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Supplementary information

Synthesis, oxide formation, dielectric properties and transistor properties of yttrium oxide and amorphous aluminium oxide using a chimie douce solution precursor route

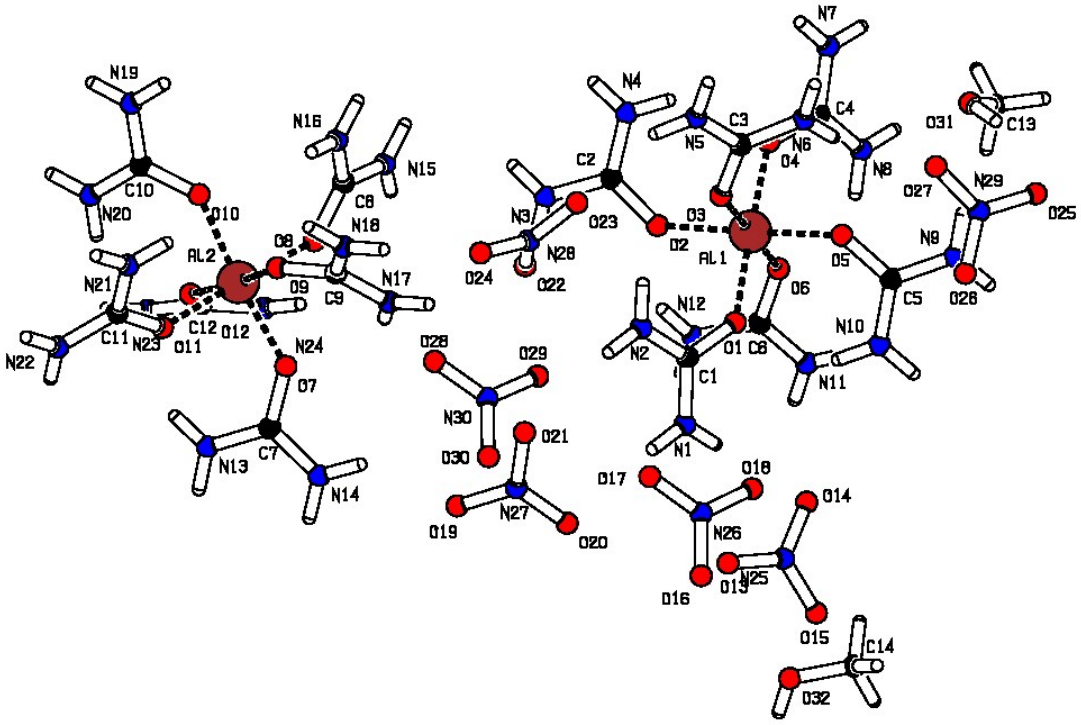

Fig.S1 Single crystal structure of Al-UN **3**. “ball and stick” illustration.

Table S1 Crystal data and structure refinement of Al-UN.

Empirical formula	C7 H28 Al N15 O16	
Formula weight	605.42	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 21.357(1) Å	□= 90°.
	b = 17.2300(7) Å	□= 106.960(7)°.
	c = 14.1833(6) Å	□ = 90°.
Volume	4992.2(4) $Å^3$	
Z	8	
Density (calculated)	1.611 Mg/m^3	
Absorption coefficient	0.183 mm^{-1}	
F(000)	2528	
Crystal size	0.400 x 0.220 x 0.220 mm^3	
Theta range for data collection	2.566 to 25.348°.	
Index ranges	-25<=h<=16, -20<=k<=19, -10<=l<=17	
Reflections collected	18866	
Independent reflections	9076 [R(int) = 0.0227]	
Completeness to theta = 25.242°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.961 and 0.930	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9076 / 13 / 706	
Goodness-of-fit on F^2	1.030	
Final R indices [I>2sigma(I)]	R1 = 0.0600, wR2 = 0.1410	
R indices (all data)	R1 = 0.0964, wR2 = 0.1626	
Largest diff. peak and hole	1.115 and -0.791 $e.Å^{-3}$	

Table S2 Crystal data and structure refinement of Y-UN.

Identification code	NK10 (Y-UN)	
Empirical formula	C4 H16 N11 O13 Y	
Formula weight	515.19	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 7.5428(7) Å	a= 112.238(8)°.
	b = 11.256(1) Å	b= 96.414(7)°.
	c = 11.976(1) Å	g = 94.215(7)°.
Volume	927.83(15) $Å^3$	
Z	2	
Density (calculated)	1.844 Mg/m^3	
Absorption coefficient	3.232 mm^{-1}	
F(000)	520	
Crystal size	0.500 x 0.480 x 0.460 mm^3	
Theta range for data collection	3.069 to 25.344°.	
Index ranges	-9<=h<=9, -13<=k<=13, -14<=l<=14	
Reflections collected	5662	
Independent reflections	3363 [R(int) = 0.0152]	
Completeness to theta = 25.242°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.318 and 0.295	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3363 / 16 / 310	
Goodness-of-fit on F^2	1.076	
Final R indices [I>2sigma(I)]	R1 = 0.0271, wR2 = 0.0681	
R indices (all data)	R1 = 0.0335, wR2 = 0.0695	
Largest diff. peak and hole	0.438 and -0.521 $e.Å^{-3}$	

