Supporting Information

Polymer-induced Self-assembly of Small Organic Molecules into Hierarchical Ultralong Microbelts with Electronic Conductivity

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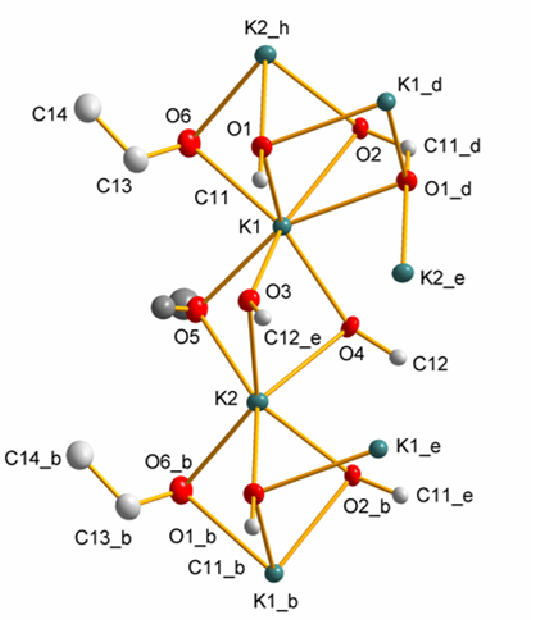

Figure S1. ORTEP-Plot of the coordination environment of **PTCAPS**
Symmetry codes: b = 1+x, y, z; d = -x, 1-y, 1-z; e = 1-x, 1-y, 1-z; h = -1+x, y, z

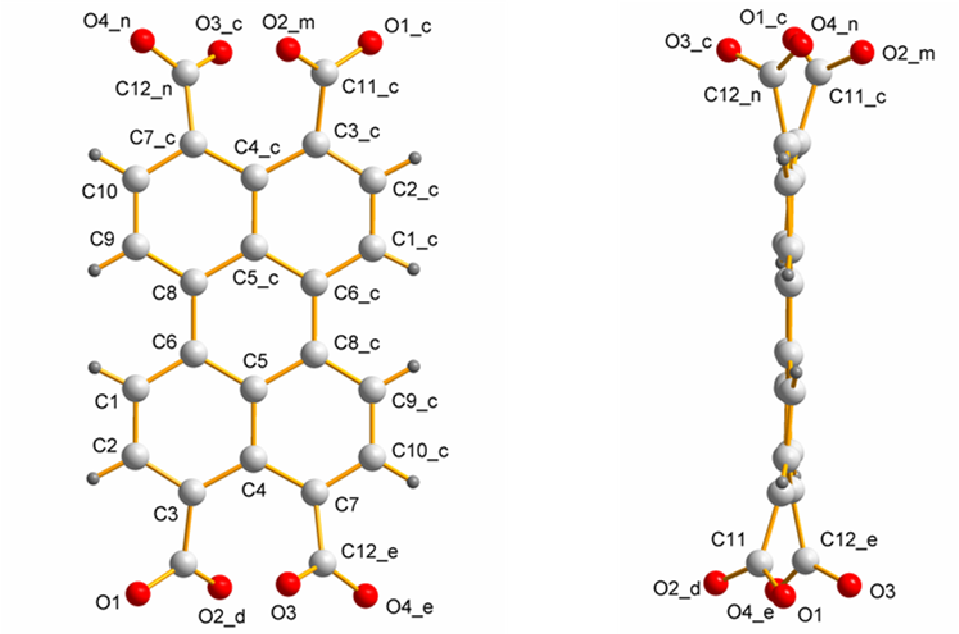

Figure S2. Numbering scheme of the perylene-tetracarboxylate moiety of **PTCAPS** Symmetry codes: m = x, -1+y, -1+z; n = -1+x, -1+y, -1+z

