Electronic Supplementary Information

Nitrogen-rich phenazine-fused hexaazatriphenylene cathode enables low-temperature potassium battery operation at -50 °C

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Table of contents

Table S1. Chemical analysis data for **TPHATP.**

Material	**C, %**	**H, %**	**N, %**	**O,%=100%-(C,%+H,%+N,%)**
Found for TPHATP	62.42	3.15	19.00	15.43
Calculated for $C_{42}H_{18}N_{12}$	73.04	2.63	24.34	0
Calculated for $C_{42}H_{18}N_{12}$•$6H_2O$	63.15	3.79	21.04	12.02

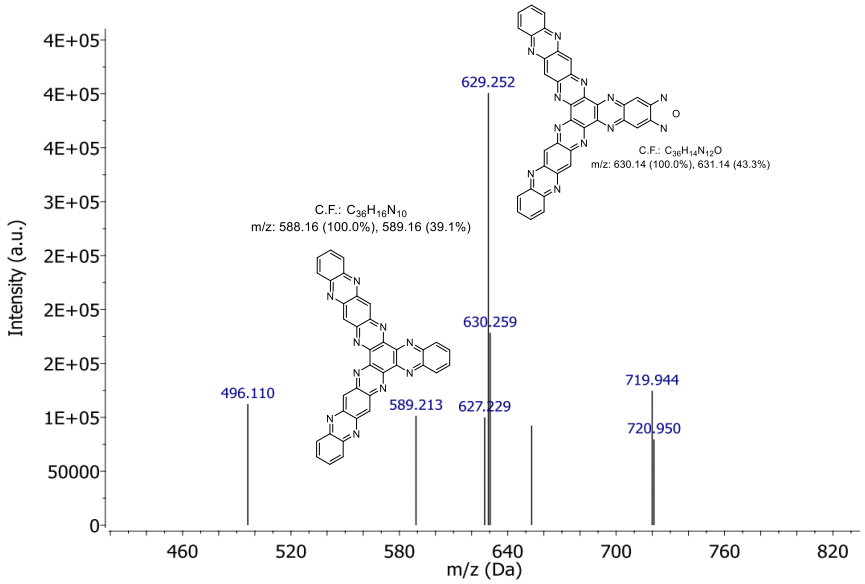


Figure S1. MALDI mass spectrum of **TPHATP** (negative ion mode).

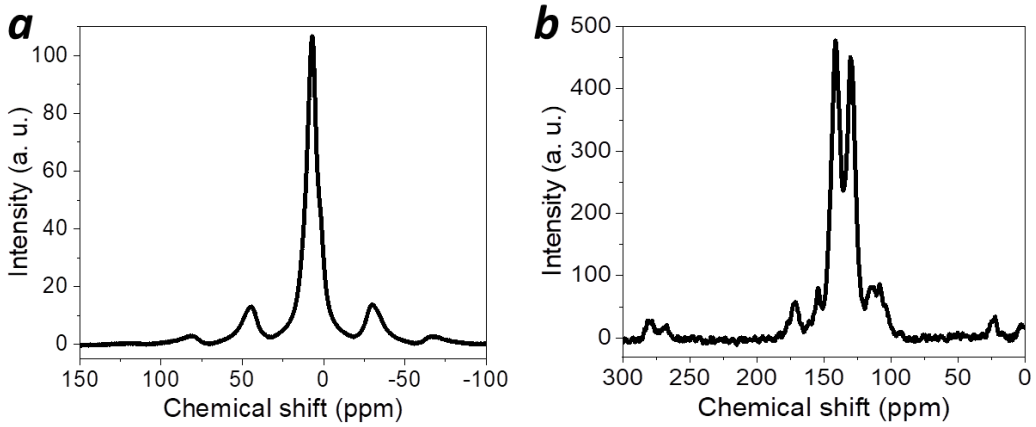


Figure S2. ^{1}H (a) and ^{13}C (b) ssNMR spectra of **TPHATP**.

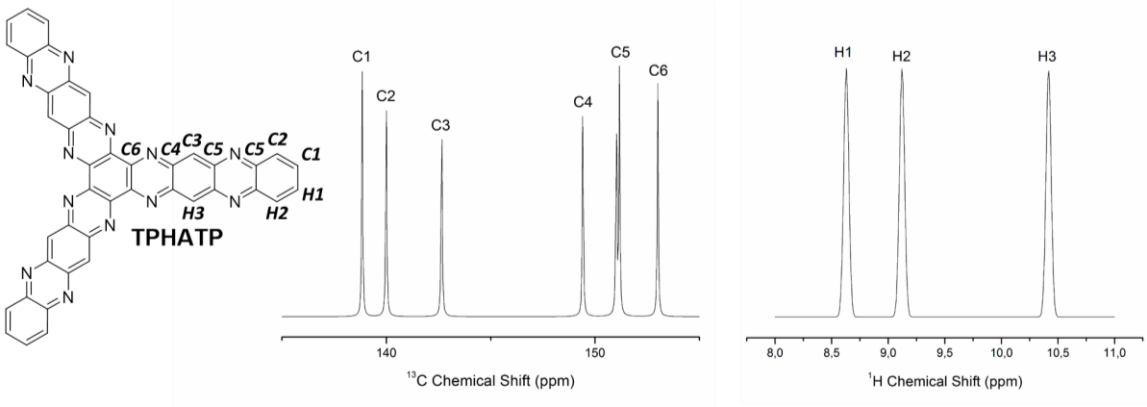


Figure S3. Calculated ^{13}C and ^{1}H NMR spectra for **TPHATP** (decoupled).

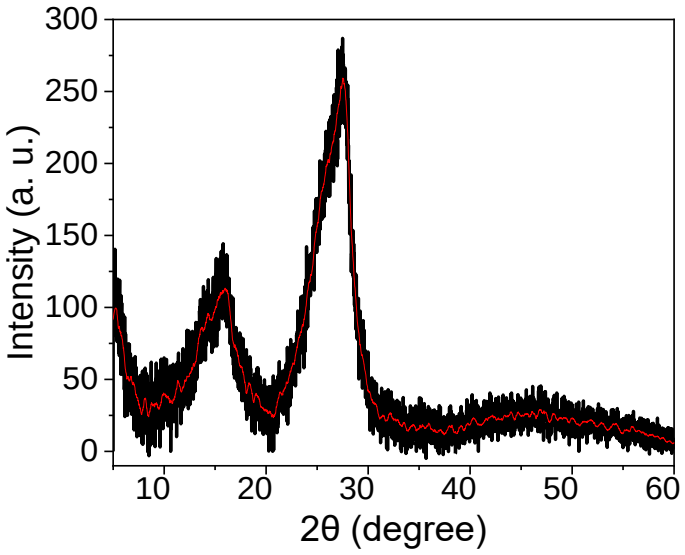


Figure S4. X-ray diffraction pattern of **TPHATP** powder.

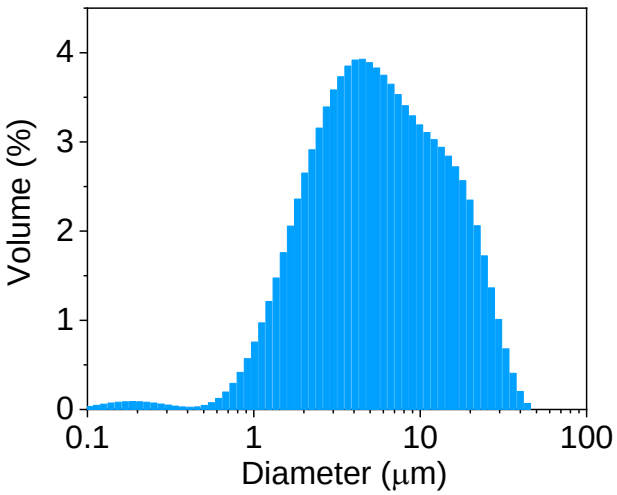


Figure S5. Particle size distribution for **TPHATP** obtained using laser diffraction.