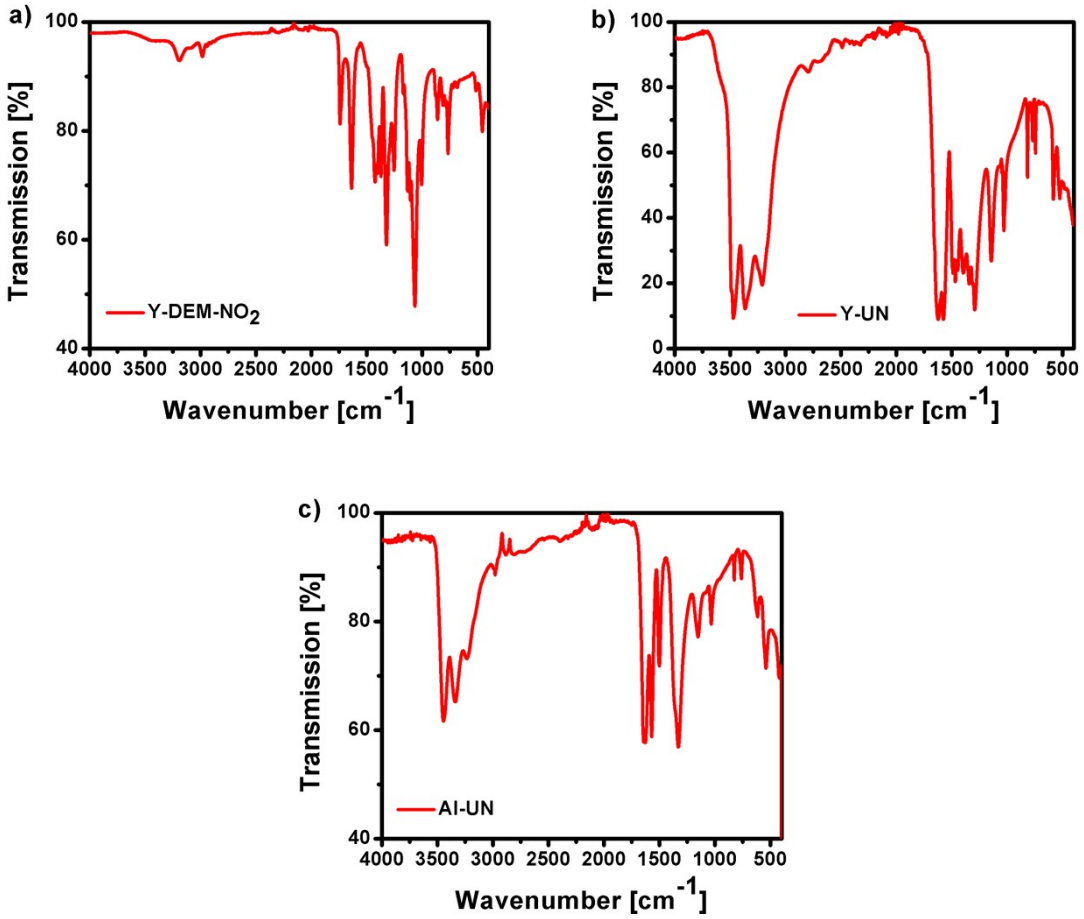

Fig.S2 FTIR-spectrum of (a) bis(diethyl-2-nitromalonato) nitrato yttrium(III) **1**, (b) dinitrato tetra(urea) yttrium(III)-nitrate **2** and (c) hexakis(urea) aluminium(III)-nitrate **3**.

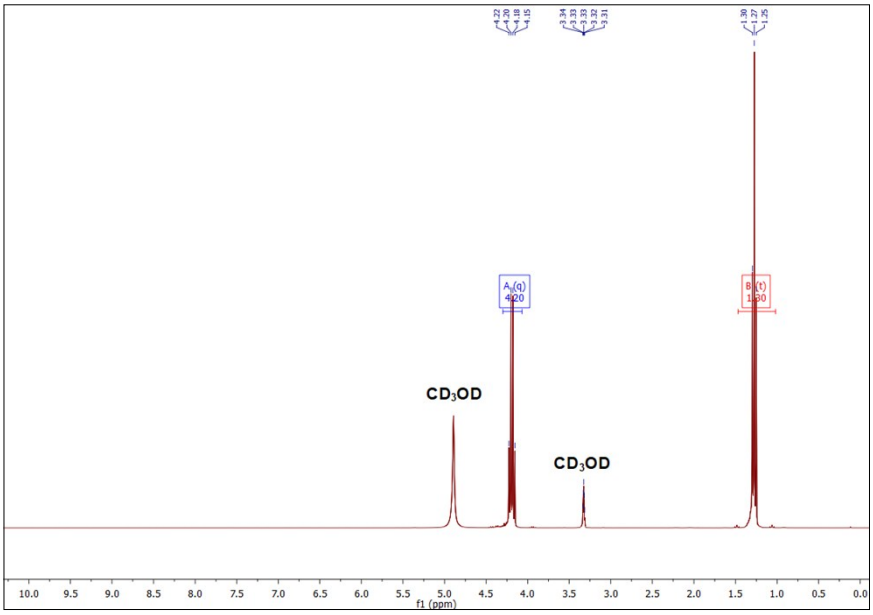

Fig.S3 ^{1}H-NMR-spectrum (CD_3OD) of bis(diethyl-2-nitromalonato) nitrato yttrium(III) **1**.

