

Supplementary Information

Self-doped polyaniline derived from poly(2-methoxyaniline-5-phosphonic acid) and didodecyldimethylammonium salt

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Calculation of the composition

The structure of the obtained mixture in the experiment can be drawn as shown in Fig. S1.

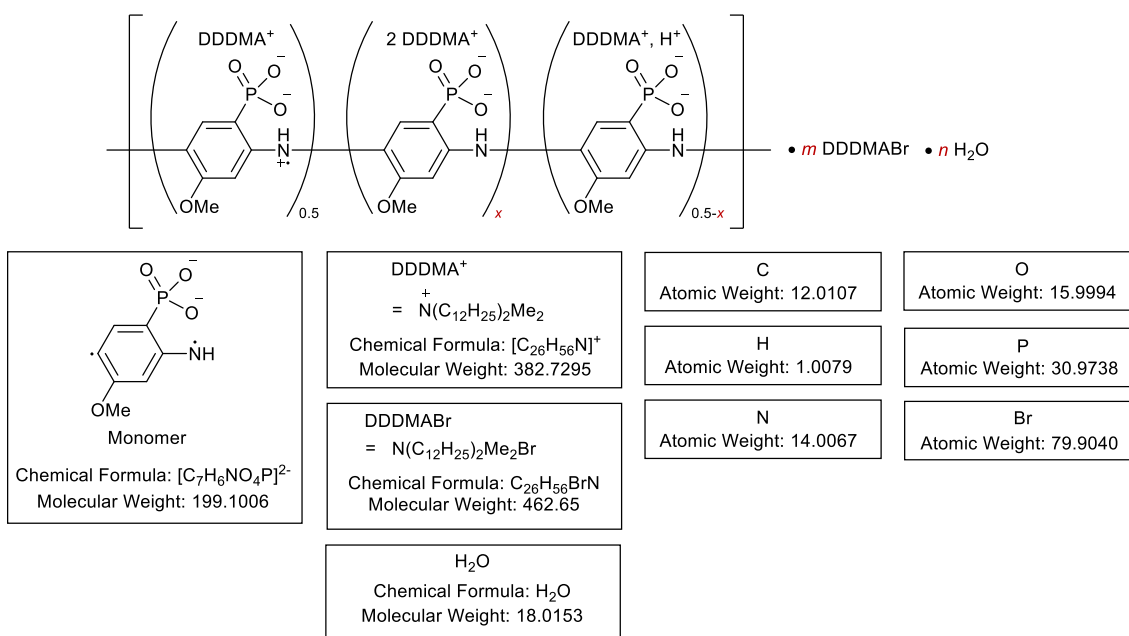


Fig. S1. Structure of the mixture.

Here, W(Atom or Molecule) means the percentage of weight (wt%) for “Atom or Molecule” in the above mixture. M_w (Molecule) and A_w (Atom) mean molecular weight and atomic weight for “Molecule” and “Atom”, respectively.

PMAP-DDDMA before washing

$W(P) = [1.75 \cdot (20/1000)] / 1.9068 \cdot 100 = 1.835$ wt%, the value of ppm for phosphorus was obtained from the ICP-AES analysis [1.75 ppm (average number of the three experiments) in the concentrated nitric acid solution of the above mixture (1.9068 mg in 20 mL)].

W(Br) = 8.76 wt%, the value was obtained from the ion-chromatography.

W(O) = 100 - {W(C)+W(H)+W(N)+W(Br)+W(P)} = 8.68 wt%, the values for W(C), W(H) and W(N) were obtained from the elementary analysis {W(C), W(H) and W(N) = 65.58, 11.88 and 3.70 wt%, respectively}.

$$m = \{W(\text{DDDMABr})/M_w(\text{DDDMABr})\} / \{W(\text{P})/A_w(\text{P})\} = 1.85, \text{ where } W(\text{DDDMABr}) = W(\text{Br}) * M_w(\text{DDDMABr}) / A_w(\text{Br})$$

$$M_w(\text{all}) = M_w(\text{monomer}) + (1+x) * M_w(\text{DDDMA}^+) + (0.5-x) * A_w(\text{H}^+) + m * M_w(\text{DDDMABr}) + n * M_w(\text{H}_2\text{O})$$

W(O) = 100 * {4 * A_w(O) + n * A_w(O)} / M_w(all), because oxygen is included in the components for monomer and H₂O in the above mixture.