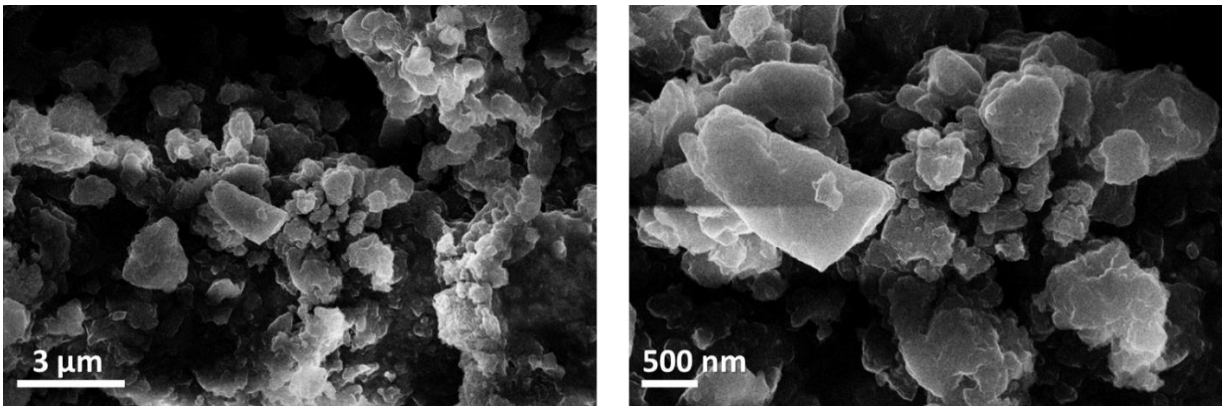


Figure S6. SEM images of **TPHATP** powder.

Table S2. Surface properties of **TPHATP**.

Compound	S_{BET} (m^2/g)	V pore P/P_0=0.99 (cm^3/g)	V (cm^3/g)	d (nm)
TPHATP	57.4	0.32	0.32	23.9

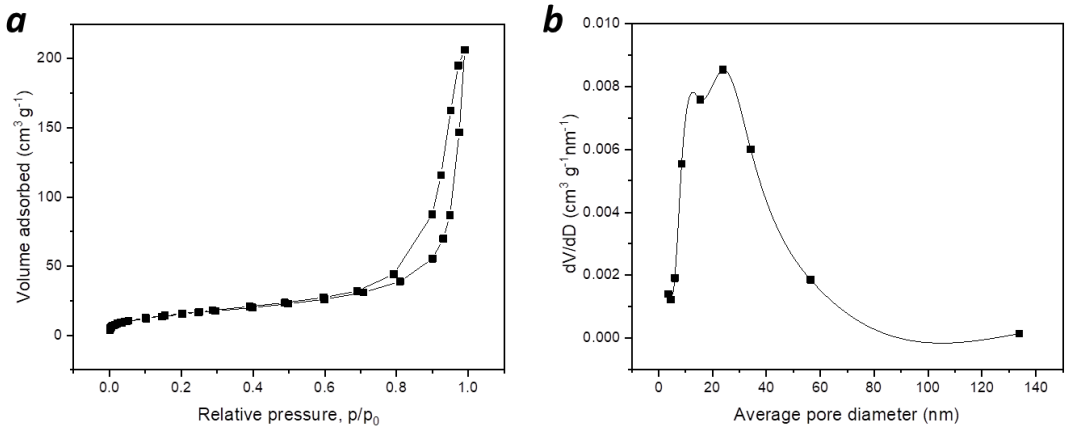


Figure S7. Adsorption-desorption isotherms for **TPHATP** (a); pore size distribution calculated from the desorption curve (b).

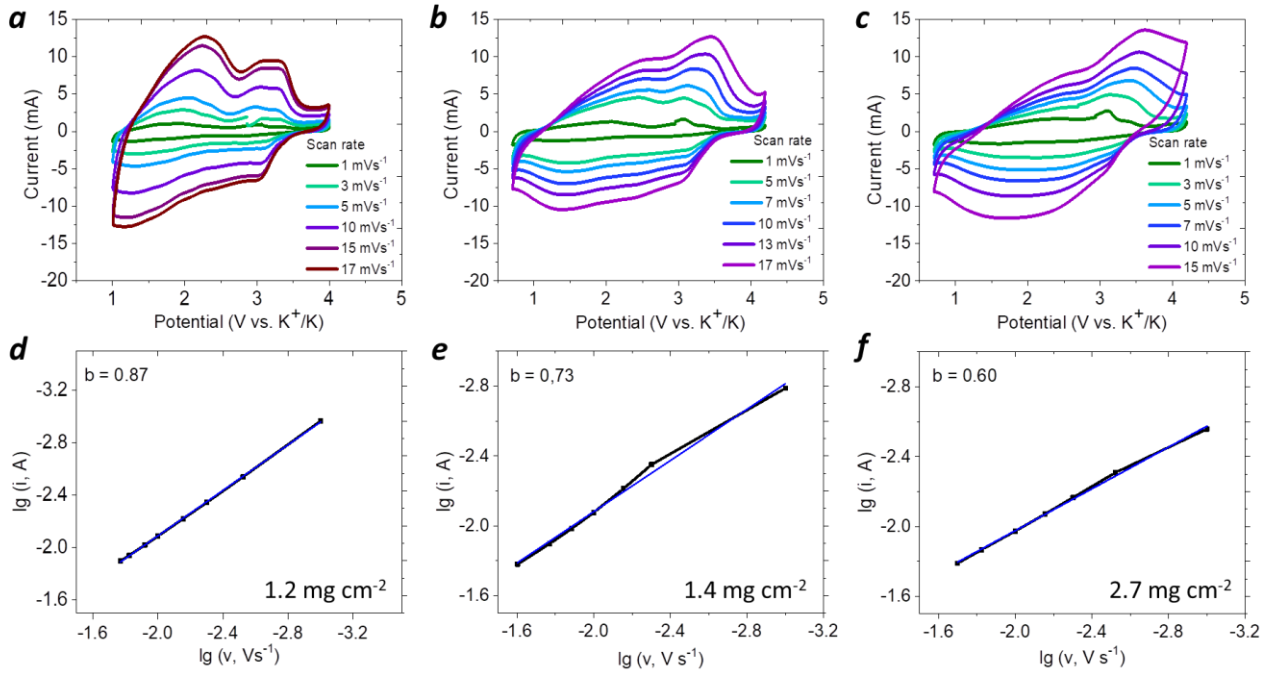


Figure S8. K// **TPHATP** half-cells: CVA curves at various scan rates from 1 to 17 mV s^{-1} (a-c) and plot of log i (current) versus log *v* (scan rate) (d-f) for the cells with **TPHATP** loading of 1.2 (a, d), 1.4 (b, e) and 2.7 mg cm^{-2} (c, f).