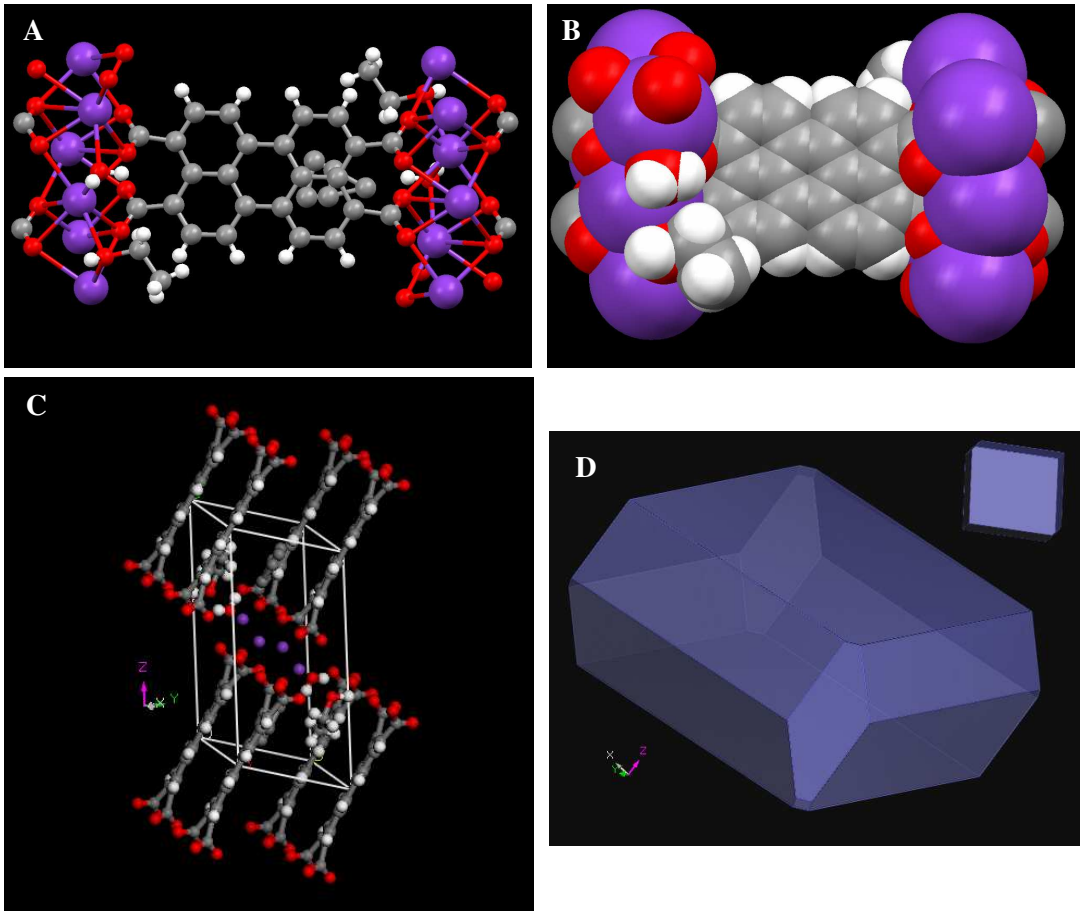

Figure S3. (A) Ball and stick presentation, and (B) space filling representation of the PTCAPS molecule with associated potassium ions and ethanol molecules in the triclinic crystal structure. Grey = carbon, white = hydrogen, red = oxygen, purple = potassium. (C) the unit cell of the crystal with 8 PTCAPS molecules at the corner of the unit cell, and (D) the default equilibrium morphology calculated in vacuum with MS Modelling Materials studio (Accelrys). The inset is a view from the most exposed crystal face.

