Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C

SUPPORTING INFORMATION FOR

A NEW $(TTF)_{11}I_8$ ORGANIC MOLECULAR CONDUCTOR: FROM SINGLE CRYSTALS TO FLEXIBLE ALL-ORGANIC PIEZORESISTIVE FILMS

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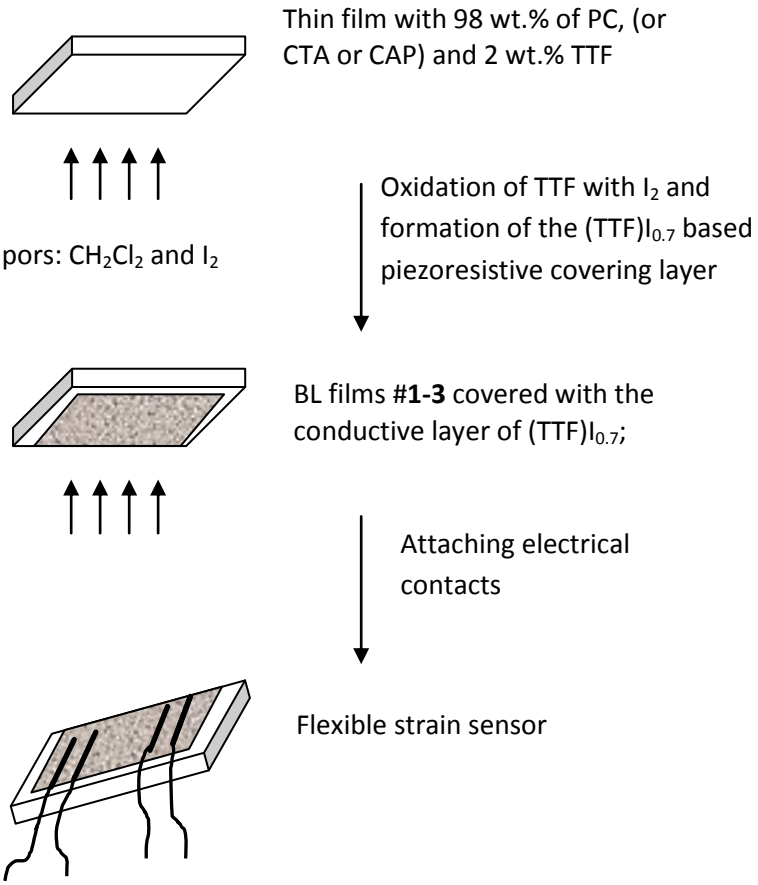

Figure S1. Scheme of the preparation method of bilayer (BL) thin films #1-3. PC=polycarbonate, CTA=cellulose triacetate, and CAP=cellulose acetate propionate.

An additional BL film (film #4), which contained copolymer of polycarbonate and siloxane as a polymeric support, was additionally prepared using this method. This BL film was only characterized by X-ray diffraction data (Fig S2b).

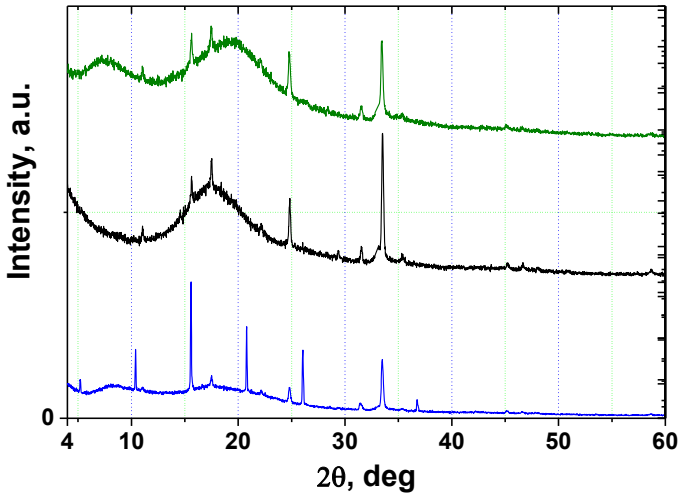

Figure S2a. X ray diffraction patterns of BL film #1 (black line), BL film #2 (blue line), and BL film #3 (green line). The film samples with dimensions 2x3 cm^2 were attached to a glass support and X-ray diffraction data were recorded on a Rigaku "Rotaflex" RU-200B diffractometer in reflection mode with monochromatic CuKα radiation (λ = 1.540598 Å). The generator was activated at 50 kV and 80 mA