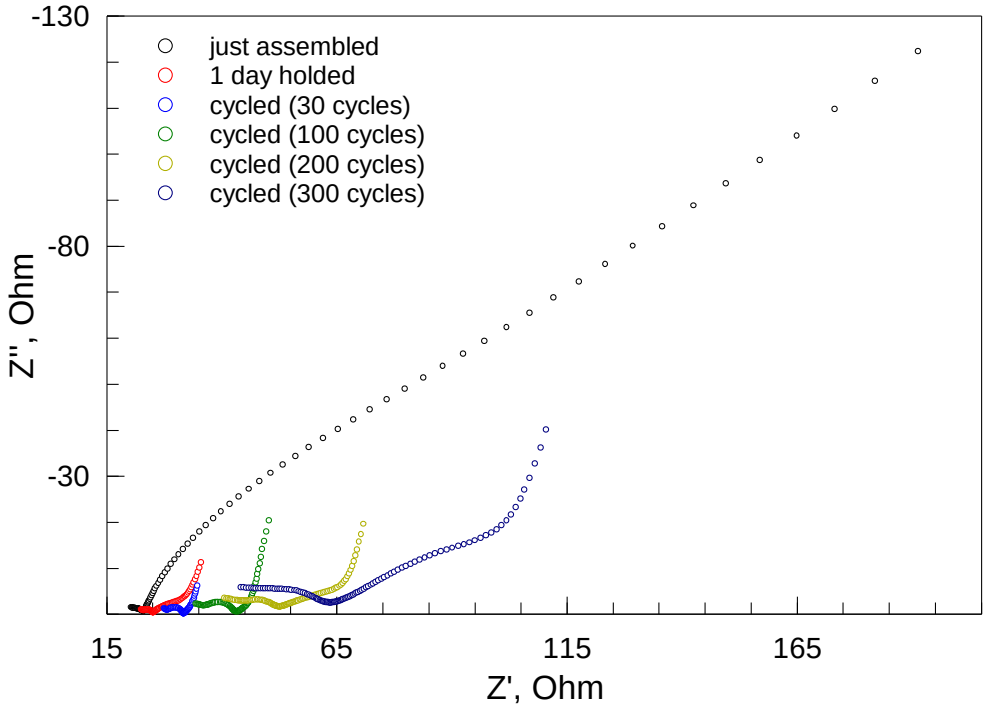


Figure S9. Nyquist plots before and after cycling of K// **TPHATP** half-cell with 1 M KPF_6 in DME electrolyte for 30-300 cycles.

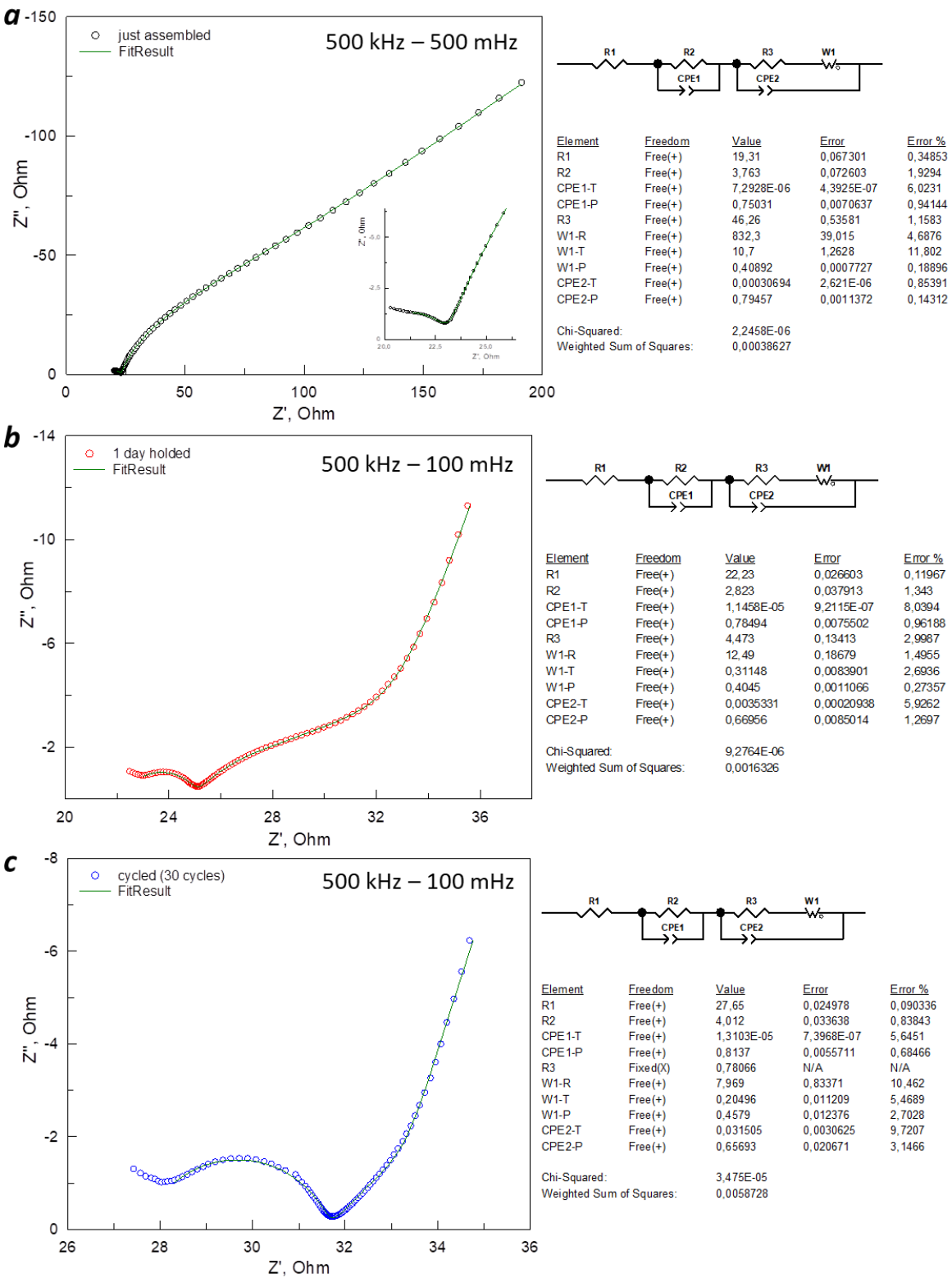


Figure S10. Equivalent circuit fitting results for the Nyquist plots presented in Fig. S8 for the just assembled cell (a), 1 day holded cell (b), cell after 30 cycles (c).