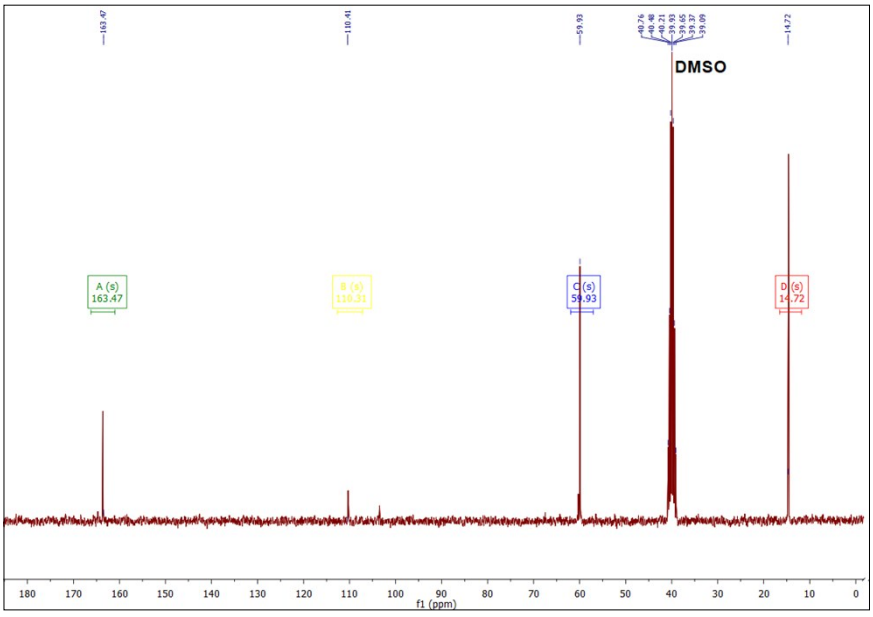

Fig.S4 ^{13}C-NMR-spectrum (DMSO) of bis(diethyl-2-nitromalonato) nitrato yttrium(III) **1**.

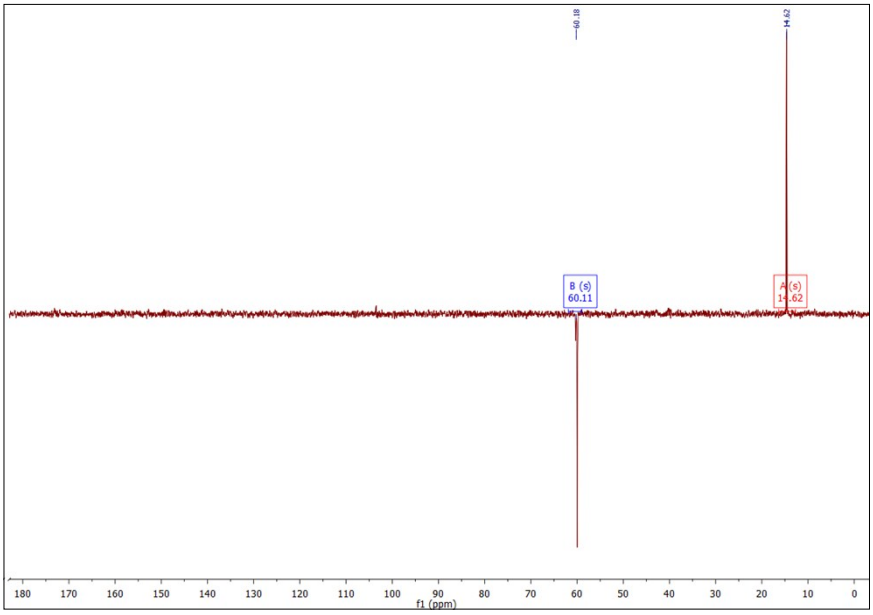

Fig.S5 DEPT-spectrum (DMSO) of bis(diethyl-2-nitromalonato) nitrato yttrium(III) **1**.

