

## Supplementary Materials to

Article

# Evaluation of Electrochemical Stability of Sulfonated Anthraquinone-Based Acidic Electrolyte for Redox Flow Battery Application

Petr Mazúr <sup>1,2,\*</sup>, Jiří Charvát <sup>1</sup>, Jindřich Mrlík <sup>1</sup>, Jaromír Pociďč <sup>2</sup>, Jiří Akrman <sup>3</sup>, Lubomír Kubáč <sup>3</sup>, Barbora Řeháková <sup>4</sup> and Juraj Kosek <sup>1,2</sup>

<sup>1</sup> University of Chemistry and Technology, Prague, Technická 5, 166 28 Praha 6, Czech Republic; [mazurp@vscht.cz](mailto:mazurp@vscht.cz) (P.M.); [charvatj@vscht.cz](mailto:charvatj@vscht.cz) (J.C.); [mrlikj@vscht.cz](mailto:mrlikj@vscht.cz) (J.M.); [jkk@vscht.cz](mailto:jkk@vscht.cz) (J.K.)

<sup>2</sup> New Technologies—Research Centre, University of West Bohemia, Univerzitní 8, 306 14 Plzeň, Czech Republic; [pocidicj@ntc.zcu.cz](mailto:pocidicj@ntc.zcu.cz) (J.P.)

<sup>3</sup> Centre for Organic Chemistry, Rybitví 296, 533 54 Rybitví, Czech Republic; [jiri.akrman@cocltd.cz](mailto:jiri.akrman@cocltd.cz) (J.A.); [lubomir.kubac@cocltd.cz](mailto:lubomir.kubac@cocltd.cz) (L.K.)

<sup>4</sup> Synthesia, a.s., Semtín 103, 530 02 Pardubice, Czech Republic; [Barbora.Rehakova@synthesia.cz](mailto:Barbora.Rehakova@synthesia.cz) (B.Ř.)

\* Correspondence: [mazurp@vscht.cz](mailto:mazurp@vscht.cz)

## List of content

Figure S1: HPLC chromatogram of anthraquinone sulfonation mixture after synthesis.

Figure S2: UV-vis spectrum of initial electrolyte and electrolyte after electrochemical test, both samples diluted 50 000 times by demineralized water, measured in cuvette with the optical length of 1 cm.

Figure S3: Equivalent circuit used for evaluation of EIS spectra of RFB full-cell consisting of: R1 – ohmic resistance of the cell, R2 and R3 – charge transfer resistance of both electrodes, Q2 and Q3 – constant phase elements representing electrode-electrolyte interface on both interfaces.

Table S1: Composition of the AQDS negolyte before and after electrochemical test in the redox flow battery obtained by HPLC

Table S2: Composition of AQDS electrolyte after 5 days in different SOC and temperatures

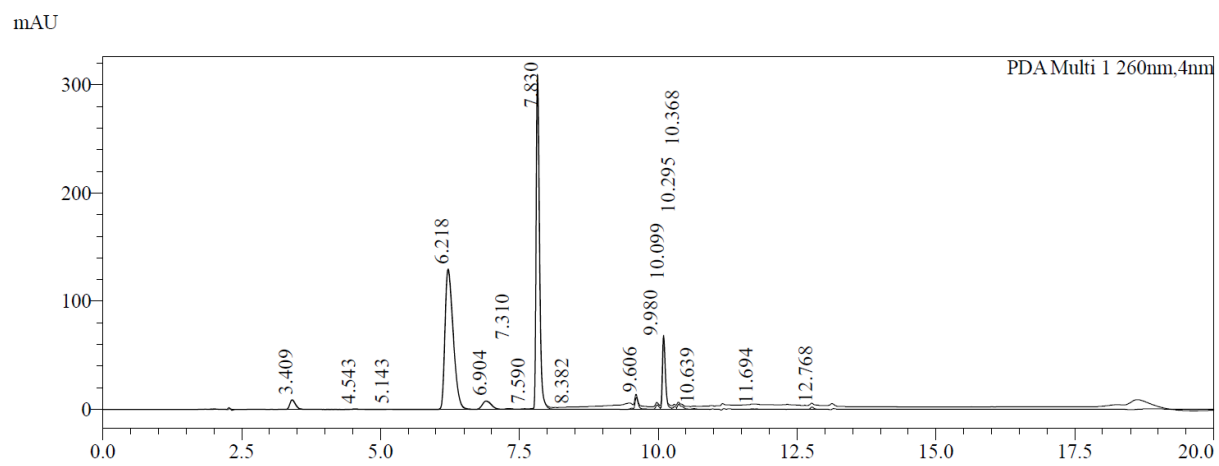


Figure S1: HPLC chromatogram of anthraquinone sulfonation mixture after synthesis.