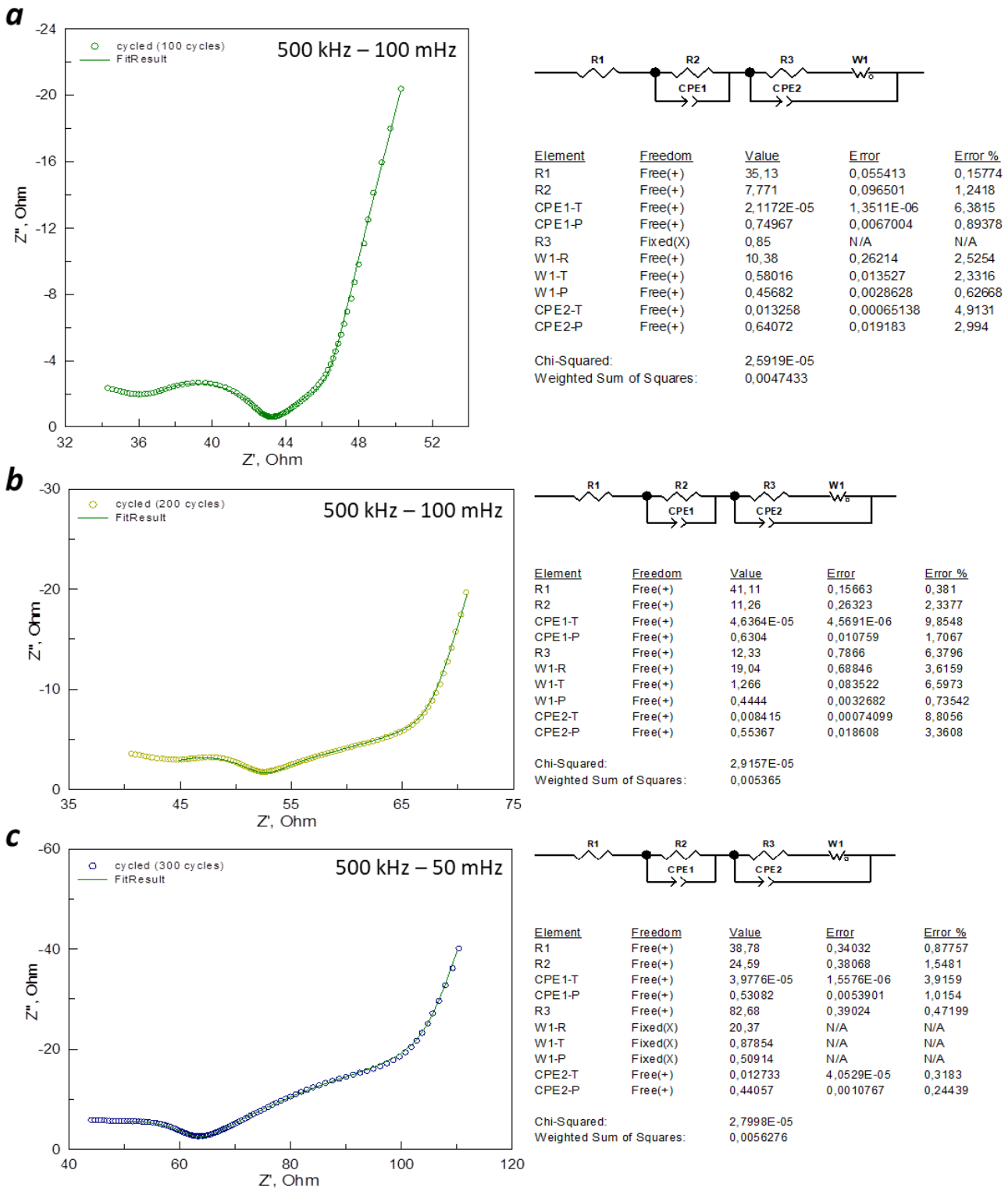


Figure S11. Equivalent circuit fitting results for the Nyquist plots presented in Fig. S8 for the cell after 100 (a), 200 (b) and 300 (c) cycles.

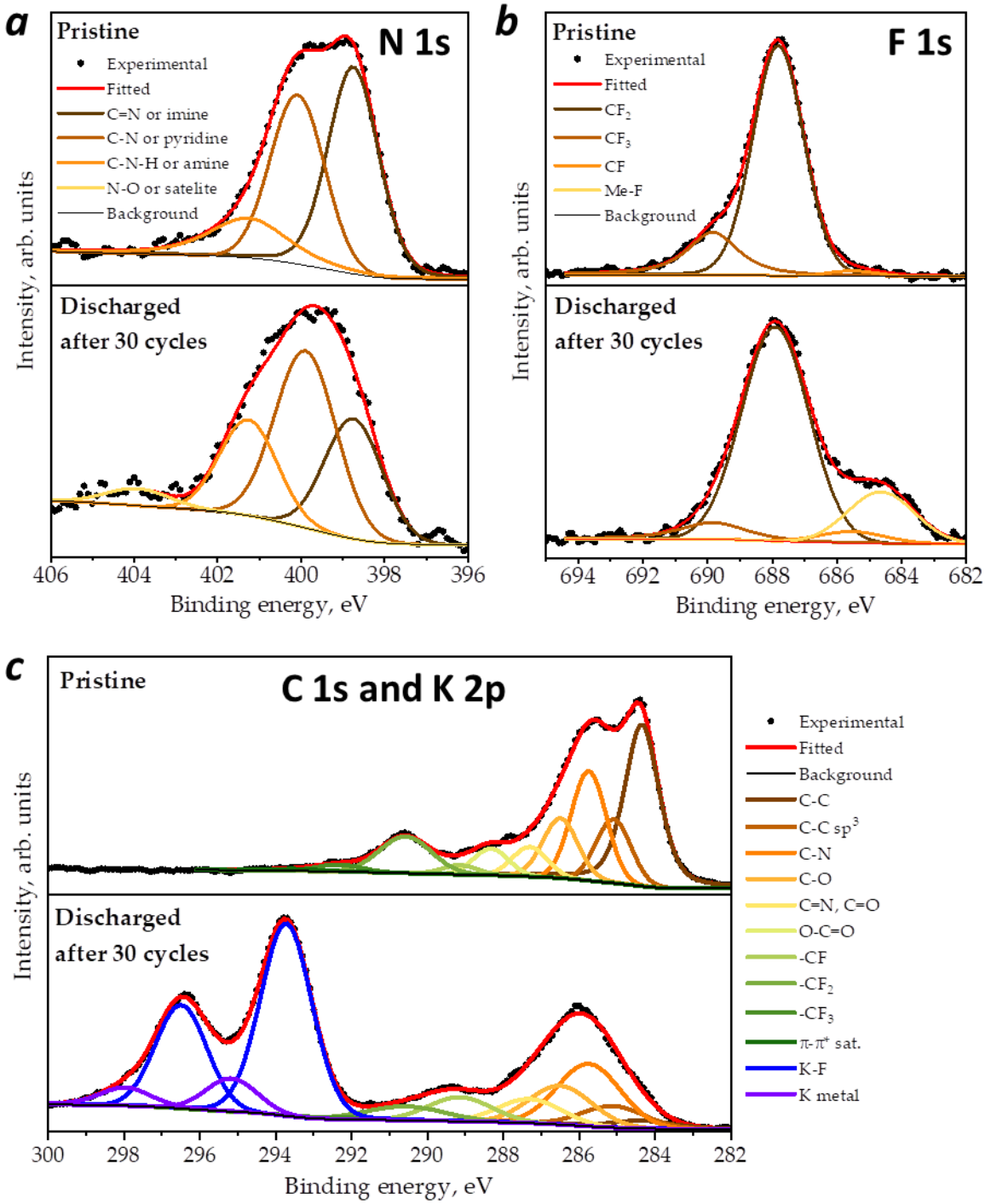


Figure S12. High-resolution core-level XPS N1s (a), F1s (b) C1s and K2p (c) spectra of the pristine and discharged to 1V (after 30 cycles) electrodes based on **TPHATP**.

Signals for metal fluorides in both the F 1s and K 2p spectra indicate the formation of potassium fluoride as a component of the cathode electrolyte interface (CEI).