$$W(\text{P}) = 100 * A_w(\text{P}) / M_w(\text{all})$$

From the above two equations concerning the percentage of weight for oxygen and phosphorous, x and n were calculated.

$$\text{i.e. } M_w(\text{all}) = 100 * A_w(\text{P}) / W(\text{P})$$

$$n = \{W(\text{O}) * M_w(\text{all}) - 100 * 4 * A_w(\text{O})\} / (100 * A_w(\text{O})) = \{W(\text{O}) * 100 * A_w(\text{P}) / W(\text{P}) - 100 * 4 * A_w(\text{O})\} / (100 * A_w(\text{O}))$$

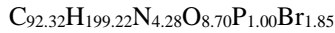
$$= 4.70$$

$$x =$$

$$\{M_w(\text{all}) - M_w(\text{monomer}) - M_w(\text{DDDMA}^+) - 0.5 * A_w(\text{H}^+) - m * M_w(\text{DDDMABr}) - n * M_w(\text{H}_2\text{O})\} / \{M_w(\text{DDDMA}^+) - A_w(\text{H}^+)\} = \{100 * A_w(\text{P}) / W(\text{P}) - M_w(\text{monomer}) - M_w(\text{DDDMA}^+) - 0.5 * A_w(\text{H}^+) - m * M_w(\text{DDDMABr}) - n * M_w(\text{H}_2\text{O})\} / \{M_w(\text{DDDMA}^+) - A_w(\text{H}^+)\}$$

$$= 0.431$$

Therefore, molecular formula of the above mixture is described as shown below.



The percentage of weight for each element is described as shown below (elementary analysis).

C, 65.71; H, 11.90; N, 3.55

Cf. the experimental values: C, 65.58; H, 11.88; N, 3.70.

PMAP-DDDMA after washing

W(P) = [3.50 * (20/1000)] / 2.1865 * 100 = 3.20 wt%, the value of ppm for phosphorus was obtained from the ICP-AES analysis [3.50 ppm (average number of the three experiments) in the concentrated nitric acid solution of the above mixture (2.1865 mg in 20 mL)].

W(Br) = 5.43 wt%, the value was obtained from the ion-chromatography.

$W(O) = 100 - \{W(C) + W(H) + W(N) + W(Br) + W(P)\} = 11.74 \text{ wt\%}$, the values for $W(C)$, $W(H)$ and $W(N)$ were obtained from the elementary analysis $\{W(C), W(H), \text{ and } W(N) = 64.38, 11.16 \text{ and } 4.09 \text{ wt\%}$, respectively}.

The values for m , n and x were calculated in the same way as **PMAP-DDDMA before washing**.

$m = 0.66$, $n = 3.10$ and $x = 0.0660$

Therefore, molecular formula of the above mixture is described as shown below.

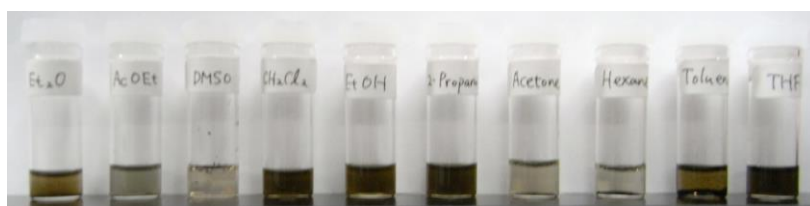
$C_{51.81}H_{109.14}N_{2.72}O_{7.10}P_{1.00}Br_{0.66}$

The percentage of weight for each element is described as shown below (elementary analysis).

C, 64.32; H, 11.37; N, 3.94

Cf. the experimental values: C, 64.38; H, 11.16; N, 4.09.

(a)



(b)



Fig. S2 Pictures of PMAP-DDDMA (a) before and (b) after washing in various solvents (from left to right, diethyl ether, ethyl acetate, DMSO, CH_2Cl_2 , ethanol, 2-propanol, acetone, hexane, toluene and THF).

PMAP-DDDMA before washing



Thickness: 293 nm
Transmittance at 455 nm: 79%

PMAP-DDDMA after washing



Thickness: 337 nm
Transmittance at 455 nm: 65%

Fig. S3 Photos of spin-coated film of PMAP-DDDMA before (left) and after (right) washing on glass substrates.