15-8245 • 2,6-DPPEAQ

METALS • INORGANICS • ORGANOMETALLICS • CATALYSTS • LIGANDS • NANOMATERIALS • CUSTOM SYNTHESIS • cGMP FACILITIES

U.S. Patents: 62/628,599, 62/740,526. Patent Application: PCT/US19/17479.
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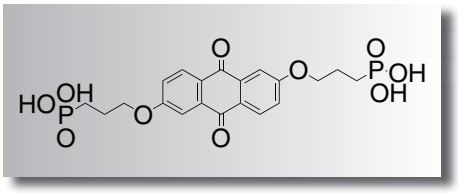
15-8245 • (((9,10-Dioxo-9,10-dihydroanthracene-2,6-diyl)bis(oxy))bis(propane-3,1-diyl))bis(phosphonic acid), 98%, 2,6-DPPEAQ



A highly stable phosphonate-functionalized anthraquinone used as a redox-active material in a negative potential electrolyte (negolyte) for aqueous redox flow batteries operating at nearly neutral pH.[1,2]

By pairing item **15-8245** with a potassium ferri/ferrocyanide positive electrolyte across an inexpensive, nonfluorinated permselective polymer membrane, this near-neutral quinone flow battery exhibits an open-circuit voltage of 1.0 V and a capacity fade rate of 0.00036% per cycle and 0.014% per day, which is the lowest ever reported for any flow battery in the absence of rebalancing processes. It is further demonstrated that the negolyte pH drifts upward upon atmospheric oxygen penetration but, when oxygen is excluded, oscillates reversibly between 9 and 12 during cycling. These results enhance the suitability of aqueous-soluble redox-active organics for use in large-scale energy storage, potentially enabling massive penetration of intermittent renewable electricity.

Based on cyclic voltammetry (CV), **2,6-DPPEAQ** exhibits a reversible redox peak at -0.47 V versus a standard hydrogen electrode (SHE) (E1/2) in pH 9 unbuffered aqueous solution and at -0.49 V versus SHE (E1/2) in pH 12 unbuffered aqueous solution (Figure 1A)