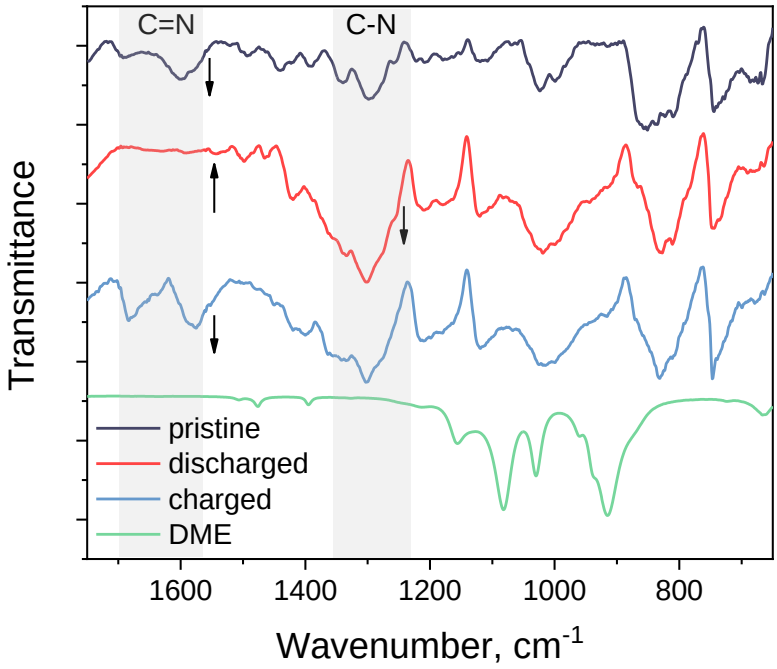


Figure S13. FTIR spectra of the pristine, charged and discharged electrodes (after 30 cycles) based on **TPHATP.** Metalation of the cathode (discharge) led to the depletion of C=N bonds and increase of the intensity of C-N bonds. Spectra of the charged and pristine electrodes were rather similar. Cycled electrodes had no noticeable signals of DME-derived CEI components.

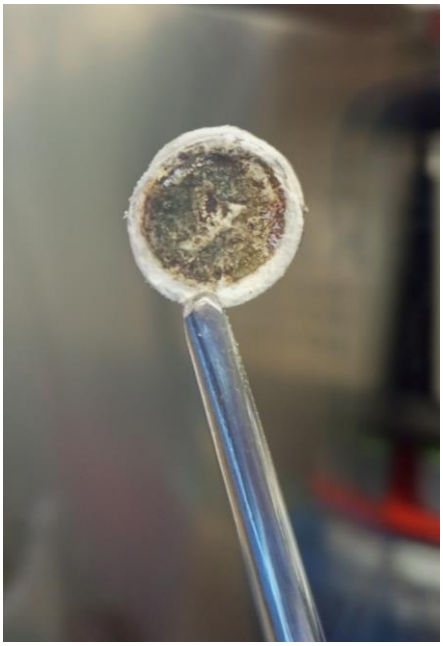


Figure S14. Separator, extracted from the cell after 300 charge-discharge cycles.

Table S3. Characteristics of low-temperature LIBs with inorganic and organic cathodes.

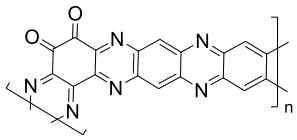
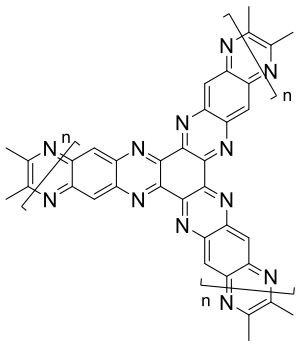
Electrodes	Electrolyte	Capacity or % of capacity at room temperature	Current, current density or cycling rate	Temperature, °C	Ref.
graphite||$LiCoO_2$	1 M $LiPF_6$/ EC:DEC:DMC (1:1:1)	~ 85%	25 mA	−20	[1]
graphite||$LiCoO_2$	1 M $LiPF_6$/ EC:DEC:DMC (1:1:3)	~ 95% ~80% ~98%	0.1 C 0.1 C 0.1 C	−30 −40 −20	[2]
graphite||$LiCoO_x$	1 M $LiPF_6$ / PC:EC:EMC (1:1:3)	~83%	0.5 mA cm^{-2}	−20	[3]
graphite||NMC111	1 M $LiPF_6$ / tetrahydrothiophene-1-oxide:PC (15:85)	~ 70 mAh g^{-1}	1 C	0	[4]
graphite||NMC111	1 M $LiPF_6$ / EC:DEC:DMC:EA (1:1:1:2)	1.49 Ah 1.24 Ah	n.i.* n.i.	−30 −40	[5]
graphite||$LiCoO_2$	1 M $LiPF_6$ / EC:EMC:EP (30:30:40)	87%–89%	0.2 C	−20	[6]
Li|| graphite	0.75 M $LiPF_6$ / EC:DEC:DMC:EA (1:1:1:1)	37 mAh g^{-1}	25 mA	−20	[7]
MCMB||$LiCoO_2$	0.75 M $LiPF_6$ / EC:DEC:DMC:EA (1:1:1:1)	~ 94%	25 mA(~C/20)	−20	[7]
MCMB||$Li_{0.8}Co_{0.2}O_2$	1 M $LiPF_6$ / EC:EMC:MP (20:60:20)	87% 74%	25 mA(~C/16) 25 mA(~C/16)	−20 −40	[8]
graphite ||$LiCoO_2$	2 M $LiPF_6$ / MP + 10% FEC	72.4% 63.2%	1 C 1 C	−40 −60	[9]
MCMB||$LiCoO_2$	1.0 M $LiPF_6$ / EC:EMC: 2,2,2- trifluoroethyl butyrate (20:60:20)	~ 88%	25 mA(C/16)	−20	[10]
MCMB||$LiCoO_2$	1.0 M $LiPF_6$ / EC:EMC: ethyl trifluoroacetate (20:60:20)	~ 90%	25 mA(C/16)	−20	[10]
$Li_4Ti_5O_{12}$||$LiCoO_2$	0.75 M / 1,3-dioxane	~ 123 mAh g^{-1} ~ 80 mAh g^{-1}	0.1 C 0.1 C	−20 −50	[11]
graphite ||$LiFePO_4$	0.8 M LiTFSI / diethyl ether of diethylene	46% (62 mAh	0.1 C	−20	[12]

