Electronic Supplementary Information

On a high-capacity aluminium battery with a two-electron phenothiazine redox polymer as positive electrode

Gauthier Studer,^{1,2} Alexei Schmidt,^{2,3} Jan Büttner,^{2,3,4} Maximilian Schmidt,¹ Anna Fischer,^{2,3,4}

Ingo Krossing,^{2,3,4,*} Birgit Esser^{1,2,4*}

¹ Institute of Organic Chemistry II and Advanced Materials, Albert-Einstein-Allee 11, 89081 Ulm, Germany

² Freiburg Materials Research Center, University of Freiburg, Stefan-Meier-Str. 21, 79104 Freiburg, Germany

³ University of Freiburg, Institute of Inorganic and Analytical Chemistry, Albertstraße 21, 79104 Freiburg, Germany

⁴ Cluster of Excellence livMatS @ FIT – Freiburg Center for Interactive Materials and Bioinspired Technologies, University of Freiburg, Georges-Köhler-Allee 105, 79110 Freiburg, Germany

Contact Information:

Prof. Dr. Birgit Esser

Address: Institute of Organic Chemistry II and Advanced Materials, Albert-Einstein-Allee 11, 89081 Ulm, Germany. * Correspondence to: <u>birgit.esser@uni-ulm.de</u>; <u>www.esserlab.com</u>

Prof. Dr. Ingo Krossing

Address: University of Freiburg, Institute of Inorganic and Analytical Chemistry, Freiburg Materials Research Center FMF, Albertstraße 21, 79104 Freiburg, Germany. * Correspondence to: <u>krossing@uni-freiburg.de</u>

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1. Investigation of fluorinated additives for chloroaluminatebased ionic liquid

1.2. Materials and methods

General procedures: All manipulations were carried out under exclusion of moisture and air within an MBRAUN glovebox (Labmaster sp) filled with argon ($O_2/H_2O < 1$ ppm) and by using standard SCHLENK techniques. All glassware used in reactions was stored in an oven at 180 °C overnight and was additionally dried with a heat gun prior to use. All solvents were stored under an argon atmosphere in sealed vessels. Fluorinated benzenes and benzene were dried over CaH₂ for two days, distilled and degassed prior to use. The water content of the solvents was below 10 ppm, as determined by KARL FISCHER titration.

AlCl₃ was purified twice by sublimation prior to use. [EMIM]Cl > 99 % was provided by IOLITEC IONIC LIQUIDS TECHNOLOGIES GMBH and dried *in vacuo* at 50 °C for 2 days until no change in pressure was observed. Benzene (absolute, stored over 3 Å molecular sieves) was purchased from SIGMA ALDRICH. Fluorobenzene (FB) and 1,2-difluorobenzene (2FB) were purchased from FLUOROCHEM. 1,2,3-Trifluorobenzene (3FB) and 1,2,3,4-Tetrafluorobenzene (4FB) were purchased from APOLLO SCIENTIFIC. Pentafluorobenzene (5FB) was purchased from ABCR. Hexafluorobenzene (6FB) was purchased from P&M INVEST. Aluminium electrodes were polished with abrasive paper under argon atmosphere prior to use.

NMR experiments: NMR samples were prepared using inert techniques and handled in 5 mm NMR tubes with J. YOUNG valves or in flame-sealed 3 mm NMR tubes (NORELL). All NMR spectra were recorded using BRUKER *DPX 200 MHz*, BRUKER *Avance III HD 300 MHz* or BRUKER *Avance II WB 400 MHz* spectrometers. Evaluation followed first order using BRUKER BIOSPIN *TopSpin 4.0.6* software. The chemical shifts of standard solvents were taken from the literature,^[1] and the shifts of the fluorinated benzenes were determined experimentally via internal reference using TMS as standard. 6FB was referenced according to the literature.^[2] NMR shifts of the pristine ionic liquids were determined experimentally by measurements of pristine IL and further addition of a small amount 2FB for reference. Calibration was then executed by setting 2FB to 6.96 ppm (Figure S 1) and then equalizing the triplet at 1.29 ppm for the [EMIM]-IL in its pristine form (Figure S 2). The electrolyte with FB additive was calibrated to 6.88 ppm (see Figure S 3).



Figure S 2 ¹H NMR spectrum (200.12 MHz, 2998 K) of 2FB (20 wt%) in [EMIM]Cl, AlCl₃ 1:1.5-IL. Peaks are broadened due to the high viscosity of the sample.



Figure S 3 ¹H NMR spectrum (400.17 MHz, 298 K) of TMS in FB.

Battery cycling: Battery cycling was performed at ambient temperatures using a LANDT INSTRUMENTS *CT2001A-5V-2mA* battery tester. LANDT INSTRUMENTS *LANDProc V7.4* was used for setting of cycling programs, LANDT INSTRUMENTS *LANDMon V7.4* was used for surveillance, control and data recording, LANDT INSTRUMENTS *LANDdt V7.4* was used for data processing and ORIGINLAB *OriginPro 2020 (9.70)* for plotting and graphics.

PTFE screw cell setup:



Figure S 4 Side perspective of a PTFE screw cell with case (1). Cell components of a symmetric cell (2): A load cell, B copper current collector with clamping point, C Al electrodes, D sealing material, E PTFE compartment as electrolyte reservoir with sealing screw.

Reusable custom-built PTFE screw cells (Figure S 4) were used for battery experiments. Assembly and measurements were performed in an argon glovebox. A polished copper current collector (**B**) was used as the first layer connected with the aluminium electrode (99% Alfa Aesar) (**C**). To prevent leakage sealing material (**D**, FREUDENBERG SEALING TECHNOLOGIES *85 Ice Cube Sealing Prototyping sheet*) with an 11 mm hole was place between electrode and PTFE inset (**E**). The inset has an 11 mm opening and is able to hold 0.55 mL of electrolyte. This setup was repeated in mirrored order (sealing material, electrode, current collector) and finished off with a LORENZ *k-22* pressure load cell (**A**) and an Al disc protecting the PTFE screw from damage. Prior to filling the cell, the screw was tightened with a force of at least 1.0 kN. After 10–20 h the pressure was reviewed and retightened if necessary.

1.3. Motivation and description

The deposition of aluminium for battery applications occurs from LEWIS-acidic ionic liquids *(ILs)*.



Scheme 1 Definition of LEWIS-basic, -neutral and -acidic chloroaluminate ILs (x(AlCl₃) is the mole fraction).