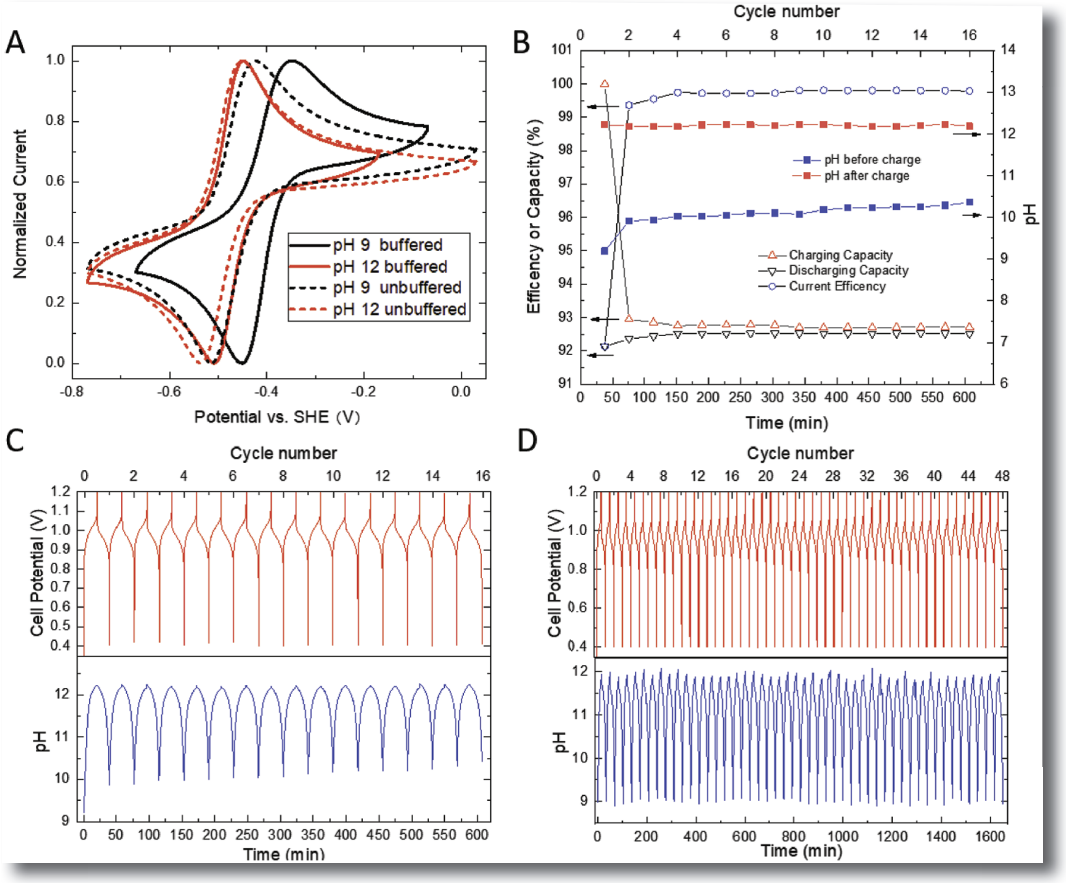


Figure 1

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Figure 1 (**A**) Cyclic voltammograms of 1 mM **2,6-DPPEAQ** at pH 9 buffered solution (black solid), pH 12 buffered solution (red solid), pH 9 unbuffered solution (black dash), and pH 12 unbuffered solution (red dash) at a scan rate of 100 mV s−1 on a glassy carbon working electrode.

(**B**) Galvanostatic cycling of the **2,6-DPPEAQ** cell at 20 mA cm−2 for 16 consecutive cycles in a glove bag. Electrolytes comprised 6.5 mL 0.1 M of the tetra-potassium salt of **2,6-DPPEAQ** (negolyte) in 1 M KCl solution at pH 9 and 40 mL 0.1 M potassium ferrocyanide and 0.01 M potassium ferricyanide (posolyte) in 1 M KCl solution at pH 9. The pH probe was immersed in the negolyte to monitor the pH of the solution. Charge/discharge capacity, CE, and pH of the negolyte before and after charging are plotted as functions of the cycle number.

(**C**) Representative curves of cell potential and negolyte pH versus time.

(**D**) Representative curves of cell potential and negolyte pH versus time for the experiment depicted in (**B**) and (**C**) repeated in a glove box instead of a glove bag.

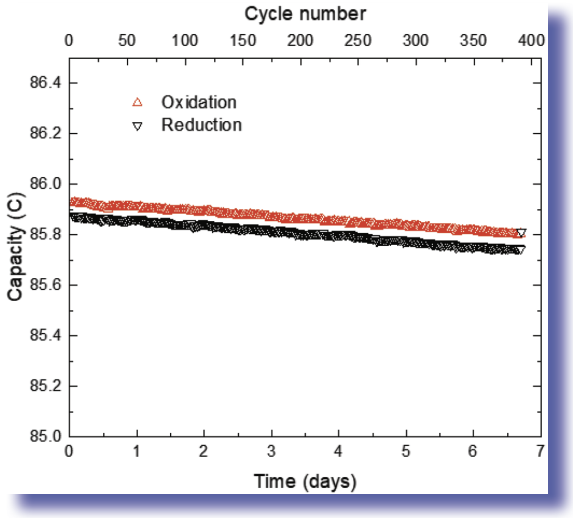

Figure 2

Unbalanced compositionally symmetric cell cycling of 0.1 m of the tetra-potassium salt of 2,6-DPPEAQ at pH 13, showing capacity as a function of time. Capacities were obtained by full potentiostatic reduction and oxidation of the capacity-limiting side at +-0.2 V.