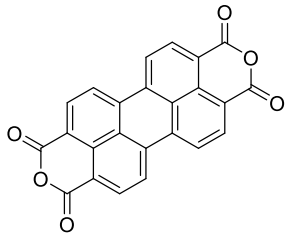
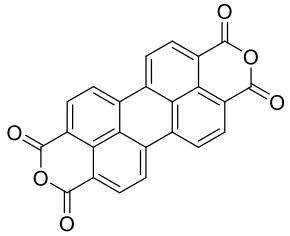
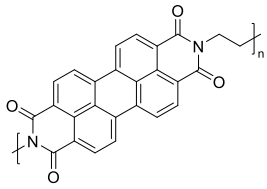
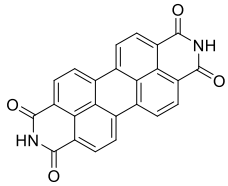
Electrodes	Electrolyte	Capacity or % of capacity at room temperature	Current, current density or cycling rate	Temperature, °C	Ref.
	glycol: methylnonafluorobutyl ether: FEC (50:45:5)	g^{-1})			
graphite ||NMC111	1 M $LiPF_6$ / PC: 1,1,2,2-tetrafluoroethyl-2,2,3,3-tetrafluoropropyl ether: FEC (60:30:30)	70% (113 mAh g^{-1})	0.1 C	−30	[13]
graphite||$LiMn_2O_4$	1 M $LiPF_6$ / 3-(2-methoxyethoxy)propanenitrile: 1,1,2,2-tetrafluoroethyl-2,2,3,3-tetrafluoropropyl ether: FEC (10:30:60)	57.1% (52.9 mAh g^{-1})	0.1 C	−20	[14]
graphite||NMC111	1 M LiBOB / GBL: 1,1,2,2-tetrafluoroethane-2,2,3,3-tetrafluoropropyl ether (70:30)	14.9 mAh g^{-1}	0.1 C	−30	[15]
Li||NCA	1.28 M LiFSI / FEC: (2,2,2-trifluoroethanol)carbonate: 1,1,2,2-trifluoro-1-(2,2,2-trifluoroethoxy)ethane	160 mAh g^{-1} 96 mAh g^{-1}	0.067 C 0.067 C	−42 −85	[16]
Li|| sulfated polyacrylonitrile	1 M LiFSI / diethyl ether	84% 76%	0.1 C 0.1 C	−40 −60	[17]
graphite ||$LiMn_2O_4$	1 M $LiPF_6$ / EC:EMC:EB (1:1:8) (polymeric)	94.61% 38.74%	0.2 C 0.2 C	−20 −60	[18]
graphite||$LiMn_2O_4$	1 M $LiPF_6$ / EC:EMC:MB (1:1:8) (polymeric)	91.72% 53.93%	0.2 C 0.2 C	−20 −60	[18]
MCMB||$LiCoO_2$	1 M $LiAsF_6$ / EC:EMC:MA:toluene (1:1:1:1) (polymeric)	~ 92%	0.2 C	−20	[19]
MCMB||$LiCoO_2$	1 M $LiPF_6$ / EC:DMC:MA (1:1:1) (polymeric)	~ 83%	0.2 C	−20	[19]
Li||polyimide	5 M LiTFSI / EA:dicloromethane (1:4)	84 mAh g^{-1}	366 mA g^{-1}	-70	[20]

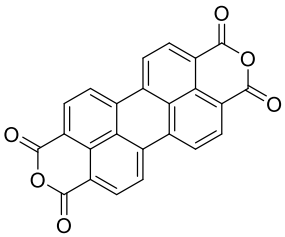
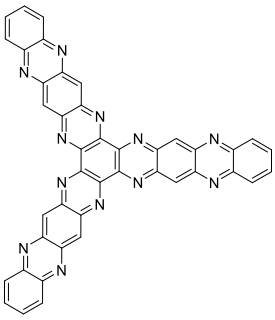
Electrodes	Electrolyte	Capacity or % of capacity at room temperature	Current, current density or cycling rate	Temperature, °C	Ref.
polyimide‖ polytriphenylamine	2 M LiFSI / EA	69 mAh g^{-1}	50 mA g^{-1}	-70	[21]

*n.i. – no information; MCMB - meso-carbon microbeads, EC - ethylene carbonate, DEC - diethyl carbonate, DMC - dimethyl carbonate, PC - propylene carbonate, EMC - ethyl methyl carbonate, EA - ethyl acetate, EP - ethyl propionate, MP - methyl propionate, FEC - fluoroethylene carbonate, GBL - gamma-butyrolactone, EB - ethyl butyrate, MB - methyl butyrate, MA - methyl acetate.

Table S4. Characteristics of low-temperature PIBs with inorganic and organic cathodes.

Electrodes	Electrolyte	Capacity or % of capacity at room temperature	Current, current density or cycling rate	Temperature, °C	Ref.
Anode: K Cathode: 	1 M KPF_6 / DME	186 mAh g^{-1}	20 mA g^{-1}	-55	[22]
Anode: K Cathode: 	1 M KPF_6 / DME	160 mAh g^{-1}	20 mA g^{-1}	-55	[22]
Anode: graphite Cathode: prepotassiated	1 M KFSI 2-methyltetrahydrofuran	64.1 mAh g^{-1}	0.1 C	−30	[23]

Electrodes	Electrolyte	Capacity or % of capacity at room temperature	Current, current density or cycling rate	Temperature, °C	Ref.
					
Graphite || carbon nanofiber	1 M KFSI / THF	200 mAh g^{-1}	50 mA g^{-1}	0	[24]
Graphite || Prussian blue	0.91 M KFSI / 1,2-bis(2-chloroethoxy)ethane	65.5 mAh g^{-1}	20 mA g^{-1}	-5	[25]
Anode: hard carbon Cathode: 	1 M KPF_6 / DME+20 mM $LiNO_3$	89 mAh g^{-1}	65 mA g^{-1}	-40	26]
Anode:  Cathode: $Cu_2[Fe(CN)_6]$	2 M CF_3SO_3K / H_2O+2-hydroxypropyl-β-cyclodextrin	>80 mAh g^{-1}	-	-20	[27]
Anode:  Cathode: $K_{1.55}Fe[Fe-$	10 mol/kg CF_3COOK / H_2O	>90 mAh g^{-1}	-	-35	[28]

Electrodes	Electrolyte	Capacity or % of capacity at room temperature	Current, current density or cycling rate	Temperature, °C	Ref.
$(CN)_6]_{0.95}\cdot 1.03H_2O$					
Anode:  Cathode: tyramine-modified hyaluronic acid @ red P@ B, N modified carbon spheres	KFSI-laponite filler	>60 mAh g^{-1}	100 mA g^{-1}	-40	[29]
$K\|\|K_3V_3(PO_4)_4/C$	0.8 M KPF_6 / EC:DEC (1:1)	52.2 mAh g^{-1}	100 mA g^{-1}	−10	[30]
Anode: K Cathode: 	1M KPF_6 / DME	147 mAh g^{-1}	50 mA g^{-1}	-50	This work

*DME - 1,2-dimethoxyethane, THF - tetrahydrofuran

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Experimental

Materials and equipment

All utilized materials (chemicals and solvents) were purchased from Acros Organics or Sigma Aldrich. Solid-state NMR spectra were acquired at room temperature on a Bruker Avance spectrometer (400 MHz for ^{1}H, 101 MHz for ^{13}C; Bruker, Billerica, MA, USA) equipped with a 3.2 mm MAS probe. FTIR spectra were recorded in ATR mode using PerkinElmer Spectrum 100 (ZnSe prism) spectrometer (PerkinElmer, Waltham, MA, USA). Thermogravimetric analysis was performed using a TGA/DSC3+ Star system from Mettler Toledo. The scanning electron microscopy images were obtained using a ZEISS LEO Supra25 scanning autoemission electron microscope (Carl Zeiss AG, Oberkochen, Germany). The surface properties of the materials were analysed using Quadrasorb SI instrument (USA). X-ray photoelectron spectroscopy (XPS) measurements were performed on a ULVAC-Physical Electronics PHI 5000 VersaProbe spectrometer equipped with a quartz monochromator and analyzer guaranteed working in the range of binding energies from 0 eV to 1500 eV with an energy resolution of $E \leq 0.5$ eV for Al Kα radiation (1486.6 eV) and a vacuum of 10^{-7} Pa. The Al Kα X-ray spot size was 200 μm in diameter. The X-ray power was less than 50 W. The energy scale was calibrated by using external gold foil reference (84 eV for Au 4f level). The spectra were processed using ULVAC-PHI MultiPak Software v. 9.8.0.2.