Even though they are comprised of ions, these ILs suffer from relatively low conductivity due to their high viscosity. Chemically and electrochemically stable molecular solvents could be used as additives reducing the viscosity and therefore increasing the conductivity of the electrolytes. However, the highly LEWIS-acidic nature of such electrolytes renders the majority of solvents incompatible with the ILs. Yet, PARK *et al.* have shown the positive effect of benzene towards overpotentials as an additive in LEWIS-acidic chloroaluminate ILs.^[3] We anticipated that the more polar fluorinated benzenes could be superior candidates due to their higher polarity. The inclusion of electron-withdrawing fluorine substituents should also provide protection towards side reactions, such as FRIEDEL-CRAFTS type reactions.^[4]

Table S 1Selected physical properties of fluorinated benzenes.

Fluorobenzenes →	F F	F F	F F F	F F F	F
↓ Properties	FB	2FB	3FB	َ F 4FB	F 5FB
<i>E</i> _{1/2} (NO ⁺) ^a vs. Fc ⁺ /Fc / V	1.11	1.23	1.42	1.52	1.47
<i>E</i> _{1/2} (Ag ⁺) ^a vs. Fc ⁺ /Fc / V	0.62	0.87	1.14	1.35	1.38
Ionization Energy /	9.20	9.29	9.40	9.53	9.63
eV					
Dielectric Constant ${m arepsilon_r}^{ extsf{b}}$	5.7	13.8	21.2	12.7	4.6
Dipole moment ^{b,c} / D	1.9	3.5	4.6	3.5	1.8

a) CV measurement at a scan rate of 100 mV s⁻¹ (C. Friedmann, unpublished results). b) Own measurements (C. Friedmann) at

(22.0 \pm 0.5) °C in cooperation with Dr. J. Hunger (MPI Mainz). c) Taken from relaxation strengths of the liquid phase – typically higher than gas phase due to induced dipoles.^[4]

A suitable molecular solvent could further allow the use of alternative cations, which form ionic liquids that are not liquid at room temperature. A broadened variety of cations could further increase conductivity due to the possibility of using smaller ions.

Therefore, we investigated first 2FB as an additive in an ionic liquid comprised of [EMIM]Cl and AlCl₃ in a 1:1.5 ratio in detail. Experiments using AlCl₃ in 2FB showed no indication of a reaction between the components by NMR spectroscopy. Subsequently, symmetric screw cells using an IL electrolyte with 20 wt% 2FB were measured for 100 cycles at a current density of 0.25, 0.5, 0.75 and 1 mA cm⁻². The results of these cells were compared with similar cells containing the pristine electrolyte, unfortunately showing for the 2FB/IL electrolyte an inferior electrochemical behaviour as well as side reactions observed by NMR spectroscopy, if compared to a pristine IL electrolyte. IL electrolytes with benzene, FB, 2FB, 3FB, 4FB, 5FB and 6FB were then additionally investigated in symmetric screw cells at current densities of 0.25, 0.75 (25 cycles each) and 1 mA cm⁻¹ (until measurement was aborted). The voltage profiles of these experiments after in total 100 cycles are collected in Figure S 5.



- Figure S 5 Symmetric cell experiments in a screw cell at 0.25, 0.5, 0.75 and 1.0 mA cm⁻² with 0.55 mL IL electrolyte [EMIM]Cl/AlCl₃ 1:1.5 with 20 wt% (fluorinated) benzene as additive. Each curve consists of the median of 25 cycles at given current density with a total of 100 cycles. Error bars are not included for clarity.
- Table S 2Potential range of symmetric screw cells with IL electrolytes containing
(fluorinated) benzenes at 0.25, 0.5, 0.75 and 1.0 mA cm $^{-2}$.

	Charge	Discharge	Charge	Discharge	Charge	Discharge	Charge	Discharge
	potential							
	@ 0.25	@ 0.25	@ 0.5	@ 0.5	@ 0.75	@ 0.75	@ 1.0	@ 1.0
	mA cm ⁻²							
	/mV							
Pristine(P)	37 - 40	-3456	48 - 55	-5066	65 - 71	-6484	76 - 91	-79108
P+ Benzene	25 - 32	-2432	35 - 43	-3543	48 - 59	-4960	64 - 73	-6474
P+FB	23 - 29	-2431	35 - 43	-3543	48 - 59	-4957	60 - 72	-6069
P+2FB	43 - 55	-4349	69 - 83	-6381	86 - 108	-80108	100 - 129	-95133
P+3FB	30 - 36	-2734	42 - 49	-4047	55 - 63	-5362	64 - 75	-6474
P+4FB	42 - 49	-3745	51 - 59	-4960	60 - 73	-6282	64 - 101	-74101
P+5FB	27 - 33	-2329	43 - 49	-4146	58 - 67	-5562	71 - 81	-6875
P+6FB	33 - 36	-2835	46 - 51	-4450	61 - 69	-6069	77 - 87	-7686

Overall, the observed overpotentials were quite low. Benzene, along with FB, 3FB, 5FB and 6FB, all showed slightly lowered overpotentials compared to the pristine electrolyte, while 4FB showed overpotentials in a similar magnitude as the pristine electrolyte. This positive effect could be based on the reduced viscosity in these cells. Only 2FB showed overpotentials higher than the pristine electrolyte. The reason for this negative effect is yet unknown. After finishing the measurement (see Table S 3 for total number of cycles) the electrolyte was investigated by NMR spectroscopy. FB, while exhibiting a slight decrease in overpotential, shows a contamination after cycling in the NMR spectrum (see Figure S 8). This contamination might occur due to side reactions with the sealing material used in these long-term experiments. ILs with higher fluorinated and therefore less electron-rich benzenes indicated no such contaminant, allowing the assumption of a possible FRIEDEL-CRAFTS-type reaction. The NMR spectrum of the benzene-containing electrolyte displays a possible impurity *post cycling*, which cannot unambiguously be assigned (see Figure S 10). These findings along with the unknown interactions of (fluorinated) benzenes and the organic positive electrode material led to the decision to work with a pristine IL electrolyte.

Table S 3Cycles completed in symmetric screw cells with IL electrolyte with 20 wt%
(fluorinated) benzenes as additive. Cells were cycled with 0.25, 0.5, 0.75 mA
cm⁻² (25 cycles each) and 1.0 mA cm⁻². The measurement was aborted after
779 cycles for most cells. Cells with 2FB, 4FB and 6FB showed signs of short
circuit but the measurement continued until the number of cycles in brackets
were accomplished.

Additive	Number of cycles
Benzene	779
Fluorobenzene	779
1,2-difluorobenzene	308 (788)
1,2,3-trifluorobenzene	779
1,2,3,4-tetrafluorobenzene	480 (781)
1,2,3,4,5-pentafluorobenzene	779
Hexafluorobenzene	41165)

1.4. Synthetic manipulations

Preparation of the [EMIM]-ionic liquid: [EMIM]Cl (5.40 g, 36.85 mmol, 1 eq) was slowly added to AlCl₃ (7.38 g, 55.31 mmol, 1.5 eq) while stirring. During the addition of [EMIM]Cl a liquid formed in the reaction vessel. The formed liquid was used as received (Figure S 7).