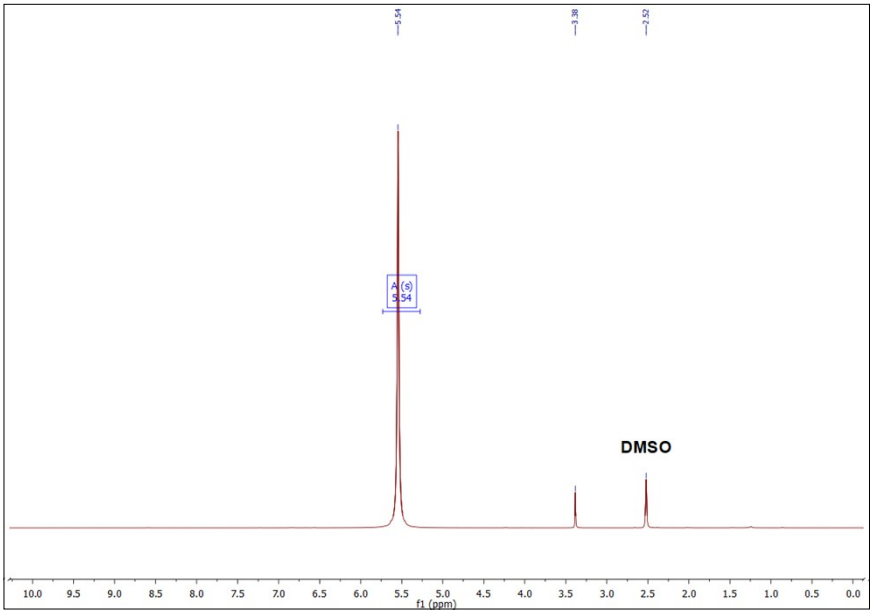

Fig.S6 ^{1}H-NMR-spectrum (DMSO) of dinitrato tetra(urea) yttrium(III)-nitrate **2**.

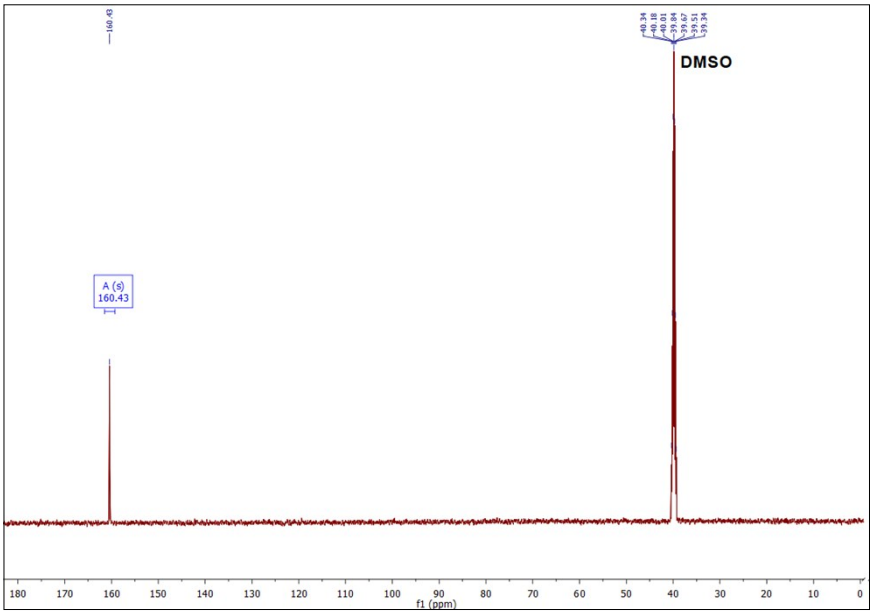

Fig.S7 ^{13}C-NMR-spectrum (DMSO) of dinitrato tetra(urea) yttrium(III)-nitrate **2**.

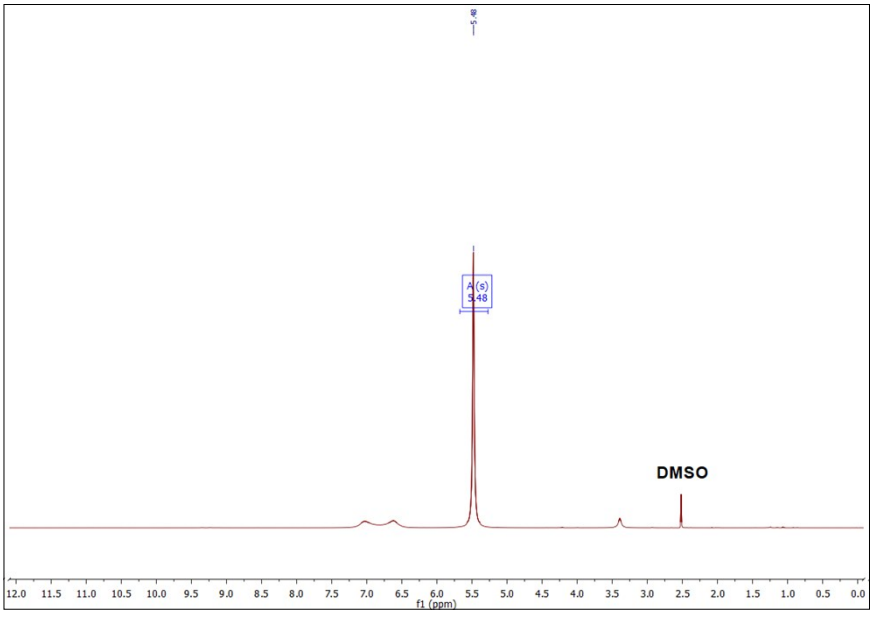

Fig.S8 ^{1}H-NMR-spectrum (DMSO) of hexakis(urea) aluminium(III)-nitrate **3**.