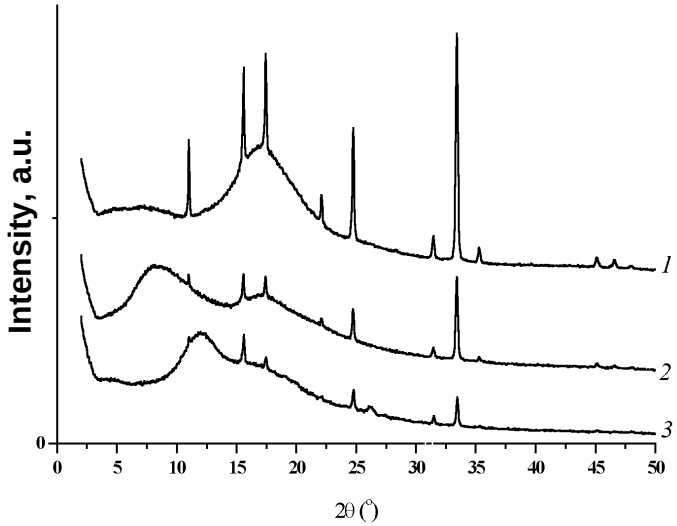

Figure S2b. X-ray patterns of BL thin films with conductive layer crystal of $(TTF)I_{0.71+d}$ crystals on different polymeric substrates: polycarbonate (*1*) (replica of BL film #1), cellulose triacetate (*2*) (replica of BL film #2) and copolymer of polycarbonate and siloxane (*3) (*BL film #4*).* Data were collected in reflection mode using a Panalytical EMPYREAN instrument with a linear X'celerator detector using non-monochromated CuK_α radiation

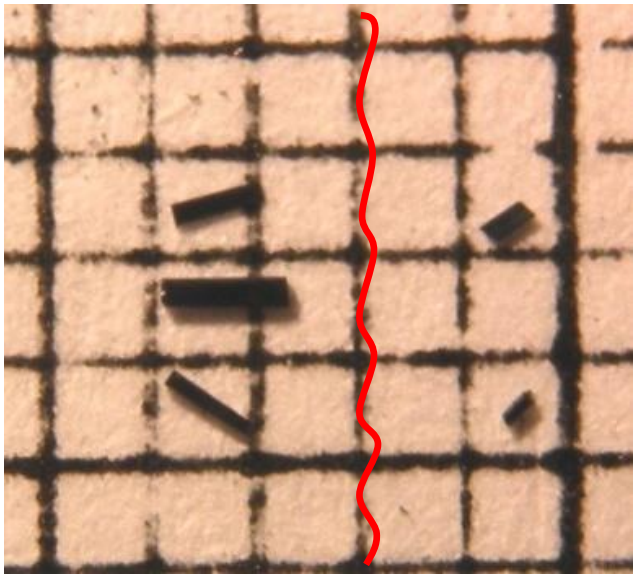

Figure S3. Photograph of $TTF_{11}I_8$ (left) and $(TTF)I_3$ (right) crystals obtained using oxidation of TTF with iodine (see experimental part of the article). Dimension of cells: 1 x1 mm^2