Preparation of the IL electrolyte with additives: For battery experiments [EMIM]-IL (800 mg) was added to benzene, 1FB, 2FB, 3FB, 4FB, 5FB or 6FB (200 mg), respectively, and stirred for a short period of time. No change in colour after adding XFB (X=0–6) occurred except for 6FB, which instantly turned reddish brown (see Figure S 6).



Figure S 6 [EMIM]Cl/AlCl₃ 1:1.5 with 20 wt% fluorinated benzenes.

Of these electrolytes, 0.55 mL were filled into symmetric screw cells for electrochemical investigation. After cycling samples of the used electrolytes were taken and investigated by NMR spectroscopy.

1.5. NMR-Data and spectra

Pristine [EMIM]Cl/AlCl₃ 1:1.5 electrolyte



9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm

Figure S 7 ¹H NMR-spectrum (400.17 MHz, 298 K) of pristine IL EMIM/AlCl₃ 1:1.5. Calibration was executed according to 2FB signals in spectra with additional 2FB.

¹H NMR (400.17 MHz, 298 K, 2FB calibrated to 6.96 ppm, t calibrated to 1.29 ppm): δ = 8.11 (s, 1H, NCHN), 7.14 (m, 1H, H₃CNCH=CH), 7.09 (m, 1H, HC=CH-NEt), 3.99 (q, 2H, NCH₂CH₃), 3.68 (s, 3H, H₃C-N), 1.29 (t, NCH₂CH₃).

NMR data of the electrolytes post cycling that did show indications for degradation reactions

In the following, we include selected NMR spectra of those electrolyte systems, that did show signs of degradation after the number of cycles given in the caption.



Figure S 8 ¹⁹F NMR spectrum (188.31 MHz, 298 K) of a [EMIM]Cl/AlCl₃ 1:1.5 electrolyte containing 20 wt% 2FB after cycling. The cell ran for 788 cycles but short circuit was observed after 308 cycles. Two new signals at -139.53 and -144.12 ppm were observed after cycling.



Figure S 9 ¹⁹F NMR spectrum (188.31 MHz, 298 K) of a [EMIM]Cl/AlCl₃ 1:1.5 electrolyte containing 20 wt% FB after cycling for 779 cycles. New signal is marked at 118.72 ppm.



Figure S 10 ¹H NMR spectrum (300.18 MHz, 298 K) of a [EMIM]Cl/AlCl₃ 1:1.5 electrolyte containing 20 wt% benzene after cycling for 779 cycles. Possible impurity is marked at 7.38 ppm.

2. Investigation of AI/X-PVMPT cells

2.2. Characterization data of X-PVMPT



Figure S 11 Thermogravimetric analysis curves of **X-PVMPT** measured under N_2 and O_2 atmosphere at a heating rate of 10 °C min⁻¹.



Figure S 12 Differential scanning calorimetry curves of **X-PVMPT** measured under air atmosphere at a heating rate of 10 °C min⁻¹.

2.3. Battery cell housing



Figure S 13 Aluminium/X-PVMPT Swagelok[®] cell setup in a) exploded view and b) fully assembled view.

2.4. Electrochemical investigations

2.4.1. Current collector

Graphite could not be used as positive electrode current collector since **X-PVMPT** shows electrochemical activity until 2 V *vs.* Al/Al³⁺. Molybdenum was used as current collector since it showed no electrochemical activity of from 0.3 to 2.3 V *vs.* Al/Al³⁺ (Figure S 14).

Figure S 14 Cyclic voltammetry of graphite and molybdenum disks vs. Al. electrolyte: AlCl₃ : [EMIm]Cl (1.5 : 1.0). Potential window: $0-3 \vee vs. Al/Al^{3+}$. Scan rate: 10 mV s⁻¹.

2.4.2. Potential limit optimization

Since constant current measurement at higher current densities caused larger polarization of the electrochemical processes, several potential limits were investigated in order to get a wider stable potential window and to a reach higher capacity without side reactions.

Figure S 15 Constant current cycling of **X-PVMPT**-based electrodes *vs*. Al with various potential limits at 10 C rate (2.9 mA cm⁻², 2.2 A g⁻¹). Electrolyte: AlCl₃ : [EMIm]Cl (1.5 : 1.0) in different potential windows.

Figure S 16 Differential capacity curves for **X-PVMPT**-based electrodes *vs*. Al with various upper potential limits at 10 C rate (2.9 mA cm⁻², 2.2 A g⁻¹). Electrolyte: AlCl₃ : [EMIm]Cl (1.5 : 1.0).

Figure S 17 Differential capacity curves for **X-PVMPT**-based electrodes *vs*. Al with various lower potential limits at 10 C rate (2.9 mA cm⁻², 2.2 A g⁻¹). Electrolyte: AlCl₃ : [EMIm]Cl (1.5 : 1.0).

With the lower limit at 0.3 V and the upper limit at 2.3 V still some additional electrochemical activity appeared which can be attributed to adsorption of $AICl_4^-$ on the conductive carbon or a process from the molybdenum current collector. For all the further measurements shown in the main text the potential window was set to 0.3–2.2 V vs. AI/AI^{3+} .

2.4.3. Capacity contribution of carbon additive

Figure S 18 Constant current cycling of a acetylene black (90 wt%) and PVdF (10 wt%)based electrode vs. Al at a current density of 3.7 mA cm⁻² (similar current density used for constant current cycling of **X-PVMPT**-based electrodes at 10 C rate). Electrolyte: AlCl₃ : [EMIm]Cl (1.5 : 1.0). Potential window: 0.3 - 2.2 V vs.Al/Al³⁺.

Figure S 19 Cyclic voltammograms of an acetylene black (90 wt%) and PVdF (10 wt%)-based electrode vs. Al at varying scan rates. Electrolyte: AlCl₃ : [EMIm]Cl (1.5 : 1.0). Potential window: 0.3 – 2.2 V vs. Al/Al³⁺.

2.4.4. Precycling/preconditioning

Figure S 20 Constant current cycling, preconditioning/precycling of **X-PVMPT**-based electrodes vs. Al at 0.5 C for 50 cycles. Electrolyte: $AlCl_3 : [EMIm]Cl (1.5 : 1.0)$. Potential window: $0.3-2.2 V vs. Al/Al^{3+}$.

Figure S 21 Differential capacity curves for **X-PVMPT**-based electrodes *vs.* Al at 0.5 C during the preconditioning. Electrolyte: $AlCl_3$: [EMIm]Cl (1.5 : 1.0). Potential window: 0.3–2.2 V *vs.* Al/Al^{3+} .