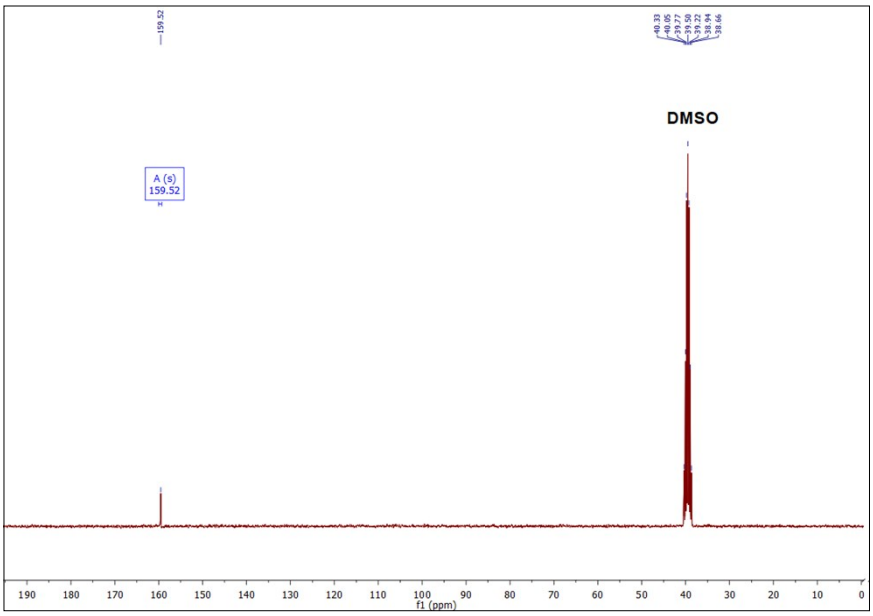

Fig.S9 ^{13}C-NMR-spectrum (DMSO) of hexakis(urea) aluminium(III)-nitrate **3**.

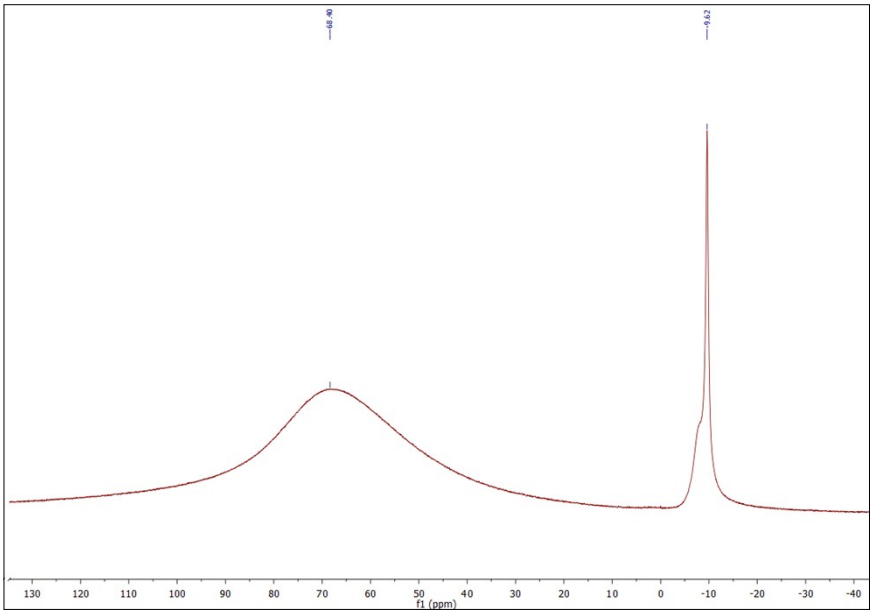

Fig.S10 ^{27}Al-NMR-spectrum (CD_3OD) of hexakis(urea) aluminium(III)-nitrate **3**.

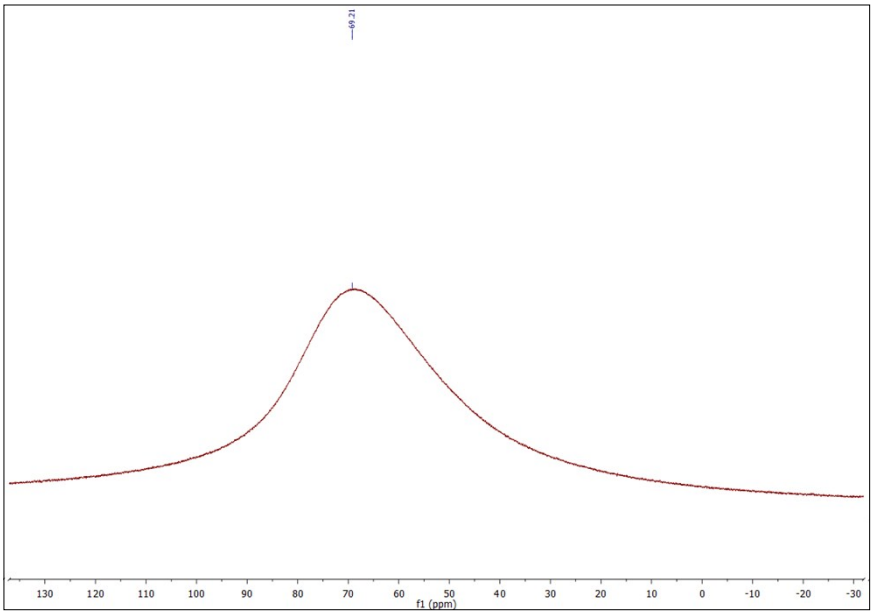

Fig. S11 ^{27}Al-NMR-spectrum of empty crucible.