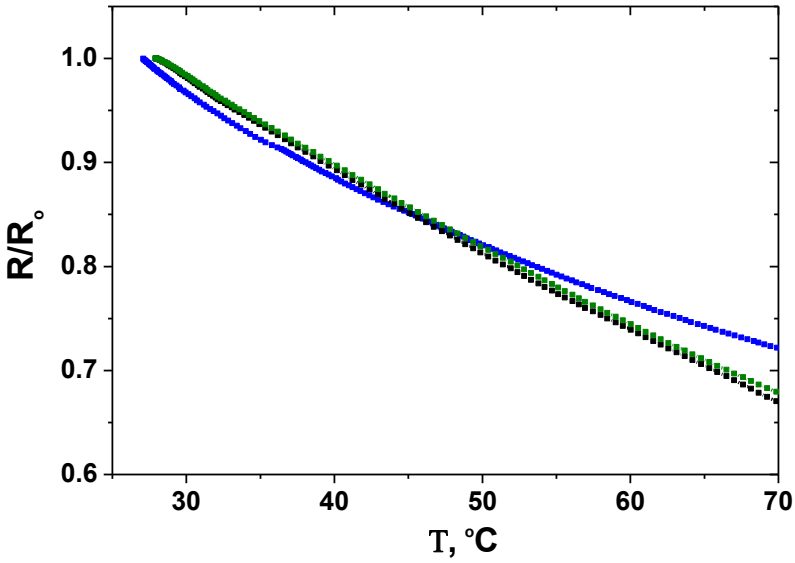

Figure S4. Temperature dependences of normalized electrical resistance of the BL film #1 (black line), film #2 (blue line), and film #3 (green line).

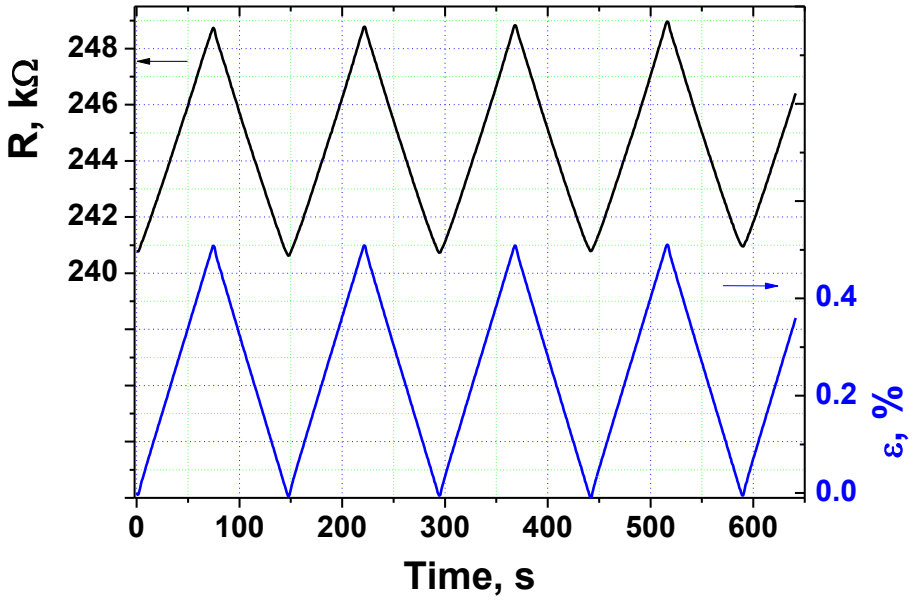

Figure S5. Electrical resistance response of the BL film #2 (CTA polymeric matrix) to perform cyclic elastic elongations using a maximum strain of ε_{max} = 0.5%.