Figure S 22 Cyclic voltammograms X-PVMPT-based electrodes vs. Al of the first 20 cycles at 0.2 mV s⁻¹. Electrolyte: AlCl₃ : [EMIm]Cl (1.5 : 1.0). Potential window: 0.3–2.2 V vs. Al/Al³⁺.

2.4.5. Calculation of standard deviation

The standard deviation and the error bars for the constant current cycling and rate capability test were calculated from the next equation:

$$\sigma = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (x_i - \mu)^2}$$
 (Eq. S1)

With σ the standard deviation, x_i the individual values and μ the mean.

2.4.6. Electrochemical characterization

Figure S 23 Differential capacity curves for **X-PVMPT**-based electrodes *vs.* Al at varying Crates. Electrolyte: AlCl₃ : [EMIm]Cl (1.5 : 1.0). Potential window: 0.3 - 2.2 V vs.Al/Al³⁺.

Figure S 24 Charge/discharge profiles of **X-PVMPT**-based electrodes *vs*. Al at varying Crates (solid lines charge, dashed lines discharge). Electrolyte: AlCl₃ : [EMIm]Cl (1.5 : 1.0). Potential window: 0.3 – 2.2 V *vs*. Al/Al³⁺.

Figure S 25 Constant current cycling of **X-PVMPT**-based electrodes *vs.* Al at 10 C rate. Electrolyte: AlCl₃ : [EMIm]Cl (1.5 : 1.0). Potential window: 0.3–2.2 V *vs.* Al/Al³⁺.

Figure S 26 Differential capacity curves for **X-PVMPT**-based electrodes *vs*. Al at 10 C until 5000 cycles. Electrolyte: AlCl₃ : [EMIm]Cl (1.5 : 1.0). Potential window: 0.3 – 2.2 V *vs*. Al/Al³⁺.

2.4.7. SEM/EDX data of X-PVMPT electrodes

The **X-PVMPT** electrodes for SEM/EDX investigations were preliminary pre-conditioned for 50 cycles at 0.5 C, then fully charged until the 2.2 V vs. Al/Al³⁺ potential limit or fully discharged until the 0.3 V vs. Al/Al³⁺ potential limit at 0.5 C. The cells were disassembled in an Ar-filled Glovebox with H₂O and O₂ levels <0.1 ppm, then the **X-PVMPT** electrodes were carefully rinsed several times with 1,2-difluorobenzene and dried at ambient temperature in the glovebox overnight. The electrodes were then transferred in the SEM chamber under inert conditions.

Charged electrode

Figure S 27 SEM of a charged electrode (charged to 2.2 V vs. Al|Al³⁺) with coloured element-specific overlays based on the energy-dispersive X-ray spectroscopy.

- Figure S 28 SEM of a charged electrode (charged to 2.2 V vs. Al|Al³⁺) with atomic concentration heat map overlays based on the energy-dispersive X-ray spectroscopy. All elements are quantitatively identified and their respective atomic concentration is indicated by the rainbow colour and can be converted into a percentage value using the axis on the right.
- Table S 4Quantification results of the energy-dispersive X-ray spectroscopy for the
whole area shown in Figure S 27 and Figure S 28.

Elomont	Impulsos	Mass concentration	Atomic concentration
Element	Impuises	normalized (%)	normalized (%)
С	1023457	58.94	75.09
Ν	27396	2.94	3.21
0	150467	7.29	6.97
F	7662	0.28	0.22
S	63657	2.90	1.39
Si	5359	0.26	0.14
AI	375372	8.53	4.84
Cl	295520	18.87	8.14

Discharged electrode

Figure S 29 SEM of a discharged electrode (discharged to 0.3 V vs. Al|Al³⁺) with coloured element-specific overlays based on energy-dispersive X-ray spectroscopy.

- Figure S 30 SEM of discharged (discharged to 0.3 V vs. Al|Al³⁺) electrode with atomic concentration heat map overlays based on energy-dispersive X-ray spectroscopy. All elements are quantitatively identified and their respective atomic concentration is indicated by the rainbow colour and can be converted into a percentage value using the axis on the right.
- Table S 5Quantification results of the energy-dispersive X-ray spectroscopy for the
whole area shown in Figure S 29 and Figure S 30.

Elomont	Impulsos	Mass concentration	Atomic concentration
Element	impuises	normalized (%)	normalized (%)
C	649193	66.16	80.88
N 11552		2.50	2.62
0	48967	4.70	4.32
F	1731	0.12	0.09
S	40642	3.57	1.63
Si	1567	0.15	0.08
Al	158101	7.20	3.92
Cl	127075	15.60	6.46

Pristine electrode

Figure S 31 SEM of a pristine **X-PVMPT**-based electrode with coloured element-specific overlays based on energy-dispersive X-ray spectroscopy.

- Figure S 32 SEM of a pristine **X-PVMPT**-based electrode with atomic concentration heat map overlays based on energy-dispersive X-ray spectroscopy. All elements are quantitatively identified and their respective atomic concentration is indicated by the rainbow colour and can be converted into a percentage value using the axis on the right.
- Table S 6Quantification results of the energy-dispersive X-ray spectroscopy for the
whole area shown in Figure S 31 and Figure S 32.

Element	Impulses	Mass concentration normalized (%)	Atomic concentration normalized (%)
C	1285087	89.29	93.83
N	10770	3.13	2.62
0	4128	0.45	0.36
F	8694	0.64	0.43
S	50758	6.31	2.48
Si	2322	0.17	0.08

The Al/S ratio and the Cl/Al data are based on the atomic concentration data shown in the tables above.

2.4.8. Electrochemical kinetics investigations

Diffusion-controlled vs. surface-controlled current deconvolution

The total current I_{tot} at a specific potential V is the sum of the diffusion-controlled and the surface-controlled current and is described by the following equation:

$$I_{tot}(V) = k_1 v + k_2 v^{0.5}$$
(Eq. S2)

Where $k_1 v$ corresponds to the surface-controlled current (proportional to the scan rate v) and $k_2 v^{0.5}$ the diffusion-controlled current.

The equation (Eq. S3) can be rearranged to:

$$\frac{I_{tot}(V)}{v^{0.5}} = k_1 v^{0.5} + k_2$$
(Eq. S3)

Linear fitting of $\frac{I_{tot}(V)}{v^{0.5}}$ vs. $v^{0.5}$ will give the k_1 (slope) and k_2 (intercept) values, which are the fraction of surface-controlled and diffusion-controlled current, respectively.

