## **Electronic Supplementary Information**

## Multifunctional cadmium single source precursor for the selective deposition of CdO or CdS films from a solution route

Graziella Malandrino,<sup>\*a</sup> Sebastiana T. Finocchiaro,<sup>a</sup> Patrizia Rossi,<sup>b</sup> Paolo Dapporto,<sup>b</sup> and Ignazio L. Fragalà<sup>a</sup>

 <sup>a</sup>Dipartimento di Scienze Chimiche, Università di Catania, and INSTM, UdR Catania, V.le Andrea Doria 6, I-95125 Catania, Italy
<sup>b</sup> Dipartimento Energetica "S. Stecco", Università di Firenze, Via Santa Marta 3, I-50139 Firenze, Italy

E-mail: gmalandrino@dipchi.unict.it

**Experimental.** Elemental microanalyses were performed in the Analytical Laboratories of the University of Catania. <sup>1</sup>H NMR spectra were recorded on a Varian Inova 500 spectrometer. Infrared spectra were recorded on a Perkin Elmer FTIR 1720 spectrometer as nujol mulls between NaCl plates. Thermogravimetric analyses were performed by using a Mettler Toledo TGA/SDTA 851<sup>e</sup>. Weights of the samples were between 10-15 mg (TGA). Analyses were made under prepurified nitrogen using a 5°C/min heating rate.

The <sup>1</sup>H NMR spectrum of the Cd(tta)<sub>2</sub>•tmed adduct shows a singlet at  $\delta = 6.12$  ppm, whose integration accounts for the two protons, one for each tta ring. The multiplets at  $\delta = 7.07$ ,  $\delta = 7.47$  and  $\delta = 7.60$  represents the resonance of the protons of the tiophene ring. In addition, multiplets at  $\delta = 2.51$  and  $\delta = 2.63$  represent resonances of the six and four protons, respectively, of the tmed methylic and methylenic groups.

The <sup>13</sup>C NMR spectrum of the Cd(TTA)<sub>2</sub>•tmed adduct shows a singlet at  $\delta = 47.06$  and a singlet at  $\delta = 56.82$ , associated with carbons of the methylic and methylenic groups, respectively, of the

<sup>\*</sup> E-mail: gmalandrino@dipchi.unict.it

tmed. Singlet at  $\delta = 90.30$  represents the resonance of the alchenic C of the tta ring, while the singlets between  $\delta = 128$  and  $\delta = 132$  represent the resonances of the carbons of the tiophene ring of the same ligand. The singlet at  $\delta = 147.11$  is associated with the resonance of the thiophene carbons linked to the carbonilic groups, while the quartet at  $\delta = 119.89$  (<sup>1</sup>J = 286.2 Hz) is associated with the resonance of carbons of the -CF<sub>3</sub> groups. Finally, the singlet at  $\delta = 185.27$  and the quartet at  $\delta = 173.04$  (<sup>2</sup>J=31.4 Hz) represent resonances of the carbonilic carbons linked, respectively, to the thiophene ring and to the -CF<sub>3</sub> group.

**Details of film deposition.** Films were deposited through spin coating of a 0.3 M solution of  $Cd(tta)_2$ •tmed complex on glass or Si substrates. Afterwards the films were treated under different temperatures and atmosphere, reactive using  $O_2$  or inert using  $N_2$ . The experimental conditions are summarized in Table S1.

Temperature	Atmosphere	Treatment Time	Phase nature assessed through XRD	Elements of the films detected through EDX
300-700°C	O <sub>2</sub>	1 h	CdO	Cd, O
300-450 °C	$N_2$	1 h	CdF <sub>2</sub>	Cd, F, S
450-550°C	N <sub>2</sub>	1 h	CdS, CdF <sub>2</sub>	Cd, F, S
550-600 °C	N <sub>2</sub>	1 h	CdS	Cd, S

Table S1. Relationship between conditions of thermal treatments and nature of Cd containing films.

**Table S2.** Crystal data and structure refinement parameters for  $Cd(tta)_2$ ·tmed.

Empirical formula	$C_{22}H_{24}CdF_6N_2O_4S_2\\$	
М	670.95	
T (K)	293	
$\lambda$ (Å)	0.71069	
Crystal system, space group	Monoclinic, P2 <sub>1</sub> /c	
Unit cell dimensions (Å, °)	a = 17.582(5)	
	$b = 8.335(2), \beta = 92.61(3)$	
	c = 18.610(7)	
Volume (Å <sup>3</sup> )	2724.4(14)	
Z, $d_{calc}$ (g/cm <sup>3</sup> )	4, 1.636	
$\mu (mm^{-1})$	1.026	
F(000)	1344	
$2\theta$ range for data collection (°)	5-50.	
Reflections collected / unique	4804 / 4640 [R(int) = 0.0327]	
Data / parameters	4640 / 339	
Final R indices $[I \ge 2\sigma(I)]$	R1 = 0.0510, wR2 = 0.1414	
R indices (all data)	R1 = 0.0553, wR2 = 0.1469	

**Table S3.** Selected bond lengths [Å] and angles  $[\circ]$  for  $Cd(tta)_2$ ·tmed.

Cd(1)-O(1)	2.284(3)
Cd(1)-O(2)	2.281(3)
Cd(1)-O(3)	2.255(3)
Cd(1)-O(4)	2.258(3)
Cd(1)-N(1)	2.393(4)
Cd(1)-N(2)	2.401(4)
O(1)-Cd(1)-O(2)	79.61(12)
O(1)-Cd(1)-O(3)	97.24(12)
O(1)-Cd(1)-O(4)	167.77(13)
O(1)-Cd(1)-N(1)	94.25(13)
O(1)-Cd(1)-N(2)	97.98(14)
O(2)-Cd(1)-O(3)	103.57(14)
O(2)-Cd(1)-O(4)	88.97(13)
O(2)-Cd(1)-N(1)	165.52(15)
O(2)-Cd(1)-N(2)	90.43(16)
O(3)-Cd(1)-O(4)	81.08(12)
O(3)-Cd(1)-N(1)	90.15(15)
O(3)-Cd(1)-N(2)	160.94(15)
O(4)-Cd(1)-N(1)	97.86(14)
O(4)-Cd(1)-N(2)	86.38(14)
N(1)-Cd(1)-N(2)	77.35(17)

Figure S1. EDX spectra of films obtained under different processing conditions: (a) CdO obtained at 600°C under  $O_2$ , (b) CdF<sub>2</sub> obtained at 350°C under  $N_2$ , (c) CdS obtained at 600°C under  $N_2$ .