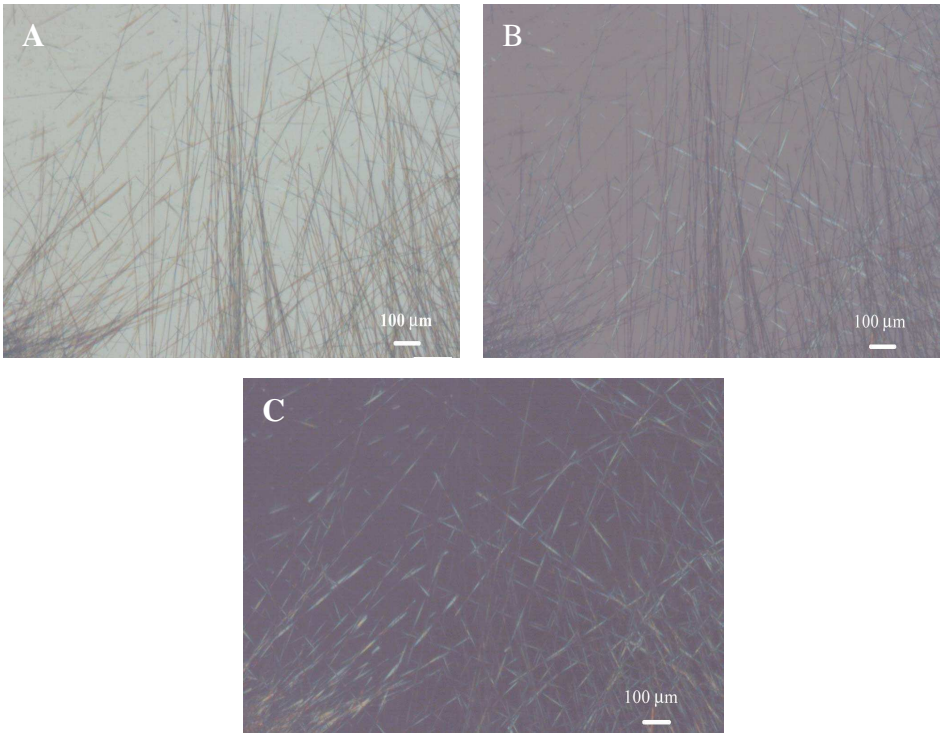

Figure S4. Polarized optical microscopy images of the belts with different relative angle of the polarizer and the analyzer: (A) 0 °, (B) 45 °, and (C) 90 °**.** It shows a rather perfect pleiochromism of the belts.

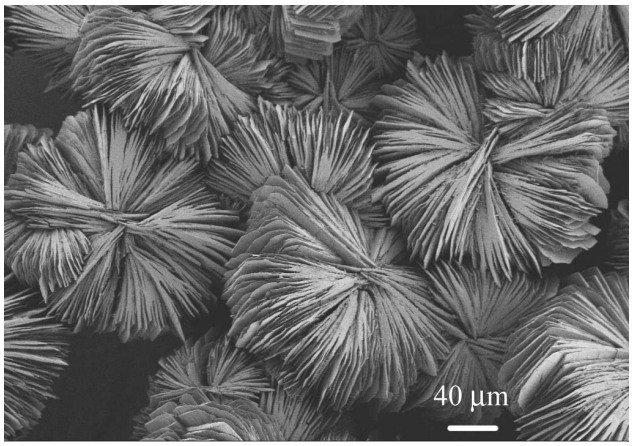

Figure S5. SEM images of PTCAPS crystal in the presence of PEG-b-PEI (1.0 g/L) at the pH of 9.6.

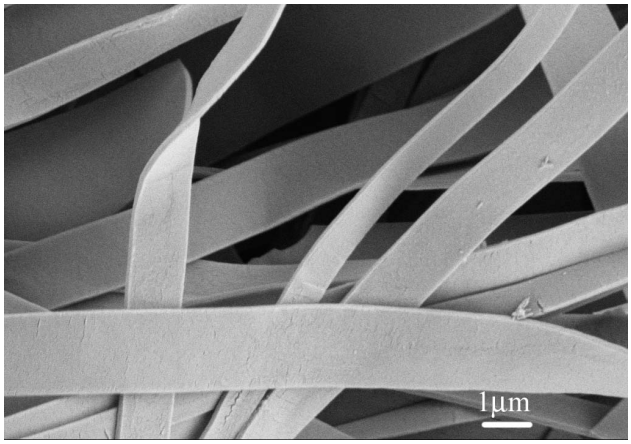

Figure S6. High magnification SEM image of PTCAPS crystal in the presence of PEG-b-PEI (1.0 g/L) at the pH of 8.4 after cooling from 65 °C to 4 °C.

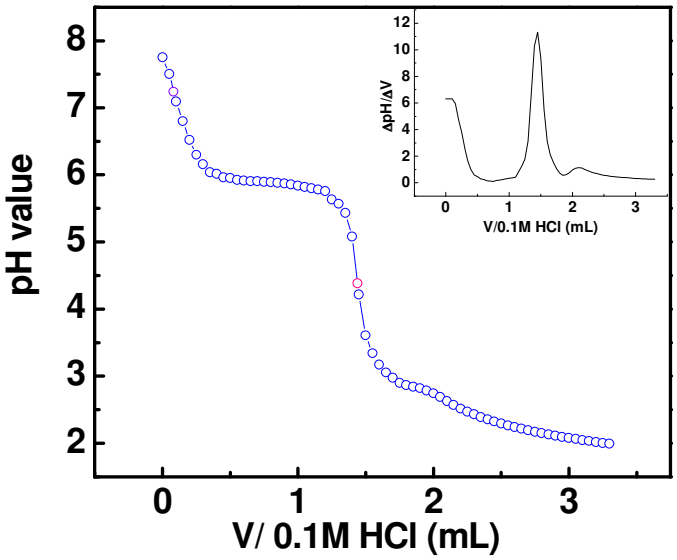

Figure S7. Titration curve of PTCAPS. pK_a was determined by titration curve and corresponding 1 order derivative curve shown in the inset. pKa values from this curve are pH = 5.9 and less clearly pH 2.6.