Figure S 33 Surface-controlled current contribution calculation of **X-PVMPT**-based electrodes vs. Al at 1.4 mV s⁻¹. Electrolyte: $AlCl_3$: [EMIm]Cl (1.5 : 1.0). Potential window: 0.3–2.2 V vs. Al/Al^{3+} .

Diffusion coefficient

Figure S 34 Galvanostatic intermittent titration technique measurements of **X-PVMPT**based electrodes vs. Al. Electrolyte: AlCl₃ : [EMIm]Cl (1.5 : 1.0). Procedure of pulses: 0.5 C for 6 min followed by 1 h OCV step.

2.5. Energy density calculation

The reactions occurring in the Al/X-PVMPT battery can be described as followed:

Negative electrode
$$4Al_2Cl_7^- + 3e^- \leftrightarrow 7AlCl_4^- + Al$$
 (I)

(with
$$Al_2Cl_7^- \leftrightarrow AlCl_3 + AlCl_4^-$$
) (II)

$$\frac{4}{3}\text{AlCl}_3 + e^- \leftrightarrow \text{AlCl}_4^- + \frac{1}{3}\text{Al}$$

Positive electrode

electrode
$$\frac{1}{2}$$
XPVMPT + AlCl₄⁻ $\leftrightarrow \frac{1}{2}$ XPVMPT(AlCl₄)₂ + e⁻ (IV)

Overall reaction
$$\frac{1}{2}$$
XPVMPT + $\frac{4}{3}$ AlCl₃ $\leftrightarrow \frac{1}{2}$ XPVMPT(AlCl₄)₂ + $\frac{1}{3}$ Al (V)

The energy density of the Al/**X-PVMPT** battery can be calculated considering the mass of the active material and the minimal required mass of electrolyte:

$$Energy \ density, E = C_{total}V \tag{Eq. S4}$$

with *E* the energy density in Wh kg⁻¹, *V* the average voltage of the battery and C_{total} the total specific capacity in mAh g⁻¹, which can be determined using the following equation:^[5]

$$C_{total} = \frac{xF(r-1)C_C}{xF(r-1) + C_C \left(rM_{AlCl_3} + M_{EMImCl}\right)}$$
(Eq. S5)

Where $F = 26,800 \text{ mAh mol}^{-1}$ (Faraday constant), x is number of electrons used to reduce one mole of the anodic material (here $AlCl_3$), r the molar ratio of $AlCl_3$ to EMImCl, C_C the specific capacity of the **X-PVMPT** positive electrode, M_{AlCl_3} and M_{EMImCl} are the molecular weights in g mol⁻¹ of $AlCl_3$ and EMImCl, respectively.

According to equation V, the x value for **X-PVMPT** is $\frac{3}{4}$, and with r = 1.5, the C_{total} and the energy density can be calculated:

$$C_{total} = \frac{\frac{3}{4} * 26,800 * 0.5 * 161}{\frac{3}{4} * 26,800 * 0.5 + 161(1.5 * 133.33 + 146.62)}$$
(Eq. S6)
$$C_{total} = 24.6 \ mAhg^{-1}$$
Energy density = 30 Wh kg^{-1}

Calculated from the data experiment Figure S 24 with the average voltage of 1.22 V (at 0.5 C)

(III)

2.6. AI/X-PVMPT batteries put to work

Figure S 36 Red LED lighting with series-connected Al/**X-PVMPT** batteries.

3. Literature comparison

Table S 7Comparison of specific discharge capacity of aluminium-organic batteries at
similar current densities (with r the molar ratio of AlCl₃ to EMImCl).

Anode/Cathode	r	Current density / A g ⁻¹	Specific discharge	Reference	
			capacity / mail g		
Al/X-PVMPT	1.5	4.4	136	This work	
AI/X-PVMPT	1.5	11	105	This work	
AI/X-PVMPT	1.5	22	64	This work	
Al/Graphita	2.0	5.0	105	[6]	
Al/Graphite	2.0	(up to 20.0)	(100)		
AL/Cranhana	1 2	10	120	[7]	
Al/Graphene	1.5	(up to 200)	(120)		
Al/Δ-PQ	1.5	5	80	[8]	
Al/PI-MOF	-	5	55	[9]	
AI/TDK	1.5	2	70	[10]	
Al/(N4) _n	1.5	2	120	[11]	
AI/PTDCA	-	5	40	[12]	
AI/ANP	1.5	5	120	[13]	
AI/DANP	1.5	5	110	[13]	
Al/Pyr	1.5	5	40	[13]	

4. DFT calculations

All calculations were performed on Justus High Performance Computing Cluster (JUSTUS 2). DFT calculations were performed with the TURBOMOLE v7.5.0 program package.^[14] The resolution-of-identity^[15] (RI, RIJDX for SP) approximation for the Coulomb integrals was used in all DFT calculations employing matching auxiliary basis set def2-XVP/J.^[16] Further, the D3 dispersion correction scheme^[18,19] with the Becke-Johnson damping function was applied.^[17,18]

The geometries were first optimized without symmetry restrictions (in neutral oxidation state for *N*-methylphenothiazine (**MPT**) and oxidized state C for (*N*-methylphenothiazine dimer) **MPT-dimer**) using the PBEh-3c composite scheme^[19] followed by harmonic vibrational vibrational frequency analysis to confirm minima as stationary points. These geometries were used as an input for further geometry optimizations of the neutral (A), half oxidized (B), oxidized (C) and fully oxidized form (D). They were each optimized on the B3LYP-D3BJ/def2-TZVP level of theory^[20,21] for **MPT** and BP86-D3BJ/def2-TZVP^[21–23] for the model compound **MPT-dimer** (It was shown before, that BP86 gives similar results as B3LYP with less computational effort).^[22–24] In all further calculations the COSMO solvation model, as implemented in TURBOMOLE^[25] (ε = 18.0) was used. Structures were optimized with unrestricted orbitals for the radical cation forms and with restricted orbitals for the neutral and the dication form. For vibrational contributions and the free energy calculations the rigidrotor-harmonic-oscillator (RRHO^[26]) approximation was made using the FREEH tool (default scaling factor of 0.9914) from TURBOMOLE. Single point energies were obtained in the gas phase on the B3LYP-D3BJ/def2-TZVP level of theory^[20,21] for all compounds.

Detailed calculations for *N*-methylphenothiazine MPT

Figure S 37 Selected frontier molecular orbitals of **MPT** in the neutral, radical cationic and dicationic form (B3LYP-D3BJ/def2-TZVP+COSMO).

Detailed calculations for the *N*-methylphenothiazine dimer MPT-Dimer

Figure S 38 Optimized structures of **MPT-dimer** in the oxidation states A (neutral), B (charge 1+), C (charge 2+) and D (charge 4+) (BP86-D3BJ/def2-TZVP+COSMO).

