Supporting Information

Highly Hydrophobic Metal–Organic Framework for Self-Protecting Gate Dielectrics

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1.0 SEM images

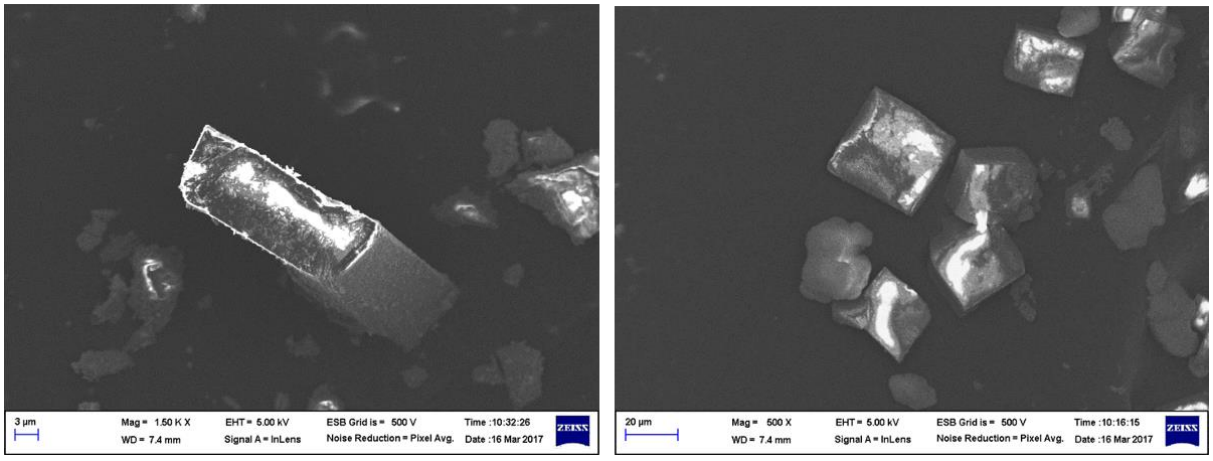

Fig. S1 Scanning electron microscope images of compound **1**.

2.0 Crystal structure, PXRD and contact angle images

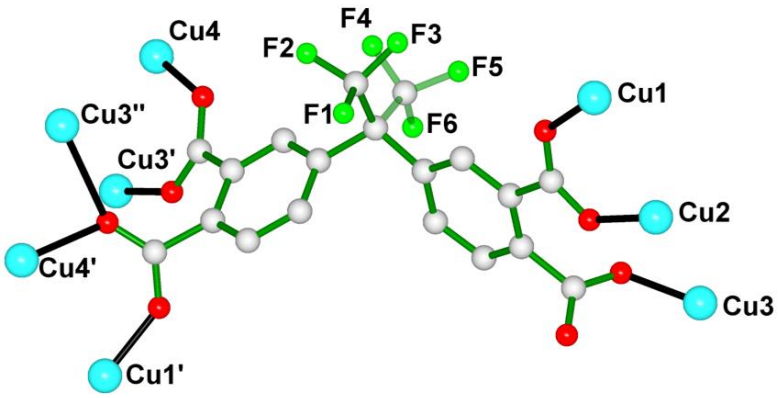

Fig. S2 Coordination of four diffrent copper atoms.

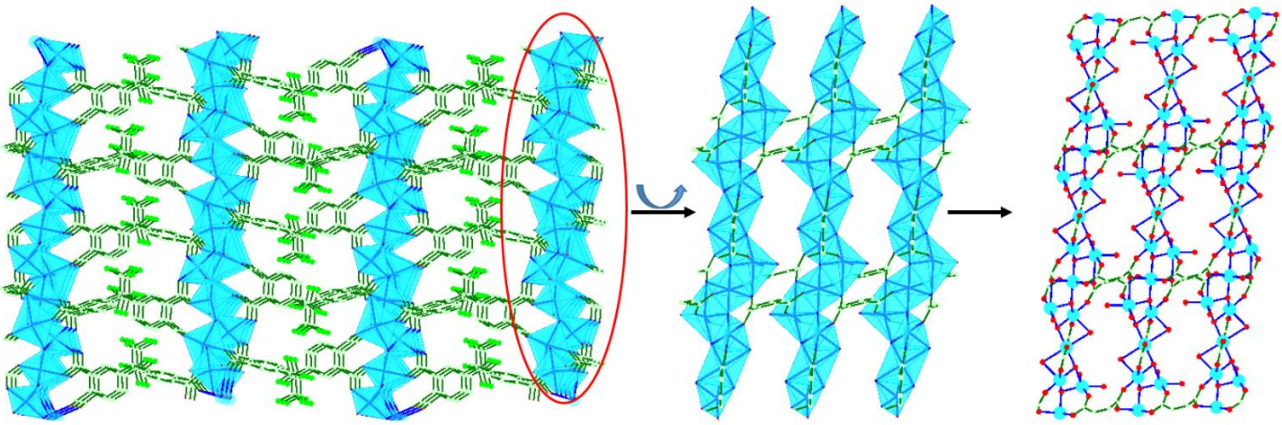

Fig. S3 Two dimensional layer of the metal oxide chain.