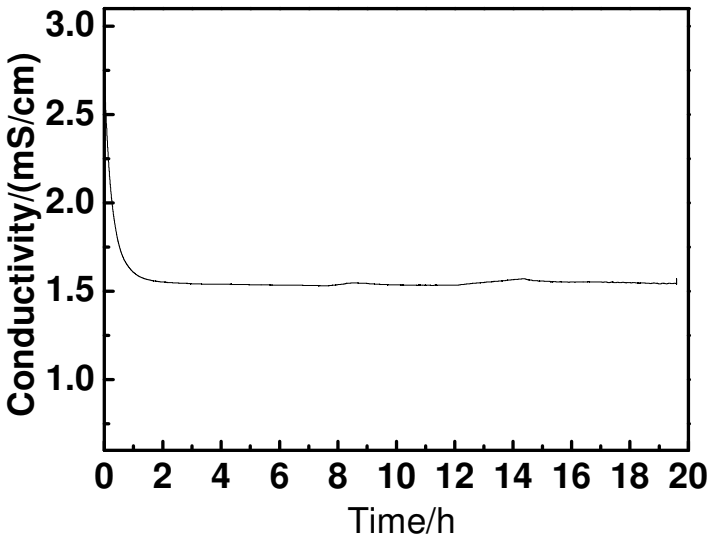

Figure S8. Time-dependent conductivities of PTCAPS crystallization solutions in the presence of PEG-b-PEI (1.0 g/L) at the pH of 8.4 after cooling from 65 °C to room temperature.

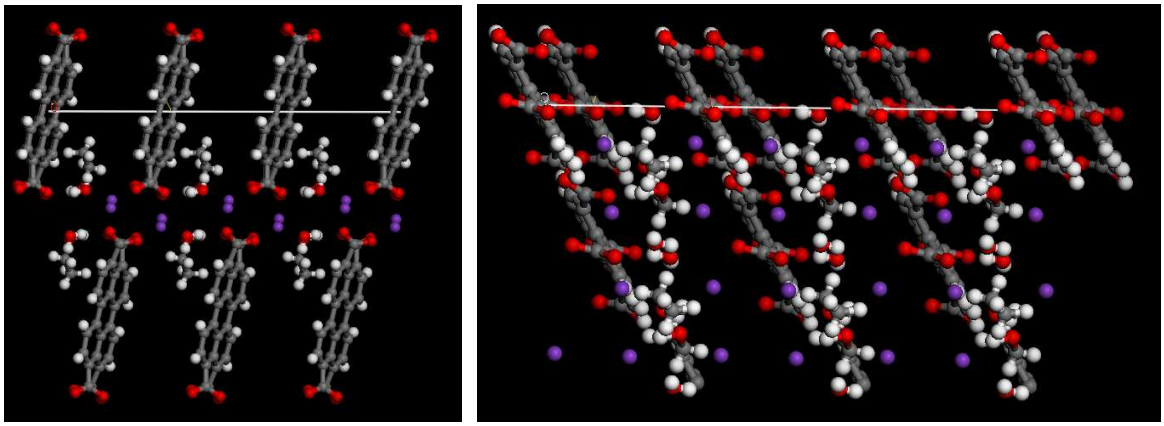

Figure S9. Surface slices of the (001) and (10-1) faces of PTCAPS. The surfaces are indicated by the white line.

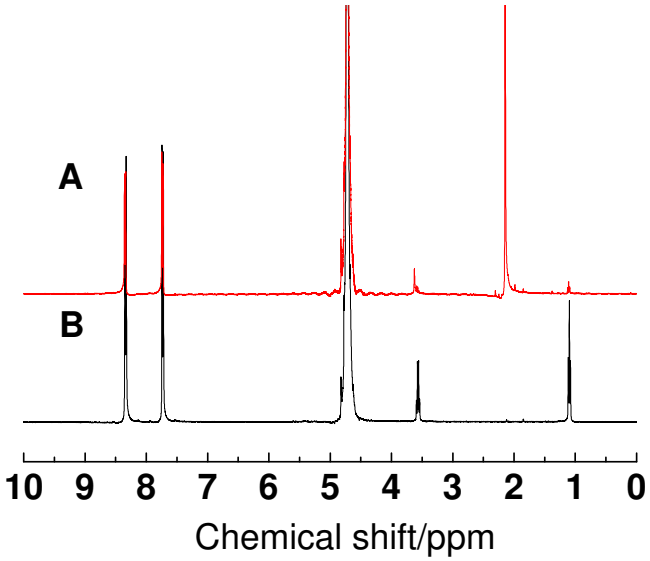

Figure S10. ^{1}HNMR spectra of (A) the PTCAPS microbelts and (B) PTCAPS powder in D_2O.