Figure S 39 Selected frontier molecular orbitals of **MPT-dimer** in oxidation state A, B, C and D (BP86-D3BJ/def2-TZVP+COSMO).

Calculations of redox potentials

The electrochemical redox potentials were calculated as described by GRIMME and coworkers.^[27]

The redox potential relative to the vacuum level is calculated by the Nernst equation given as

$$E_{\rm R/O}^{\rm o} = -\frac{\Delta_r G_{\rm R/O}^{\rm o}}{n_e \rm F}$$
(Eq. S7)

where $\Delta_r G^o_{R/O}$ is the free energy change of the investigated oxidation process at standard conditions, n_e is the number of transferred electrons, and F is the Faraday constant.

Differences in the Gibbs free energy were calculated based on a thermodynamic Born-Haber cycle according to

$$\Delta_r G^o_{\rm R/O} = \rm{IP} + \Delta G^o_{\rm RRHO} + \Delta \delta G^o_{\rm solv}$$
(Eq. S8)

Where IP is the adiabatic electronic ionization potential (calculated from the energies of a reduced and an oxidized species) of the reduced species, $\Delta G_{\rm RRHO}^{0}$ is the difference of the thermostatistical correction obtained by a modified rigid-rotor-harmonic-oscillator approximation (RRHO)^[26] of a reduced and an oxidized species, and $\Delta \delta G_{\rm solv}^{0}$ is the difference of the solvation free energies of a reduced and an oxidized species obtained from a COSMO-calculation.

MPT:

Table S 8Electronic energies (B3LYP-D3BJ/def2-TZVP//BP86-D3BJ/def2-TZVP), zero-
point vibration energies, G^o_{RRHO} from vibrational frequency calculations and
 δG^o_{Solv} from COSMO calculations (BP86-D3BJ/def2-TZVP) (ϵ = 18.0)) of **MPT** in
oxidation state A (neutral), C (radical cation) and D (dication).

Oxidation state	E(B3LYP) (Hartree)	ZPE (Hartree)	$\delta G_{ m solv}^{ m o}$ (Hartree)	G _{RRHO} (kJ/mol)
A (neutral)	-954.8388	0.2057	-0.0106	566.1800
C (radical cation)	-954.6594	0.2066	-0.0644	568.7000
D (dication)	-954.4361	0.2070	-0.2440	570.6100

Table S 9 Redox potentials and free energy changes for the oxidation processes of **MPT** (B3LYP-D3BJ/def2-TZVP ($\epsilon = 18.0$)).

Redox	ID (keel/mel) ^a	$\Delta \delta G_{ m solv}^{ m o}$	$\Delta G^{o}_{\rm RRHO}$	$\Delta_r G^{o}_{\rm R/O}$	
Process		(kcal/mol) ^b	(kcal/mol) ^c	(kcal/mol) ^d	$L_{\rm R/O}$ (V)
$A \rightarrow C$	113.08	-33.78	0.60	79.90	-3.46
$C \rightarrow D$	140.44	-112.73	0.46	28.16	-1.22
$A \rightarrow D$	253.52	-146.51	1.06	108.07	-4.69

^a IP = Difference in the calculated energies (E_{EI} + ZPE) of the two species; ^b Difference in δG_{solv}^{o} values of the two species; ^c Difference in G_{RRHO}^{o} values of the two species; ^d Calculated according to Eq. S8; ^e Calculated according to Eq. S7.

MPT-dimer:

Table S 10Electronic energies (B3LYP-D3BJ/def2-TZVP//BP86-D3BJ/def2-TZVP), zero-
point vibration energies, G^o_{RRHO} from vibrational frequency calculations and
 δG^o_{solv} from COSMO calculations ((BP86-D3BJ/def2-TZVP ($\epsilon = 18.0$)) of **MPT-**
dimer in oxidation state A (neutral), B (radical-cation), C (dication) and D ("di-
dication").

Oxidation state	E(B3LYP) (Hartree)	ZPE (Hartree)	$\delta G_{ m solv}^{ m o}$ (Hartree)	G ^o _{RRHO} (kJ/mol)
А	-2105.0179	0.5183	-0.0188	1431.31
В	-2104.8518	0.5197	-0.0582	1434.96
С	-2104.6651	0.5213	-0.1977	1438.61
D	-2104.1744	0.5323	-0.6522	1438.86

Table S 11Redox potentials and free energy changes for the oxidation processes of MPT-
dimer (B3LYP-D3BJ/def2-TZVP//BP86-D3BJ/def2-TZVP ($\varepsilon = 18.0$)).

Redox	IP (kcal/mol) ^a	$\Delta \delta G_{ m solv}^{ m o}$	$\Delta G^{o}_{\rm RRHO}$	$\Delta_r G^{o}_{\rm R/O}$	$E^{\rm o}_{\rm R/O}$ (V) ^e
process		(kcal/mol) ^b	(kcal/mol) ^c	(kcal/mol) ^d	
$A \rightarrow B$	104.18	-24.73	0.87	81.22	-3.52
$B \rightarrow C$	117.17	-87.56	0.87	31.47	-1.36
$C \rightarrow D$	307.93	-285.17	0.06	29.75	-0.64

^a IP = Difference in the calculated energies (E_{EI} + ZPE) of the two species; ^b Difference in δG_{solv}^{o} values of the two species; ^c Difference in G_{RRHO}^{o} values of the two species; ^d Calculated according to Eq. S8; ^e Calculated according to Eq. S7.

Cartesian coordinates of calculated structures

Cartesian coordinates of **MPT** in the neutral form (A):

	х	У	Z
С	3.5146546	0.2435188	0.5276899
С	3.6255497	-1.1277887	0.3390755
С	2.5238275	-1.8422417	-0.1216518
С	1.3366283	-1.185775	-0.4213821
С	1.2109222	0.1997107	-0.2285037
С	2.3163389	0.9004269	0.2636065
S	-0.0103874	-2.0808504	-1.1392123
С	-1.3457161	-1.1811532	-0.4054623
С	-1.2128524	0.2038768	-0.2140553
Ν	-0.0017443	0.8441991	-0.5374325
С	-2.5315649	-1.8334574	-0.0916242
С	-3.6251559	-1.1151677	0.3823375
С	-3.5072232	0.2557386	0.5696083
С	-2.3098667	0.9084487	0.2911962
С	0.0002544	2.2964151	-0.624609
Н	4.358375	0.8133591	0.8954694
Н	4.5539615	-1.6415038	0.5508058
Н	2.5879162	-2.9130996	-0.2686575
Н	2.2487684	1.9630339	0.4431481
Н	-2.6011519	-2.9040844	-0.2377998
Н	-4.5526934	-1.6256846	0.6053334
Н	-4.3444671	0.8285432	0.9474476
Н	-2.2363928	1.9708441	0.4696793
Н	-0.8843095	2.6187822	-1.1695133
Н	0.879237	2.615641	-1.1802821
Н	0.0070917	2.7882686	0.3547882