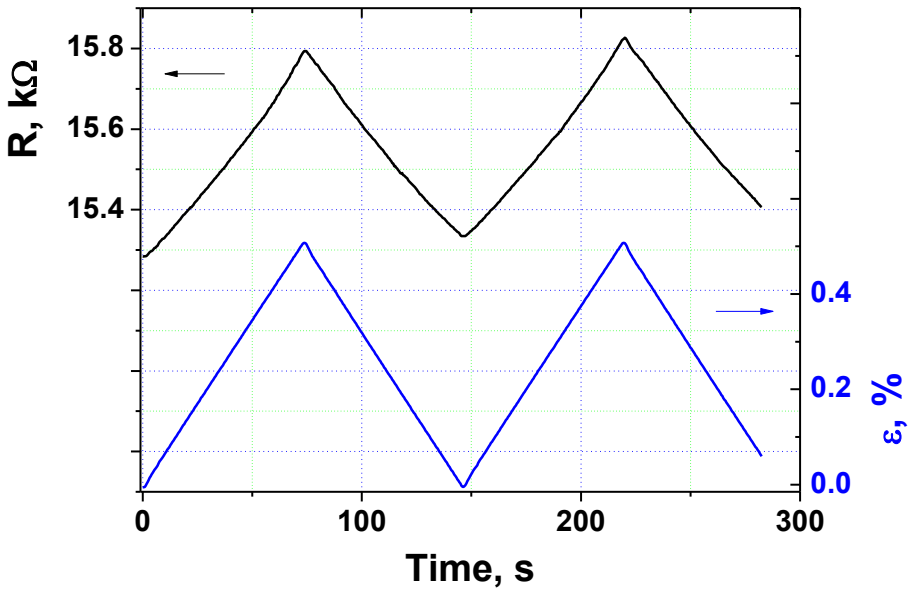

Figure S6. Electrical resistance response of BL film #3 (CAP polymeric matrix) to perform cyclic elastic elongation using a maximum of ε_{max} = 0.5%.

Table S1. Distances between iodine species extracted from the resolved crystal structure of $TTF_{11}I_8$, as well as the values of the bond length in I-I and $(I\text{-}I\text{-}I)^-$ added for comparison.

Number of I^-	Object1	Object2	Length, Å
1	I8	I3	4.883(5)
2	I4	I3	4.900(6)
3	I7	I4	4.892(6)
4	I1	I5	4.928(5)
5	I5	I6	4.864(6)
6	I6	I2	4.875(6)
I-I			**2.68-2.72**[1]
I_3^-			**2,79-3,11**[2]

Table S2. The central $C^1=C^4$ and C^4-S^4 bond length extracted from the resolved crystal structure of $TTF_{11}I_8$, the charge transfer of each molecule of TTF in asymmetric unit was calculated from Ref 3 using following equation r=0.762+0.049q, where r is ratio between bond lengths as it show in the table and q is a charge of TTF species.

Molecule TTF	Atom1	Atom2	Length, Å	ratio, r=(L($C^1=C^4$)/L(C^4-S^4))	charge, q
	S4	C4	1.723		
A	C1	C4	1.372	0,796	0,700
	S4	C4	1.722		
B	C1	C4	1.393	0,809	0,958
	S4	C4	1.712		
C	C1	C4	1.372	0,801	0,804
	S4	C4	1.722		
D	C1	C4	1.393	0,809	0,958
	S4	C4	1.732		
E	C1	C4	1.382	0,798	0,733
	S4	C4	1.722		
F	C1	C4	1.373	0,797	0,721
	S4	C4	1.722		
G	C1	C4	1.383	0,803	0,840
	S4	C4	1.722		
H	C1	C4	1.393	0,809	0,958
	S4	C4	1.712		
I	C1	C4	1.382	0,807	0,923
	S4	C4	1.712		
J	C1	C4	1.392	0,813	1,043
	C1	C4	1.414		
K	S1	C4	1.713	0,825	1,295
	S4	C4	1.722		
L	C1	C4	1.394	0,810	0,970

References

1. U. Buontempo et al., J. Chem. Phys. 107 (1997), 5720.

2. Atkins et al*Inorganic Chemistry* 5th ed.(2010) Oxford University Press. p.431.

3. T.C.Umland et al., J. Phys. Chem. 92 (1986), 6456.