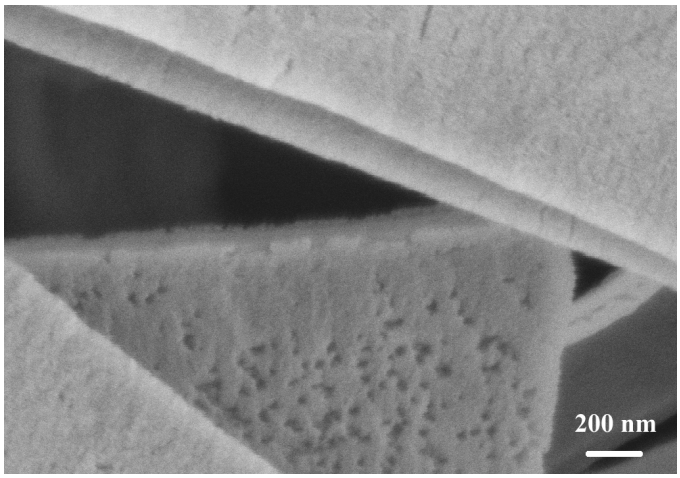

Figure S11. SEM image of belts after etching at pH 12 for several minutes.

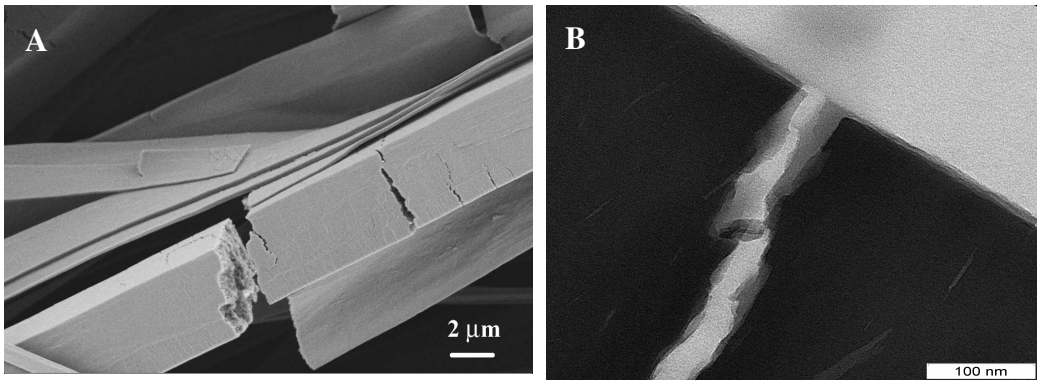

Figure S12. (A) SEM image of a cleavage plane and (B) TEM image of a cleavage plane showing the inner nanoparticular mesostructure.

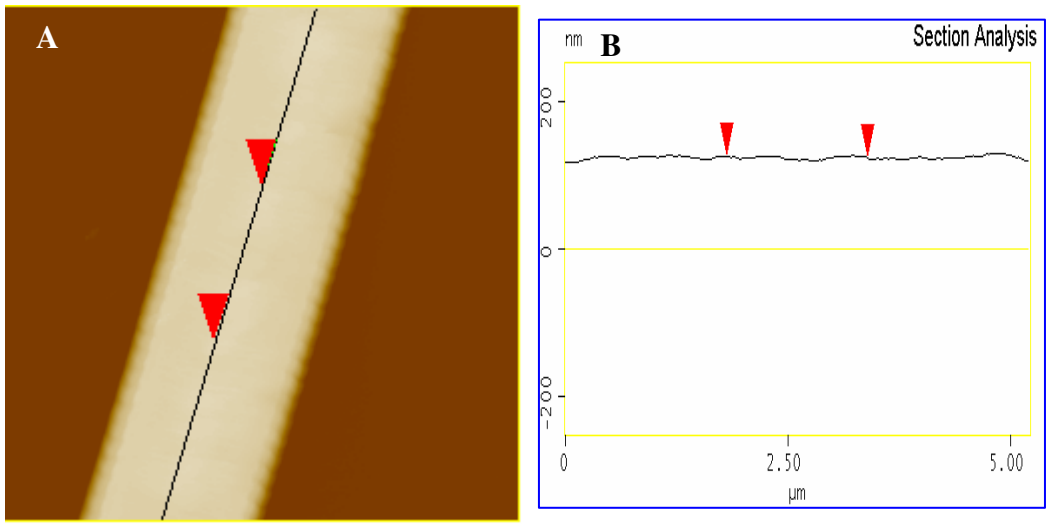

Figure S13. (A) AFM image of a single belt cast on the mica substrate. (B) Line-scan profile along the black line in (A).