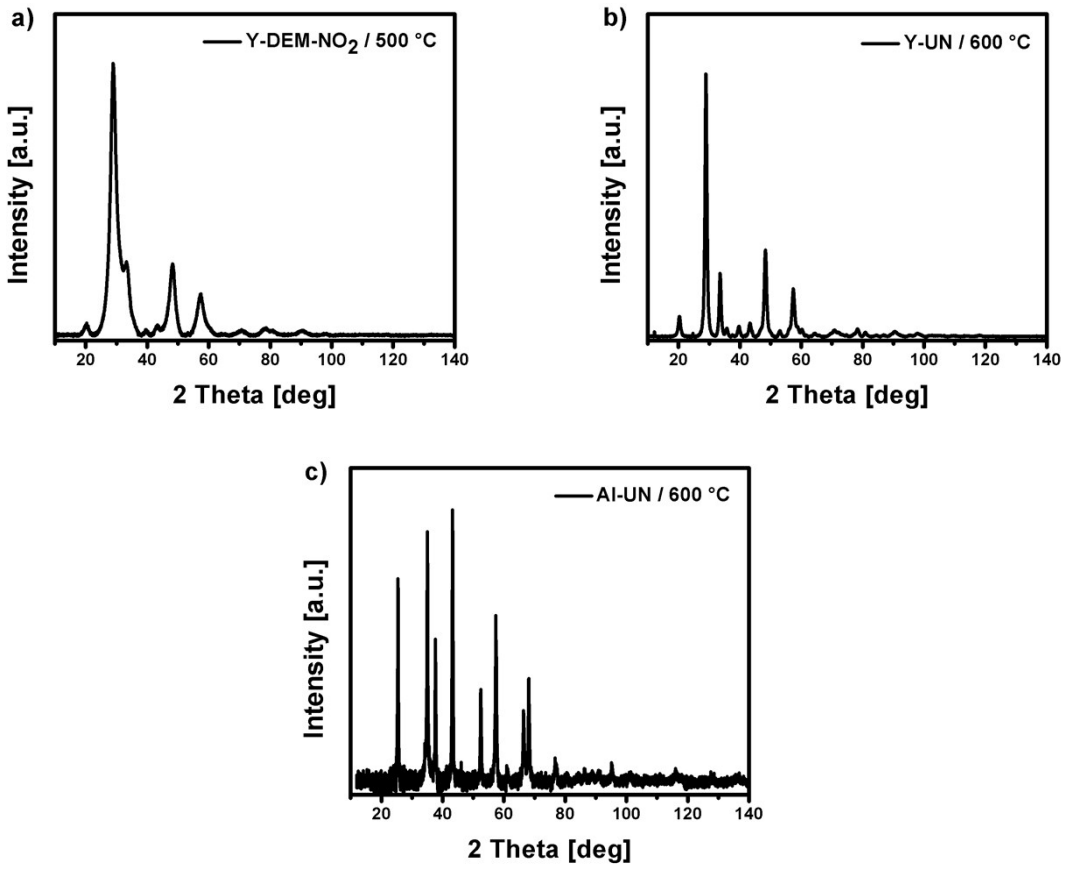

Fig. S12 XRD of (a) bis(diethyl-2-nitromalonato) nitrato yttrium(III) **1** annealed at 500 °C, (b) dinitrato tetra(urea) yttrium(III)-nitrate **2**annealed at 600 °C and (c) hexakis(urea) aluminium(III)-nitrate **3** annealed at 600°C.

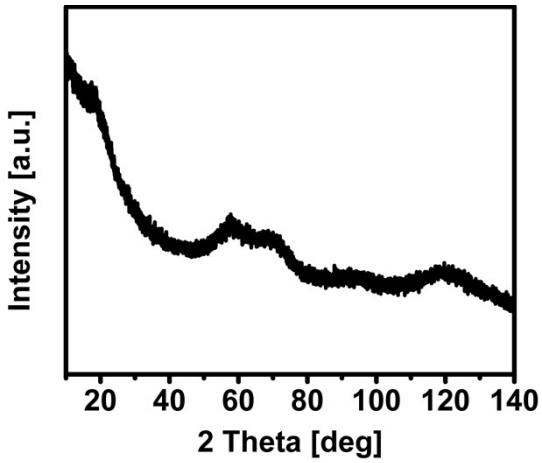

Fig. S13 XRD of empty crucible.

Table S3 Summary of spectroscopic ellipsometry measurements.

Temperature (°C)	Y-DEM-NO_2 (nm)	Y-UN (nm)	Al-UN (nm)
350	156	82	59
300	163	87	61
250	248	/	74
200	286	/	130

