrum of 1 mM Cu(II)Me_3TACN with 200 mM $NaNO_2$ in an 30% glycerol/H_2O solution, recorded at 110 K. Simulation of the experimental spectrum (red) generated using SpinCount with the following parameters: $g_x = g_y = 2.045$, $g_z = 2.25$, $A_z = 503$ MHz, $sg_x = sg_y = 0.0215$, $sg_z = 0.012$.

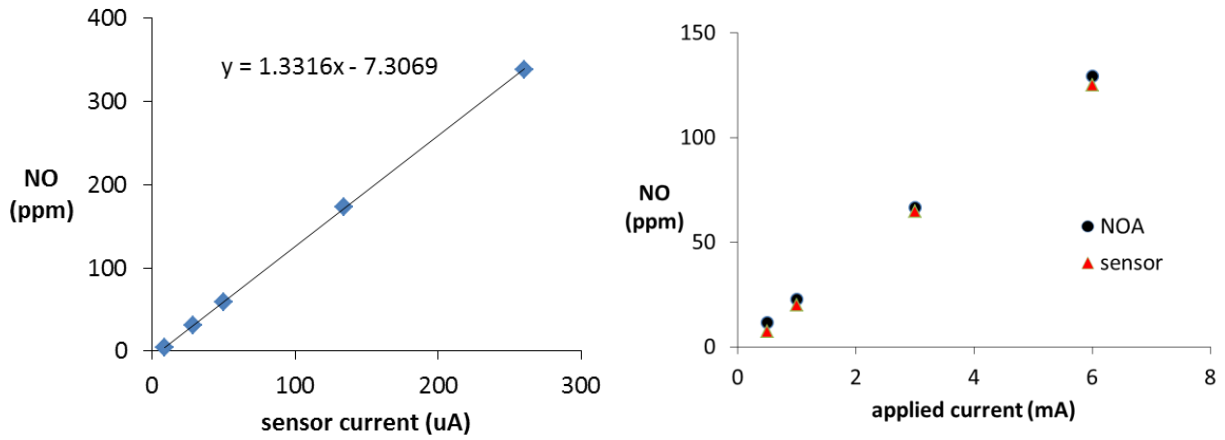


Figure S7. Left: calibration curve of amperometric NO sensor prepared in our lab. ; Right: comparison of NO levels at different applied currents measured simultaneously with NOA and the electrochemical NO sensor. The NO from the generator was split, and a gas stream of 0.2 L/min was delivered to NOA, while another stream of 0.05 L/min flowed over the surface of the sensor, with excess NO at the outlet of the sensor being scavenged by an activated carbon cartridge. The NO concentration from the sensor was calculated based on the sensor calibration curve on the left and the sensor currents.

Table 1 Potential difference between working and counter electrodes at different constant current in the two electrodes system (working electrode: 5 cm × 10 cm Au mesh; counter electrode: 5 cm × 5 cm Pt mesh)

Applied constant current (mA)	Potential difference (V)
5	-0.8
10	-0.9
20	-1.1
80	-1.3

References

1. Fiona H. F., Adam J. F., Matthew J. B., Leone S., and Joel B. Kinetics and Mechanism of Hydrolysis of a Model Phosphate Diester by $[Cu(Me_3tacn)(OH_2)_2]^{2+}$ (Me_3tacn = 1,4,7-Trimethyl-1,4,7-triazacyclononane). *Inorg. Chem.* **2005** *44* (4), 941-950.