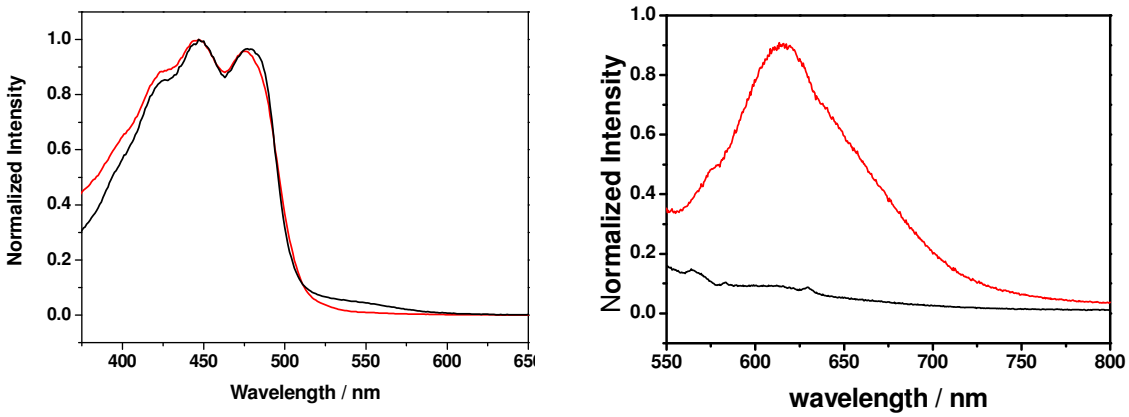

Figure S14. (A, left) Normalized diffuse reflectance spectra of the PTCAPS crytal powder (red line) and the belt powder (black line). (B, right) Normalized emission spectra of the PTCAPS crystal powder (red line) and the belt powder (black line) excited at λ_{ex} = 530 nm.

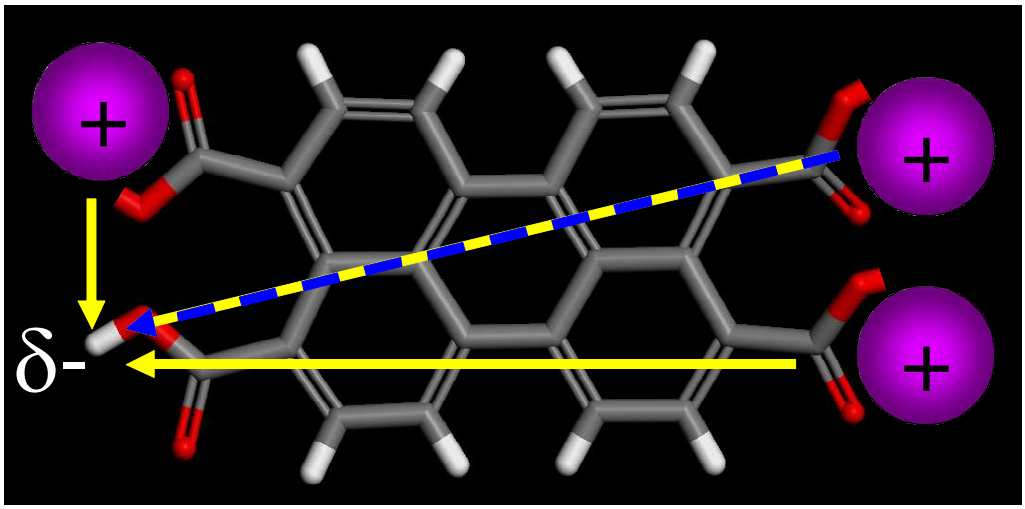

Figure S15. Development of a dipole moment from a partially non-neutralized perylene-3,4,9,10-tetracarboxylic-acid. The yellow arrows represent individual dipole fields, the dashed arrow the resulting dipole field.