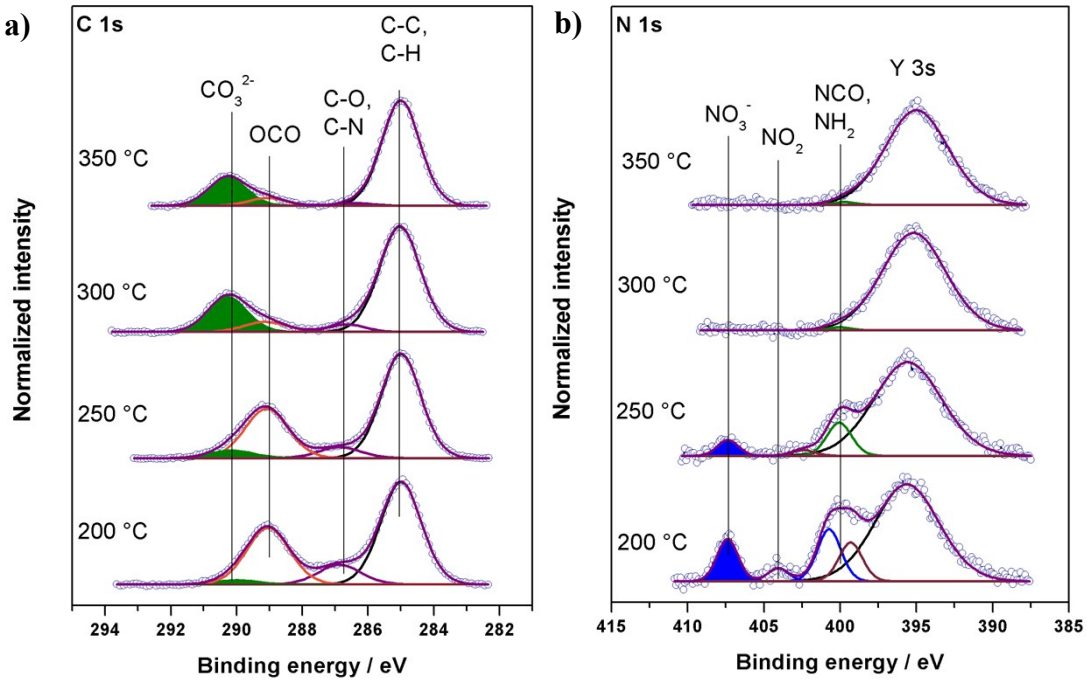

Fig. S 14 C 1s (a) and N 1s (b) XPS core spectra of samples obtained from Y-DEM-NO_2 precursor **1** annealed for 2 hours each at 200 °C, 250 °C, 300 °C and 350 °C.

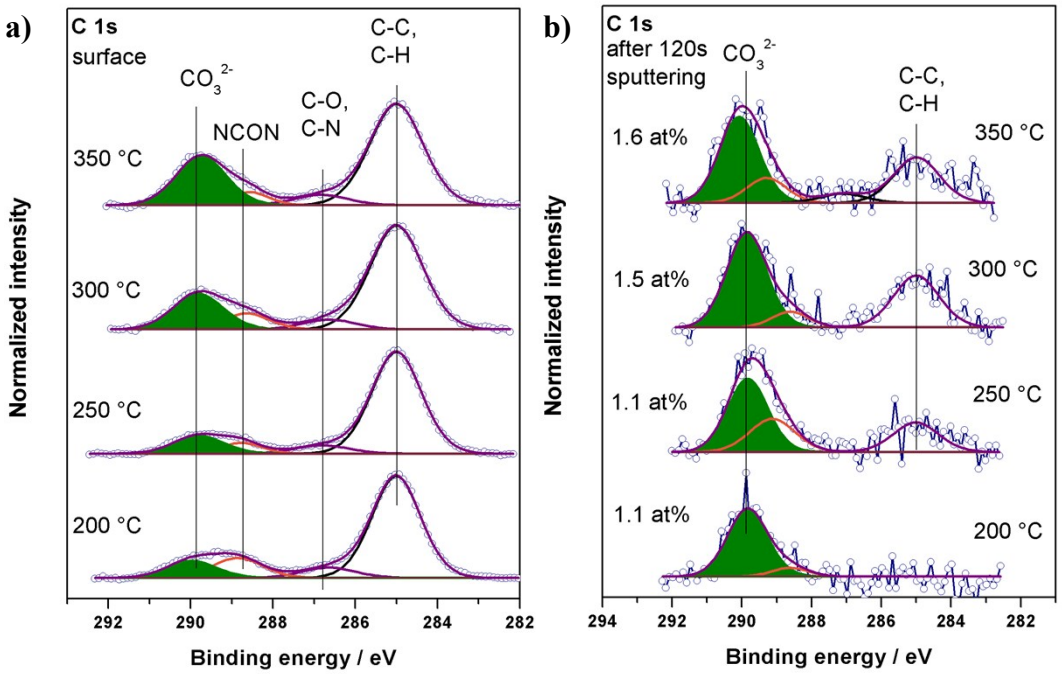

Fig. S 15 C 1s XPS core spectra of samples obtained from Y-UN precursor **2** annealed for 2 hours each at 200 °C, 250 °C, 300 °C and 350 °C. (a) initial sample without sputtering and (b) after 120 s of surface sputtering (cluster size of 300 atoms with 8000 eV).