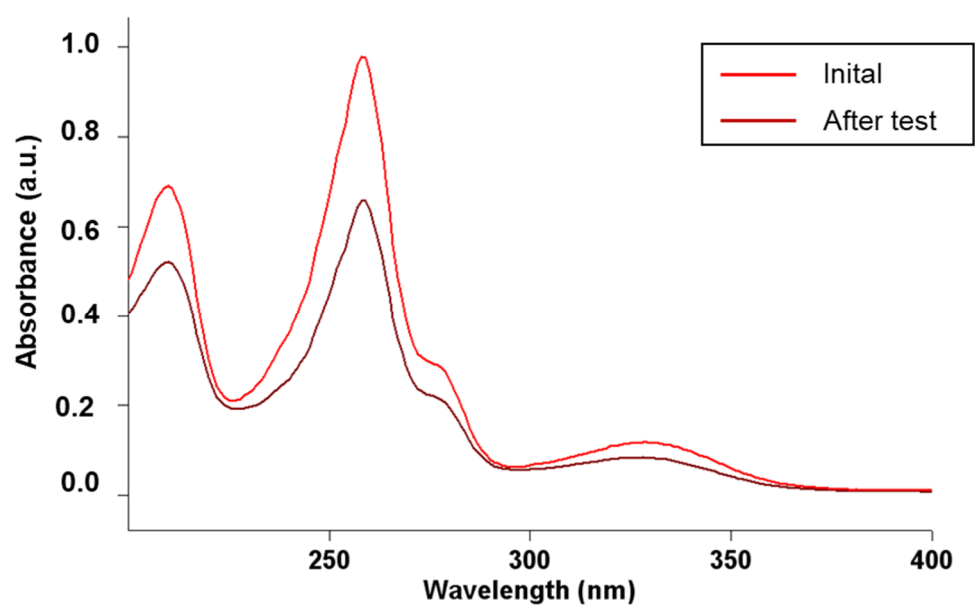


Figure S2: UV-vis spectrum of initial electrolyte and electrolyte after electrochemical test, both samples diluted 50 000 times by demineralized water, measured in cuvette with the optical length of 1 cm.

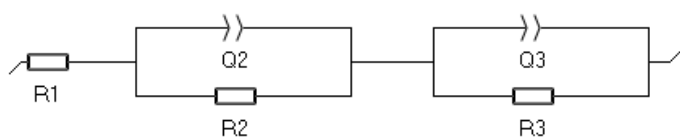


Figure S3: Equivalent circuit used for evaluation of EIS spectra of RFB full-cell consisting of: R1 – ohmic resistance of the cell, R2 and R3 – charge transfer resistance of both electrodes, Q2 and Q3 – constant phase elements representing electrode-electrolyte interface on both interfaces.

Table S1: Composition of the AQDS negolyte before and after electrochemical test in the redox flow battery obtained by HPLC

Compound	Retention time	Initial electrolyte	Electrolyte after test
	(min)	(area %)	(area %)
anthraquinone-1,7-disulfonic acid	3.4	2.1	2.0
anthraquinone-2,6-disulfonic acid	6.2	41.9	44.1
anthraquinone-1,6-disulfonic acid	6.9	2.8	3.0
unknown compound - 1	7.3	0.2	0.3
anthraquinone-2,7-disulfonic acid	7.8	41.0	43.0
unknown compound - 2	9	0.0	0.4
unknown compound - 3	9.4	0.0	0.3
anthraquinone-1-sulfonic acid	9.6	1.5	0.3
2-hydroxyanthraquinone-1-sulfonic acid	10.0	0.6	0.2
anthraquinone-2-sulfonic acid	10.1	7.7	3.2
unknown compound - 4	10.4	0.8	0.8

Table S2: Composition of AQDS electrolyte after 5 days in different SOC and temperatures

SoC / %	0	0	25	50	50	75	75	85	95	100	100
Temperature / °C	20	60	60	20	60	20	60	60	60	20	60
c AQDS <sup>(1)</sup> / mol dm <sup>-3</sup>	0.84	0.85	0.82	0.81	0.81	0.80	0.72	0.68	0.68	0.79	0.65
c H <sub>2</sub> SO <sub>4</sub> <sup>(2)</sup> / mol dm <sup>-3</sup>	1.14	1.36	1.03	1.04	1.09	1.06	1.27	1.31	1.17	1.02	1.16
c total sulphate / mol dm <sup>-3</sup>	2.82	3.06	2.67	2.66	2.71	2.66	2.71	2.67	2.53	2.60	2.46
	<b>Content <sup>(3)</sup> / Area %</b>										
anthraquinon-1,7-disulfonic acid	1.80	1.83	1.80	1.78	1.40	1.79	1.34	1.28	1.31	1.83	1.29
anthraquinon-2,6-disulfonic acid	39.15	39.30	41.28	39.20	40.11	39.54	41.70	42.14	43.95	41.49	43.96
anthraquinon-1,6-disulfonic acid	1.91	1.97	2.66	2.37	2.14	2.06	1.73	1.92	1.69	2.06	2.06
anthraquinon-2,7-disulfonic acid	43.37	43.22	42.49	42.85	43.39	43.00	44.10	44.73	45.66	44.67	45.85
anthraquinon-1-sulfonic acid	2.06	2.07	1.55	2.06	1.44	1.97	0.76	0.62	0.50	1.14	0.55
anthraquinon-2-sulfonic acid	11.72	11.61	10.22	11.74	11.53	11.65	10.38	9.31	6.90	8.82	6.30
2,6-AQDS / 2,7-AQDS / area % ratio	0.90	0.91	0.97	0.91	0.92	0.92	0.95	0.94	0.96	0.93	0.96
2,6- and 2,7-AQDS / area % ratio	0.83	0.83	0.84	0.82	0.83	0.83	0.86	0.87	0.90	0.86	0.90

<sup>(1)</sup>UV-vis spectrophotometry, <sup>(2)</sup>acido-basic titration by NaOH, <sup>(3)</sup>HPLC