X-ray structure determination

The crystal was embedded in perfluoropolyalkylether oil and mounted on a glass fibre. The X-ray analyses were performed on an Imaging Plate Diffraction System IPDS-2 (Stoe) at 210 K with graphite-monochromated MoK_α radiation (λ = 0.71073 Å) at 50 kV and 40 mA (90 frames, $\Delta\omega$=1°, 1 min exposure time per frame). Due to a decay of the crystal, for which a corresponding correction was not succesful, only the first 90 frames could be taken into account. The data were corrected for Lorentz, polarizsation and extinction effects, but no absorption correction was applied. The structure was solved with SHELXS-97 using direct methods, and refined with full-matrix least-squares on F^2 with the program SHELXL-97. The nonhydrogen atoms were refined anisotropically. All hydrogen atoms could be located from the difference Fourier map, with the exception of that ones on the carbon atoms of the disordered ethanol solvent molecule. Table S1 summarizes details of the data collection as well as of the structure refinement. CCDC-762617 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge at www.ccdc.cam.ac.uk/data_request/cif [or from the Cambridge Crystallographic Data Centre (CCDC), 12 Union Road, Cambridge CB2 1EZ, UK; fax: +44(0)1223-336033; email: deposit@ccdc.cam.ac.uk].

G. M. Sheldrick, SHELXS-97, SHELXL-97, Programs for the Crystal Structure Solution and Refinement, University of Göttingen, Germany 1997.

Table S1. Details of the data collection and the structure refinement for **PTCAPS**.

empirical formula	$C_{16}\ H_{12}\ K_2\ O_7$
formula weight	394.46
crystal system	triclinic
space group (number)	$P\bar{1}$ (#2)
cell dimensions	
a, Å	7.4228(14)
b, Å	8.1929(18)
c, Å	14.838(4)
α, deg	104.299(18)
β, deg	100.577(18)
γ, deg	95.938(17)
V, Å^3	362.94(14)
T, K	210
Z	2
D_{calcd}, g·cm^{-3}	1.543
μ, mm^{-1}	0.593
F(000)	404
radiation (λ, Å)	Mo-K_α (0.71073)
Θ range, deg	2.83 – 29.36
crystal size, mm	0.8 × 0.25 × 0.20
no. of reflns measd	4009
no. of unique reflns	3215 (R_{int}=0.0340)
no. of parameters	293
R_1 [for $I > 2\sigma(I)$]	0.0359
R (for all reflections)	0.0432
wR_2 (for all reflections)	0.1034
goodness of fit, S	1.029
Largest diff. peak and hole (e/Å^3)	0.539 and -0.452

$w = 1/[\sigma^2(F_o^2)+(0.0748P)^2+0.1462P]$ where $P=(F_o^2+2F_c^2)/3$

Table S2. Selected bond lengths (Å) and angles (°) of **PTCAPS**.

K1 - O1	2.7958(17)	C3 - C4	1.4309(18)
K1 - O3	2.7682(13)	C4 - C7	1.432(2)
K1 - O5	2.789(2)	C4 - C5	1.427(2)
K1 - O6	2.8208(19)	C5 - C6	1.428(2)
K1 - O1_d	2.9587(17)	C5 - C8	1.4308(18)
K1 - O2_d	2.7937(14)	C6 - C8_c	1.463(2)
K1 - O4_e	2.7009(16)	C7 - C12	1.503(2)
K2 - O1	2.6528(12)	C7 - C10	1.378(2)
K2 - O6	2.825(2)	C8 - C9	1.389(2)
K2 - O3_a	2.9106(17)	C9 - C10	1.389(3)
K2 - O5_a	2.7340(16)	C13 - C14	1.508(4)
K2 - O2_d	2.8261(17)	C1 - H1	0.95(3)
K2 - O4_d	2.7277(15)	C2 - H2	0.97(2)
O1 - C11	1.2545(19)	C9 - H9	0.98(2)
O2 - C11	1.267(2)	C10 - H10	0.97(3)
O3 - C12	1.265(2)	C13 - H13B	1.03(5)
O4 - C12	1.252(2)	C13 - H13A	1.00(3)
O6 - C13	1.4246	C14 - H14C	0.96(4)
O5 - H51	0.86(4)	C14 - H14A	0.98(4)
O5 - H52	0.78(4)	C14 - H14B	1.12(5)
O6 - H6	0.83(4)	C1 - C6	1.3871(19)
C1 - C2	1.391(3)	C2 - C3	1.380(2)
C3 - C11	1.513(2)		

Symmetry codes: a = -1+x, y, z; b = 1+x, y, z; c = -x,-y,-z
d = -x, 1-y, 1-z; e = 1-x, 1-y, 1-z; f = -x, 2-y, 1-z
g = 1-x, 2-y, 1-z; h = -1+x, y, z; i = x, -1+y, z
j = x, 1+y, z; k = 1+x, -1+y, z; l = -1+x, 1+y, z

Table S3. Selected bond angles (°) of **PTCAPS**.