Synthesis of TPHATP

Hexaketocyclohexane octahydrate and phenazine-2,3-diamine were used to prepare **TPHATP** by a simple condensation reaction. Hexaketocyclohexane (1.0 g) was dissolved in N-methyl pyrrolidone (20 mL) under stirring in a two-necked round-bottom flask filled with argon. Subsequently, phenazine-2,3-diamine (2.24 g) was added to the reaction mixture. The solution was heated at reflux for 24 h. Then, the suspension was filtered and washed with hot acetic acid, acetone, water and ethanol. The resulting powder was heated at reflux in 50 mL of acetic acid at 110 ^{o}C for 3 h. The reaction mixture was filtered and the residue was washed with water, ethanol, and dried in vacuum to produce **TPHATP** with 75% yield.

Fabrication of potassium half-cells

The cathode composition consisted of the active material **TPHATP** (50 wt.%), conductive carbon black (40 wt.%, Timical Super C65), and polyvinylidene difluoride (PVDF) binder (10 wt.%, Gelon). PVDF binder (10 mg) was stirred with 0.7 mL of NMP for 1 hour. Well-grinded active material (50 mg) and carbon black (40 mg) were added to the PVDF solution. The resulting mixture was vigorously stirred at room temperature for 24 h to form a slurry, which was tape-casted on a carbon-coated Al foil (Gelon Lib.). The obtained coatings were dried in air at 150°C for 10 h and then calendered at room temperature. The mass loading of active material was in the range of 1.2–2.7 mg cm^{-2}. The counter electrodes were made from metallic potassium pressed onto a stainless steel disc. Three layers of glass fiber filter (Whatman GF/A Glass microfiber filters, GE Healthcare, Chicago, IL, USA) were used as a separator. 1 M KPF_6 in DME was used as electrolytes (80 μL per cell). The CR2032 coin-type cells were assembled inside an MBraun argon-filled glove box (H_2O, $O_2 < 0.1$ ppm).

Electrochemical characterization

Cyclic voltammograms were recorded with an Elins P40 potentiostat (Elins, Russia) at scan rates of 0.5–17 mV s^{-1}. The galvanostatic measurements were carried out on a Neware BTS3000 workstation (Neware, China) at the current rates ranging from 50 mA g^{-1} to 2 A g^{-1} in a potential range of 1.0-4.0 V (vs. K^+/K). The galvanostatic cycling was started from the discharge for all potassium cells. Impedance spectra were registered using Elins P40 potentiostat (Elins, Russia) equipped with frequency response analyzer (FRA), within a frequency range from 500 kHz to 500, 100 or 50 mHz, at the cell potential of 1.8 V (± 10 mV) corresponding to state-of-charge close to 50%. Every time before measurement, the cell was held for 10 minutes at the required potential to reach equilibrium.

Quantum chemical calculations

Structures of oligomers were optimized using the PBE exchange-correlation functional [J. P. Perdew, K. Burke and M. Ernzerhov, *Phys. Rev. Lett.*, 1996, **77**, 3865] and the SBK pseudopotential [W. J. Stevens, H. Basch and M. J. Krauss, *Chem. Phys*., 1984, **81**, 6026] with an extended basis set C,N,O : [5s, 5p,2d/3s, 3p, 2d], K [4s, 1p/32, 1p] H[5s, 1p/3s, 1p] for valence electrons. The Hirschfeld method [F. L. Hirshfeld, *Theoret. Chim. Acta*., 1977, **44**, 129] was used to calculate atomic charges. All molecular structures were optimized using the PRIRODA software package [D. N. Laikov, *Chem. Phys. Lett.*, 1997, **281**, 151.], followed by the calculation of vibration frequencies to confirm their stability. Structure of **TPHATP** and its metalated forms with the lowest energies were chosen. The Cartesian coordinates of the metalated stacks of the model oligomers are also given below. All quantum chemical calculations were performed using the computing capabilities of the Joint supercomputer center of the National Research Center "Kurchatov Institute".

The calculation of the specific metallation energies ΔE_{nK} (eV) of P:

n K(metal) + P = PK_n + $n\Delta E_{nK}$

was performed based on the data for the theoretical energy of the reaction with diatomic molecules K_2

n 0.5 K_2 + P = PK_n +n Q_n

taking into account the semi-empirical correction

$E_{nK} = Q_n$ - 0.66 eV

based on the experimental values of the thermal effect of atomization of metallic potassium and the binding energy in the diatomic molecule K_2.

Cartesian coordinates

$[TPHATP]_3K_6$

C	-4.934251920000	9.569433650000	4.547021830000
C	-6.147799040000	8.827746110000	4.555361580000
H	-7.048613950000	6.864005860000	4.475821370000
C	-6.131483210000	7.454634260000	4.471246730000
C	-4.896686580000	6.752910600000	4.376457190000
C	-3.659866940000	7.508685940000	4.368718900000
C	-3.720494370000	8.928211930000	4.455208700000

H	-2.776782580000	9.475296340000	4.447258770000
N	-2.458302990000	6.901809110000	4.285076860000
N	-4.905333490000	5.406453120000	4.299676500000
C	-3.708480390000	4.798326900000	4.219623080000
C	-2.463485970000	5.558829570000	4.212675750000
C	10.804292340000	-0.405134850000	4.458732630000
C	10.766959210000	1.016358490000	4.487053040000
H	9.513831690000	2.777524430000	4.440206300000
C	9.568210950000	1.688183020000	4.420269820000
C	8.343415730000	0.969336930000	4.323980770000
C	8.381238830000	-0.479398020000	4.297685530000
C	9.642371420000	-1.135978090000	4.365745360000
H	9.645686860000	-2.226586090000	4.343029690000
N	7.255057370000	-1.216953560000	4.214621160000
N	7.180408220000	1.649427000000	4.263382740000
C	6.055710050000	0.916589710000	4.182224690000
C	6.093225420000	-0.541640630000	4.159383250000
H	4.914934040000	-2.348500720000	4.105547550000
C	4.874171770000	-1.257932580000	4.089239600000
C	4.801548740000	1.570120060000	4.127231060000
H	4.784124120000	2.660554790000	4.172336680000
C	3.612517200000	0.853278910000	4.067213070000
C	3.648966130000	-0.602870880000	4.052032680000
N	2.483588870000	-1.322193680000	3.997468840000
N	2.413727800000	1.514534380000	4.014107840000
C	1.293559660000	0.787508570000	4.049872180000
C	1.329083980000	-0.650815730000	4.048026490000
C	0.081110100000	-1.411502200000	4.067470440000
C	-1.182274030000	-0.723122760000	4.060323010000
C	-1.217685230000	0.738000140000	4.056446460000
C	0.010326730000	1.487655460000	4.053198670000
N	0.014498990000	2.823508200000	4.017439610000
N	-2.407442680000	1.345252000000	4.025231040000
C	-2.433885860000	2.713799770000	4.088174870000
C	-1.190639040000	3.472770520000	4.082867210000
C	-1.234245370000	4.860785410000	4.138196680000
C	-3.648652770000	3.385941310000	4.150646430000
H	-4.585654940000	2.827186510000	4.186728490000
N	-2.341141330000	-1.388107930000	4.026031820000
N	0.150157170000	-2.745705590000	4.057358490000
C	-1.021738350000	-3.452121800000	4.126810960000
C	-2.300924200000	-2.755903600000	4.102968940000
C	-0.995535270000	-4.839123390000	4.210032700000
H	-0.042498930000	-5.368738630000	4.262281850000
C	-2.188625610000	-5.597522430000	4.277478520000
C	-3.470169050000	-4.901130580000	4.245842800000
C	-3.480813710000	-3.488475010000	4.155020130000
H	-4.445675350000	-2.978288420000	4.165301720000
N	-4.636006050000	-5.568497270000	4.311408130000
C	-3.287132440000	-7.602736760000	4.447852730000
C	-4.560576480000	-6.911310510000	4.413265690000
N	-2.116524000000	-6.936701340000	4.377049990000
H	-0.309115830000	5.439360220000	4.163774530000
C	-5.759912340000	-7.673817020000	4.492531720000
C	-3.277263900000	-9.021468540000	4.562490800000
C	-5.708206380000	-9.044156600000	4.603577230000
H	-2.306831350000	-9.519077090000	4.587866630000
H	-6.632052700000	-9.621176580000	4.666274480000
C	-4.458611910000	-9.722440070000	4.639387470000
H	-4.442495750000	-10.809628820000	4.729799260000