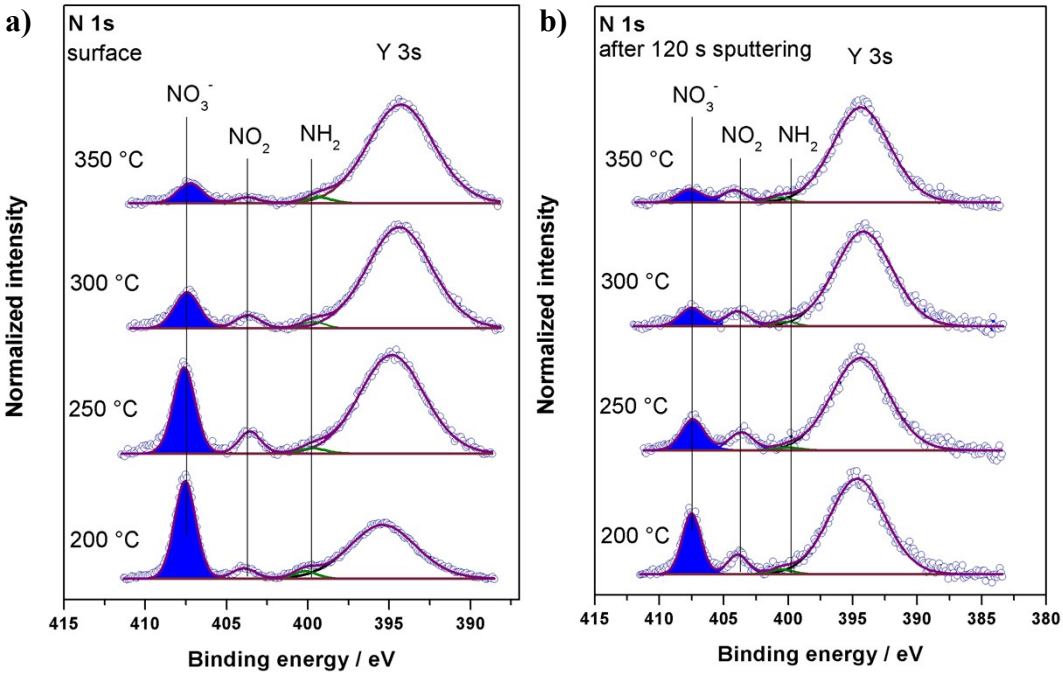

Fig. S 16 N 1s XPS core spectra of samples obtained from Y-UN precursor **2** annealed for 2 hours each at 200 °C, 250 °C, 300 °C and 350 °C. (a) initial sample surface without sputtering and (b) after 120 s sputtering (cluster size of 300 atoms with 8000 eV).

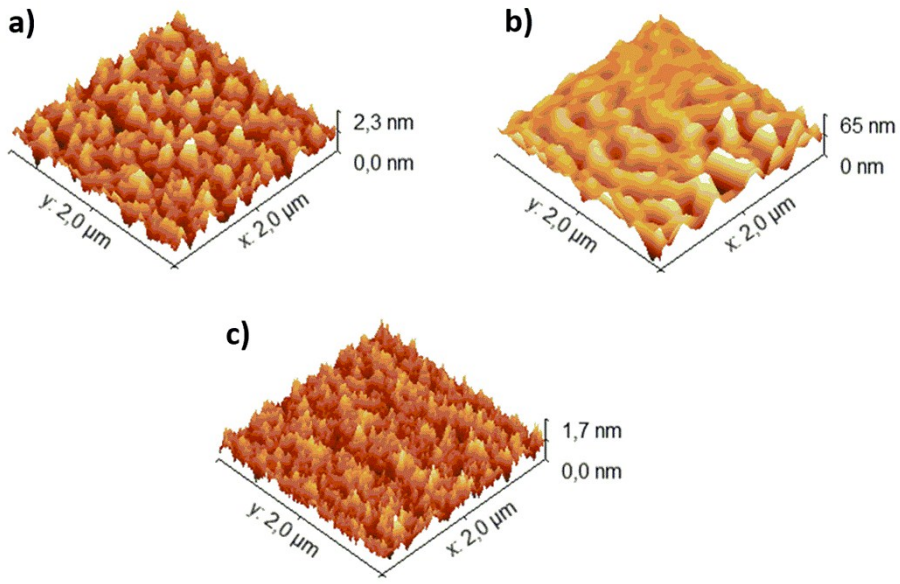

Fig. S 17 a-c) AFM images of precursor **1**, **2** and **3** prepared at 350 °C.

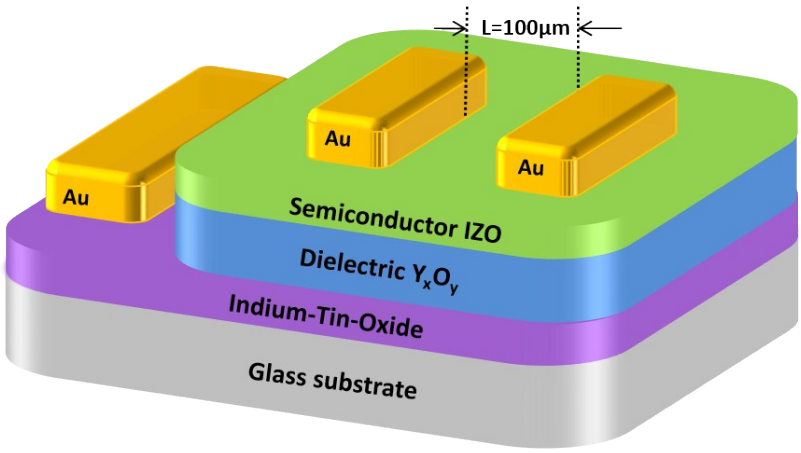

Fig. S 18 Schematic illustration of the fabricated Y_xO_y based thin film transistor.