Cartesian coordinates of **MPT** in the radical cationic form (B):

	х	У	Z
С	3.6240084	0.2927693	0.2531983
С	3.7335572	-1.095344	0.0977313
С	2.598754	-1.8471573	-0.1037787
С	1.3423315	-1.2299281	-0.1653034
С	1.2222914	0.1757055	-0.0448241
С	2.3990809	0.9167836	0.1815074
S	-0.0064834	-2.2711294	-0.4308237
С	-1.3485854	-1.2252429	-0.1499042
С	-1.2222067	0.1799217	-0.0303597
Ν	0.0004848	0.8205247	-0.1513851
С	-2.6064111	-1.838054	-0.0742343

-3.7360597	-1.0824076	0.1414583
-3.6197092	0.3051374	0.2969804
-2.3935374	0.9248909	0.2110041
0.0019354	2.2763928	-0.3575059
4.5081858	0.8865504	0.440686
4.700219	-1.5767656	0.149552
2.6612707	-2.9225906	-0.2080189
2.3477575	1.9825439	0.3314936
-2.673922	-2.913153	-0.1788136
-4.7037121	-1.5604789	0.2045054
-4.4994058	0.9018567	0.4958691
-2.3365679	1.9902768	0.3616724
-0.8786564	2.5516872	-0.926082
0.8755884	2.5479895	-0.9384696
0.0097918	2.809221	0.593845
	-3.7360597 -3.6197092 -2.3935374 0.0019354 4.5081858 4.700219 2.6612707 2.3477575 -2.673922 -4.7037121 -4.4994058 -2.3365679 -0.8786564 0.8755884 0.0097918	-3.7360597-1.0824076-3.61970920.3051374-2.39353740.92489090.00193542.27639284.50818580.88655044.700219-1.57676562.6612707-2.92259062.34775751.9825439-2.673922-2.913153-4.7037121-1.5604789-4.49940580.9018567-2.33656791.9902768-0.87865642.55168720.87558842.54798950.00979182.809221

Cartesian coordinates of **MPT** in the dicationic form (C):

	х	У	Z
С	3.6181804	0.2954051	0.1432312
С	3.7160915	-1.1118992	0.0270724
С	2.585188	-1.8698436	-0.0800312
С	1.3255906	-1.2397874	-0.0829509
С	1.2130149	0.1939673	-0.0155061
С	2.4103352	0.9351834	0.1137532
S	-0.0049817	-2.2585496	-0.1868536
С	-1.3309887	-1.2352586	-0.0684709
С	-1.2126613	0.1980857	-0.0008564
Ν	0.0008367	0.8187103	-0.0739958
С	-2.5927201	-1.8609077	-0.0521532
С	-3.719596	-1.0991691	0.069774
С	-3.6153699	0.3075612	0.1873691
С	-2.4057778	0.9431988	0.1441333
С	0.0029974	2.2961231	-0.2291887
Н	4.5192032	0.8801315	0.2648986
Н	4.6873746	-1.5859095	0.0379783
Н	2.6357667	-2.9481301	-0.1487283
Н	2.386134	2.0041702	0.2316805
Н	-2.6478472	-2.9388661	-0.1224255
Н	-4.6923062	-1.5698707	0.0919956
Н	-4.5127678	0.895157	0.3213854
Н	-2.3764406	2.0119499	0.2631631
Н	-0.8764425	2.589027	-0.7849941
Н	0.8726787	2.5837902	-0.8030183
Н	0.0145078	2.7657309	0.7527383

Cartesian coordinates of MPT-dimer in state A:

	Х	У	Z
С	-4.5346795	1.9654176	-2.3723044
С	-3.0498699	2.1752939	-2.0185442
С	-2.226689	2.3524521	-3.3099843
С	-0.787605	2.8922538	-3.1449239
С	-0.215676	3.3004099	-4.5101056
С	-2.2387418	-0.2076555	-1.5809514
С	-2.583014	1.0585528	-1.0997179
С	-2.5216603	1.2642671	0.2861486
С	-2.1392492	0.2426965	1.1566704
С	-1.7487062	-1.0171038	0.6626804
С	-1.8009534	-1.2190426	-0.7238194
S	-2.2099232	0.4920845	2.9105538
С	-0.8223314	-0.4982971	3.3899789
С	-0.5298178	-1.6708683	2.6629255
Ν	-1.3237924	-2.0267715	1.5534025
С	-0.0527898	-0.1326851	4.4953976
С	1.0026091	-0.9453787	4.9200065
С	1.3048039	-2.1038161	4.2053722
С	0.5584864	-2.4549117	3.0776165
С	-1.2102739	-3.3843443	1.0409439
С	0.0972852	1.9013701	-2.4170379
С	0.3876964	2.0882495	-1.0613765
С	1.0090534	1.0954583	-0.3053396
С	1.4132418	-0.1160631	-0.9003472
С	1.2331155	-0.2506855	-2.2866422
С	0.5646441	0.7306362	-3.0229495
S	1.1225436	1.308814	1.4398642
С	2.5138732	0.2793671	1.781377
С	2.7509989	-0.8743652	1.0013461
Ν	1.9399496	-1.1599433	-0.1119789
С	3.3067834	0.5633824	2.8940181
С	4.3229296	-0.3124827	3.2855232
С	4.5624284	-1.457799	2.5270531
С	3.801722	-1.7255019	1.3846255
С	2.0517822	-2.4765449	-0.719857
Н	-4.9226823	2.8121826	-2.9578547
Н	-5.1440852	1.8626532	-1.4633509
Н	-4.6613998	1.0491116	-2.9688336
Н	-2.9716059	3.1163523	-1.4467257
Н	-2.7754187	3.061597	-3.9515265
Н	-2.1927504	1.402184	-3.8691532
Н	-0.8488177	3.7975229	-2.5167001
Н	0.8046574	3.6961939	-4.4077816
Н	-0.8426091	4.0745691	-4.9756091