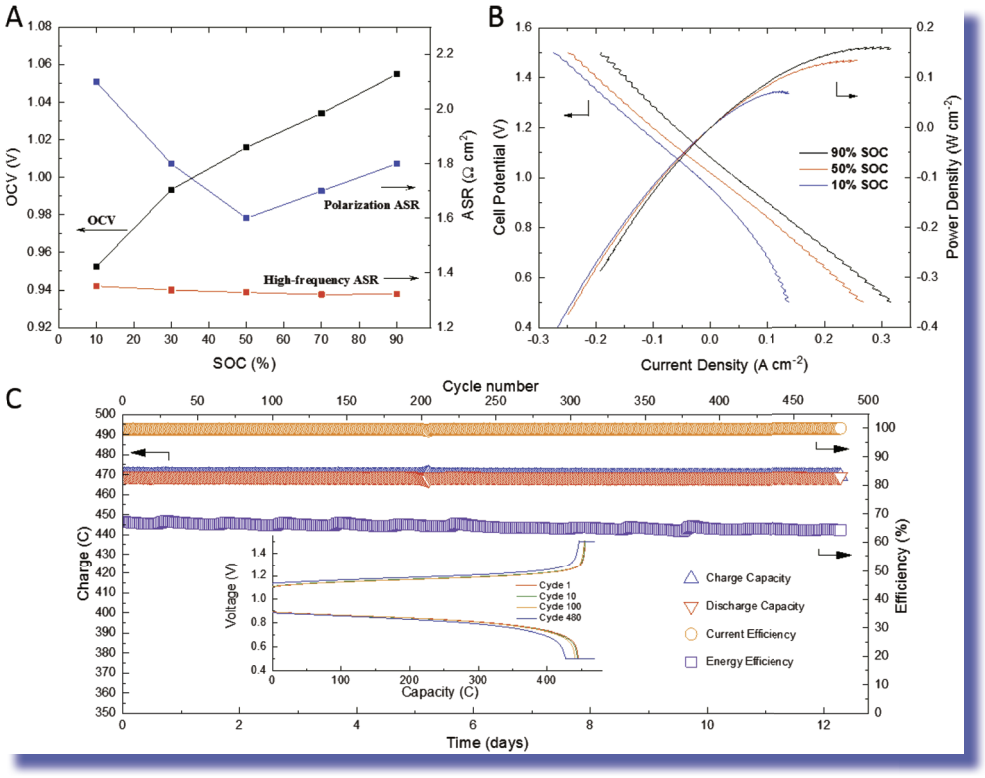

Figure 3

(A) Full cell OCV, high-frequency and polarization ASR versus SOC at room temperature at 10, 30, 50, 70, and 90% SOC. Electrolytes comprised 5 mL 0.5 M of the tetra-potassium salt of **2,6-DPPEAQ** (negolyte) at pH 9 and 80 mL 0.4 M potassium ferrocyanide and 0.1 M potassium ferricyanide (posolyte) at pH 9.

(B) Cell potential and power density versus current density.

(C) CE (circles), energy efficiency (squares), charge (upwardpointing triangles) capacity, and discharge (downward-pointing triangles) capacity versus time and cycle number. The cell was cycled galvanostatically at 100 mA cm−2 between 1.5 and 0.5 V, and each half-cycle ended with a potentiostatic hold until the magnitude of the current density fell below 2 mA cm−2. The supply of nitrogen to the glove bag ran out near cycle 202 and was replaced near cycle 211. Inset: capacity versus cell voltage at the 1st, the10th, the 100th, and the 480th cycle.

Typical Lot Specific Characterization

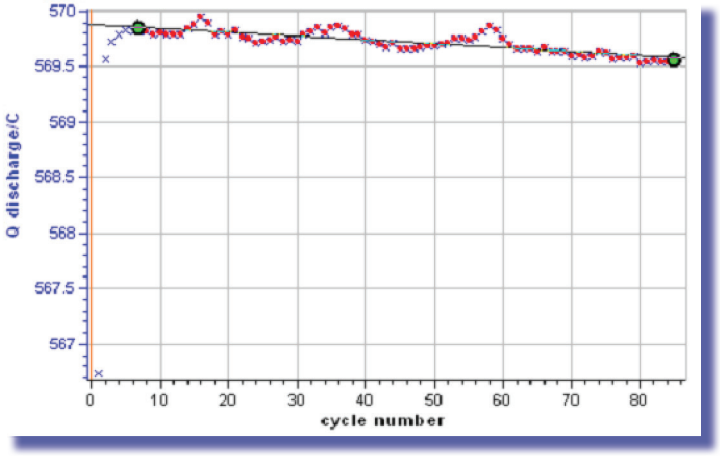

Figure 4

- Membrane: Nafion 115;
- Electrode: 2 layers Zoltek felt (0.63 mm) (800 um Viton gasket);
- Posolyte: 40 mL, 0.5 M K4Fe(CN)6, 0.05 M K3Fe(CN)6, pH=12 (KOH);
- Negolyte: 6 mL, 0.505 M STREM DPPEAQ, neutralized by KOH, pH=12;
- Flow field: IDFF, impregnated graphite;
- Flowrate: 48 mL/min, peristaltic pump;
- Temperature: 20°C;
- Atmosphere: UHP N2 glove bag;
- Charging/discharging cycling: 50 mA/cm2 till voltage cutoff reached (1.4 to 0.6 V), then hold at voltage until current density dropped to 2 mA/cm2.

References:

1. *Adv. Energy Mater.* **2019**, *9(12)*, 1900039.
2. *Joule* **2018**, *2(9)*, 1894–1906.

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