H	-7.098340430000	9.358065210000	4.630487310000
H	-4.971980960000	10.657676360000	4.615590860000
H	11.701266740000	1.574621440000	4.563520760000
H	11.766740280000	-0.916156570000	4.513048560000
H	-6.705821700000	-7.131281620000	4.463123270000
C	-4.541129060000	9.736106060000	-4.571629710000
C	-5.791920630000	9.059143150000	-4.563517020000
H	-6.794066340000	7.146374790000	-4.460833760000
C	-5.847037120000	7.687697280000	-4.469031990000
C	-4.650046960000	6.922582330000	-4.379659840000
C	-3.375371640000	7.612564930000	-4.387722150000
C	-3.361992380000	9.032572820000	-4.485138180000
H	-2.390665890000	9.529063600000	-4.489443030000
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C	10.651391310000	-1.042732300000	-4.625576390000
C	10.692340650000	0.378700770000	-4.599709370000
H	9.539260840000	2.202917430000	-4.470532830000
C	9.533415830000	1.112296630000	-4.492138410000
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H	4.669090400000	-2.672514500000	-4.234047020000
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C	4.769978840000	1.245548560000	-4.148401190000
H	4.813464700000	2.336041860000	-4.165503180000
C	3.543956730000	0.593503540000	-4.091708630000
C	3.503720330000	-0.862403110000	-4.107682320000
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N	2.381189990000	1.315397820000	-4.017668080000
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C	1.185152350000	-0.791014140000	-4.055998790000
C	-0.099392940000	-1.488150500000	-4.037358080000
C	-1.325362550000	-0.735346460000	-4.047192470000
C	-1.286524560000	0.725910000000	-4.050794400000
C	-0.021618370000	1.411447830000	-4.053222560000
N	0.050368950000	2.745209380000	-4.020908460000
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H	-4.543608400000	2.986290110000	-4.164745600000
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C	-2.546354290000	-2.707748490000	-4.065382870000
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C	-3.827415250000	-4.788820780000	-4.184116660000
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H	-4.696667330000	-2.813189260000	-4.186764330000

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H	-2.911692880000	-9.472140430000	-4.322113440000
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H	-6.713982970000	9.638122440000	-4.634119840000
H	-4.522303960000	10.824299200000	-4.648428190000
H	11.655159520000	0.887431170000	-4.667191650000
H	11.583382970000	-1.603236750000	-4.713022710000
H	-7.171672380000	-6.845155200000	-4.460721370000
C	-5.967536180000	-8.962503100000	0.005737660000
C	-4.734119120000	-9.670679490000	0.061439650000
H	-2.579430850000	-9.517061830000	0.128623630000
C	-3.536715620000	-8.996604510000	0.086373050000
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C	-4.771662420000	-6.851556020000	0.004511160000
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C	-2.372100200000	-5.589487560000	0.049887410000
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C	-4.773052170000	9.652721880000	-0.024237200000
C	-6.004325460000	8.938675650000	-0.013646220000
H	-6.950611270000	6.995737140000	0.001874420000
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C	-3.543812350000	7.561051350000	-0.018350590000
C	-3.572380140000	8.984076940000	-0.026379280000
H	-2.616680970000	9.509067860000	-0.034258410000
N	-2.356490790000	6.924543550000	-0.019631930000
N	-4.836488930000	5.486311920000	-0.002611270000
C	-3.652460970000	4.851544660000	-0.005198680000
C	-2.393461690000	5.581605860000	-0.012979870000
H	-0.245273280000	5.417227790000	-0.021489930000
C	-1.179804620000	4.852139300000	-0.013771610000
C	-3.621925400000	3.435942690000	-0.000656390000
H	-4.576598410000	2.905467980000	0.007008000000
C	-2.425355480000	2.733581890000	-0.003540370000
C	-1.164317120000	3.464696660000	-0.008167570000
N	0.034170940000	2.789162470000	-0.004903720000
N	-2.434609470000	1.357845600000	-0.004307030000
C	-1.251535830000	0.727961220000	-0.002779310000
C	-0.007089640000	1.449608120000	0.000942470000
C	1.258319590000	0.722011970000	0.007214490000
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C	-1.249060810000	-0.731531460000	-0.002270720000
N	-2.429692640000	-1.366033580000	-0.012685530000
N	0.044047670000	-2.787465630000	0.035261220000
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C	-3.608888090000	-3.449375830000	-0.018612820000

C	-1.161763330000	-4.854703660000	0.063455430000
H	-0.225194980000	-5.415570120000	0.097506980000
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N	2.395333570000	1.431535070000	0.015587190000
C	3.582072400000	0.735582100000	0.009519430000
C	3.584693670000	-0.721880860000	-0.015134870000
C	4.788776040000	1.420440550000	0.021406640000
H	4.806833960000	2.512191750000	0.045327030000
C	6.029863360000	0.739069110000	0.001698940000
C	6.032408540000	-0.715883880000	-0.033352500000
C	4.793815700000	-1.402126390000	-0.038667750000
H	4.815549570000	-2.493680390000	-0.065347970000
N	7.176814020000	-1.419079900000	-0.061333700000
C	8.319209720000	0.741565810000	-0.011452410000
C	8.321762180000	-0.709252090000	-0.052053970000
N	7.171683590000	1.446858560000	0.013384370000
H	-4.565360070000	-2.923239690000	-0.051078350000
C	9.568262570000	-1.395659330000	-0.083132490000
C	9.563294380000	1.432897410000	0.001414790000
C	10.747745610000	-0.690390830000	-0.071595750000
H	9.536112890000	2.522474330000	0.035089000000
H	11.700156620000	-1.221684690000	-0.095752520000
C	10.745266480000	0.732300360000	-0.027728120000
H	11.695830910000	1.267337910000	-0.017246780000
H	-4.745699330000	-10.761231970000	0.084105760000
H	-6.903582510000	-9.522245060000	-0.015283070000
H	-6.943118530000	9.494200320000	-0.011588930000
H	-4.788970770000	10.743427360000	-0.030686430000
H	9.544882320000	-2.485340710000	-0.116137370000
K	2.045680400000	-3.347053780000	2.216535460000
K	-3.887120640000	-0.047139810000	2.224482780000
K	1.928436550000	3.459276000000	2.182027580000
K	-3.961203690000	0.051007620000	-2.184739410000
K	1.869441960000	-3.460049280000	-2.194366500000
K	2.001672970000	3.338146130000	-2.230140900000

$[TPHATP]_3K_{18}$

C	-6.118503520000	8.940520450000	5.474386810000
C	-7.224546300000	8.078741400000	5.469150020000
H	-7.886412250000	6.018618070000	5.326658600000
C	-7.037788940000	6.707629970000	5.300918100000
C	-5.748907660000	6.158210870000	5.131570790000
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