Н	-0.1788095	2.4439085	-5.1994791
Н	-2.2622666	-0.4095953	-2.6517399
Н	-2.7778943	2.2423674	0.6995443
Н	-1.4853794	-2.170598	-1.1476236
Н	-0.2881016	0.7917366	5.0248606
Н	1.5956249	-0.6575197	5.7878428
Н	2.1477756	-2.7281065	4.5008147
Н	0.8345041	-3.3424774	2.5113762
Н	-1.1885229	-4.0820401	1.8860461
Н	-0.3078943	-3.5487832	0.4278405
Н	-2.0915435	-3.6073929	0.4283665
Н	0.0540762	2.9990239	-0.5594731
Н	1.5779374	-1.1490311	-2.7954101
Н	0.3835433	0.5522537	-4.0839567
Н	3.0967668	1.4617219	3.4761346
Н	4.9149841	-0.0982355	4.1752933
Н	5.3552125	-2.1509393	2.8111589
Н	4.0274191	-2.6110734	0.794043
Н	2.1094762	-3.2319677	0.0721395
Н	2.936266	-2.5847908	-1.3723211
н	1.1533637	-2.6672732	-1.3175461

Cartesian coordinates of **MPT-dimer** in state B:

	х	У	Z
С	-4.5493875	1.9453427	-2.3335013
С	-3.0491865	2.1404439	-2.0466364
С	-2.2770938	2.3344198	-3.3688264
С	-0.8589117	2.9317992	-3.2348841
С	-0.2673694	3.2268475	-4.6223164
С	-2.5086728	-0.3272716	-1.6523079
С	-2.532202	0.9997119	-1.1906829
С	-2.0796924	1.2325021	0.1074777
С	-1.611858	0.1964787	0.9219633
С	-1.5970256	-1.141666	0.4587482
С	-2.0499321	-1.3703486	-0.8560565
S	-1.1120459	0.6282096	2.5404271
С	-0.1773399	-0.7735975	3.0108543
С	-0.3146392	-2.0249034	2.361988
Ν	-1.1689623	-2.1983794	1.2678684
С	0.6703952	-0.6269365	4.1156945
С	1.3836789	-1.7140061	4.6106407
С	1.2648439	-2.9526347	3.9749727
С	0.4398492	-3.1054098	2.8635753
С	-1.5012821	-3.5624177	0.8571594
С	0.0387525	2.0308041	-2.4190999

С	0.5348198	2.4327549	-1.1823305
С	1.2025119	1.5369706	-0.3377195
С	1.422672	0.1938672	-0.7336386
С	1.0285115	-0.1629777	-2.0391318
С	0.3418223	0.7275549	-2.8495798
S	1.6145304	2.1242079	1.2522034
С	2.655361	0.8585642	1.8547188
С	2.7229643	-0.4263125	1.2597072
Ν	1.9766036	-0.7561945	0.1241432
С	3.3955917	1.1568403	3.0075223
С	4.2038627	0.1922496	3.5967411
С	4.2910391	-1.0752314	3.0105755
С	3.5755463	-1.3750625	1.8563415
С	1.8832112	-2.1639512	-0.2575449
Н	-4.9542811	2.8162345	-2.8680622
Н	-5.11506	1.8158255	-1.4004893
Н	-4.7161126	1.0552638	-2.9581023
Н	-2.934342	3.0649374	-1.4563834
Н	-2.8644152	3.0143908	-4.0059653
Н	-2.2230712	1.3757668	-3.9113604
Н	-0.9515897	3.8855976	-2.6895915
н	0.7322221	3.6747355	-4.5361343
н	-0.913425	3.9242875	-5.1740611
н	-0.1780282	2.3069767	-5.218681
н	-2.8349447	-0.5561278	-2.6674573
Н	-2.0686261	2.2510501	0.5002317
Н	-2.0186279	-2.3733247	-1.2745643
Н	0.7566903	0.3522747	4.5872934
н	2.0356993	-1.5906398	5.4737318
н	1.8337463	-3.8105184	4.3326728
Н	0.3907894	-4.0752839	2.3747969
н	-1.5731248	-4.1950086	1.7468161
н	-0.7514493	-3.9888322	0.1722138
Н	-2.4763431	-3.5571013	0.3616747
Н	0.3415253	3.446173	-0.8243532
н	1.2437064	-1.1579238	-2.4190747
н	0.0124854	0.3882401	-3.8320367
н	3.3176931	2.1550276	3.4405829
н	4.7654582	0.4279611	4.49989
н	4.9313617	-1.8398463	3.4497568
Н	3.688353	-2.3595155	1.4108582
Н	1.8682121	-2.7769814	0.648697
Н	2.7204973	-2.4822775	-0.8962277
Н	0.944035	-2.3236294	-0.7957371

Cartesian coordinates of **MPT-dimer** in state C:

	х	У	Z
С	-4.605558	1.8910741	-2.3616756
С	-3.1213851	2.1489786	-2.0417525
С	-2.3209162	2.3482994	-3.3472621
С	-0.8998813	2.9317129	-3.1775222
С	-0.2876694	3.2582407	-4.5501992
С	-2.5010125	-0.2942553	-1.6419028
С	-2.5721596	1.0376836	-1.1755466
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Ν	-0.9662425	-2.0996467	1.1995086
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С	0.4894034	-2.9914973	2.9332753
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Н	-2.8887615	3.0422982	-3.9852675
Н	-2.2674759	1.3964682	-3.9012196
Н	-0.990325	3.8696306	-2.6065338
Н	0.7149508	3.6926836	-4.4397137
Н	-0.9219486	3.9792856	-5.0835368

Н	-0.2039276	2.3563035	-5.1735628
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Н	-2.1982145	-3.5104385	0.2519358
Н	0.3033716	3.37443	-0.7544042
Н	1.2405069	-1.1694434	-2.521605
Н	-0.0264962	0.4041223	-3.8499937
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Н	1.9431861	-2.8818022	0.4679332
Н	2.8946836	-2.4910799	-0.9939025
н	1.1114958	-2.4048323	-1.0234225

Cartesian coordinates of **MPT-dimer** in state D:

	х	У	Z
С	-4.7553487	1.9541167	-2.7963386
С	-3.3609842	2.1709081	-2.1826532
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С	-0.0479722	3.0635057	-4.134732
С	-3.0836352	-0.2881405	-1.5880965
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С	-2.431249	1.4057201	0.0106695
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S	-1.0798268	0.9365735	2.2167191
С	-0.2469622	-0.4418727	2.7546844
С	-0.4465591	-1.7526103	2.1899176
Ν	-1.3547339	-1.9723503	1.1735632
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С	1.2375426	-2.5923321	3.7148891
С	0.3257466	-2.8202379	2.7062056

С	-1.7021928	-3.3819183	0.8654705
С	-0.0998501	1.7997244	-2.030425
С	0.6135157	2.241379	-0.9245176
С	1.4186065	1.3597726	-0.1862294
С	1.5019406	-0.0446998	-0.5298202
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S	2.256698	2.039804	1.1266062
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Н	2.9820367	-2.5885047	-0.8864065
Н	1.2150064	-2.583472	-0.6264229

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