O1 - K1 - O3	72.45(4)	O2_d - K2 - O6	81.07(5)
O1 - K1 - O5	127.25(5)	O4_d - K2 - O6	129.65(5)
O1 - K1 - O6	76.50(5)	O3_a - K2 - O5_a	76.26(5)
O1 - K1 - O1_d	73.16(5)	O2_d - K2 - O3_a	137.59(5)
O1 - K1 - O2_d	81.91(4)	O3_a - K2 - O4_d	81.08(5)
O1 - K1 - O4_e	141.65(5)	O2_d - K2 - O5_a	121.90(5)
O3 - K1 - O5	77.75(5)	O4_d - K2 - O5_a	74.55(5)
O3 - K1 - O6	115.99(5)	O2_d - K2 - O4_d	69.85(4)
O1_d - K1 - O3	100.66(5)	K1 - O1 - K2	85.49(4)
O2_d - K1 - O3	143.27(5)	O3 - K1 - O4_e	84.21(5)
K1 - O1 - K1_d	106.84(5)	O5 - K1 - O6	78.99(5)
O1_d - K1 - O5	156.17(5)	O2_d - K1 - O5	138.86(5)
O4_e - K1 - O5	74.08(5)	O1_d - K1 - O6	121.52(5)
O2_d - K1 - O6	81.71(5)	K1_d - O2 - K2_d	82.35(4)
O4_e - K1 - O6	141.83(5)	K1 - O3 - C12	146.44(33)
O1_d - K1 - O2_d	45.67(4)	O1_d - K1 - O4_e	82.09(5)
O2_d - K1 - O4_e	101.38(5)	O1 - K2 - O6	78.74(5)
O1 - K2 - O3_a	96.24(5)	K1_e - O4 - K2_d	88.90(5)
O1 - K2 - O5_a	149.22(5)	K1 - O5 - K2_b	86.99(6)
O1 - K2 - O2_d	83.87(4)	K1 - O6 - K2	81.89(5)
O1 - K2 - O4_d	134.53(5)	O3_a - K2 - O6	140.76(5)
O5_a - K2 - O6	88.39(5)	C8 - C9 - C10	121.46(14)
C7 - C10 - C9	121.90(15)	O1 - C11 - C3	117.05(16)
O2 - C11 - C3	117.69(14)	O1 - C11 - O2	125.09(16)
O4 - C12 - C7	117.94(15)	O3 - C12 - O4	124.79(17)
O3 - C12 - C7	117.09(16)	C2 - C1 - C6	121.23(16)
C1 - C2 - C3	121.97(14)	C4 - C3 - C11	124.45(15)
C2 - C3 - C11	116.39(13)	C2 - C3 - C4	118.61(15)
C3 - C4 - C7	122.40(15)	C3 - C4 - C5	118.85(15)
C5 - C4 - C7	118.74(13)	C4 - C5 - C8	120.41(14)
C4 - C5 - C6	120.31(13)	C6 - C5 - C8	119.27(14)
C1 - C6 - C8_c	121.32(15)	C5 - C6 - C8_c	120.38(12)
C1 - C6 - C5	118.29(16)	C4 - C7 - C12	124.72(13)
C10 - C7 - C12	115.77(14)	C4 - C7 - C10	119.01(16)
C5 - C8 - C6_c	120.33(14)	C6_c - C8 - C9	121.51(13)
C5 - C8 - C9	118.16(15)		

Table S4. Selected torsion angles (°) of **PTCAPS**.

C4 – C3 – C11 – O1	148.26(3)	C4 – C3 – C11 – O2	-36.12(4)
C4 – C7 – C12 – O3	-41.80(4)	C4 – C7 – C12 – O4	142.87(3)

Table S5. Hydrogen-bonding parameters (Å, °) of **PTCAPS**.

D–H···A	D–H	H···A	D···A	D–H···A
O5–H51···O7	0.86(4)	2.03(3)	2.764(3)	143(3)
O5–H52···O4_g	0.78(4)	2.01(4)	2.789(2)	175(4)
O6–H6···O2_f	0.83(4)	1.92(4)	2.755(2)	178(5)