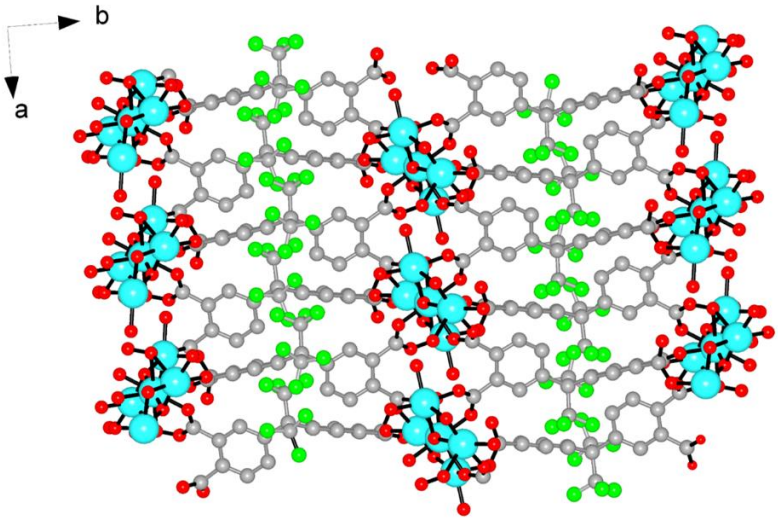

Fig. S4 Structure of compound **1** along the c-axis.

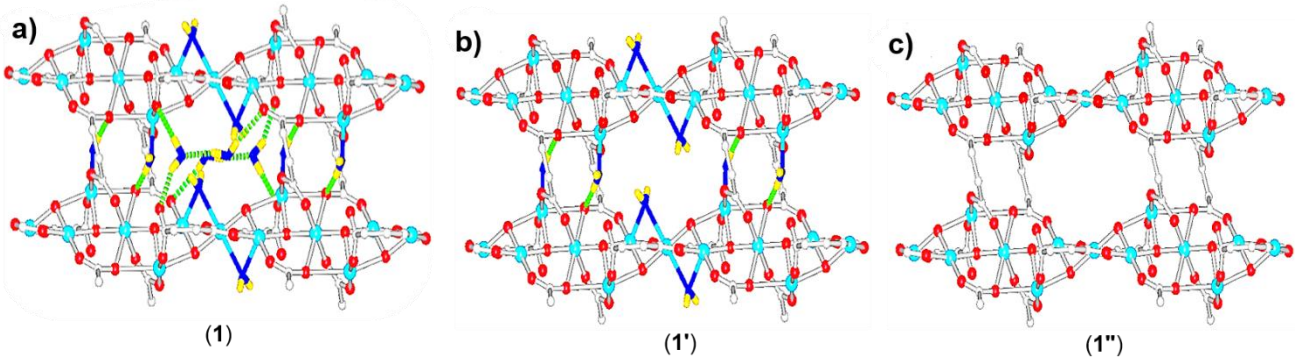

Fig. S5 a) Hydrogen bonding interactions between guest water, oxide chain and coordinated water. b) Structure of compound **1'** based on compound **1** which showing hydrogen bonding interactions of coordinated water molecules with oxide chain. c) Structure of compound **1"** based on compound **1**, oxide chain free from hydrogen bonding interactions of guest and coordinated water molecules.

3.0 Powder X-ray and thermogravimetric analysis

The powder X-ray diffraction data for the three compounds in (Fig. 2b) in precisely matched the simulated X-ray data for compound **1**. Activation of compound **1** done at two different temperatures 140 °C and 170 °C resulted in the formation of compound **1'** and compound **1"**, respectively. In the case of 170 °C, compound **1"** was in a completely dehydratd state, as evidenced by TGA data and PXRD data showed that an older peak had disappeared and a newer one was formed, indicating that this was final stage of dehydration for compound **1**. Compound **1'**, an intermediate state of compounde **1,** underwent a phase transition and a new peak was formed (Fig. S6). Thermogravimetric analyses of compound **1**, compound **1'** and compound **1"** in the temperature range 30–800 °C were performed (Fig. 2a). The TGA data for compound **1** showed a one step weight loss of 9.50% between 155–267 °C. The percentage weight loss coincides with the calculated value of guest and coordinated water molecules.

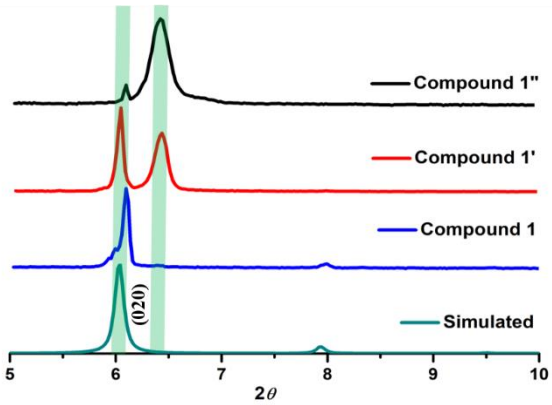

Fig. S6 Enlarged picture of the PXRD for compounds **1**, **1'**, and **1"**.

4.0 BET surface area and FT-IR

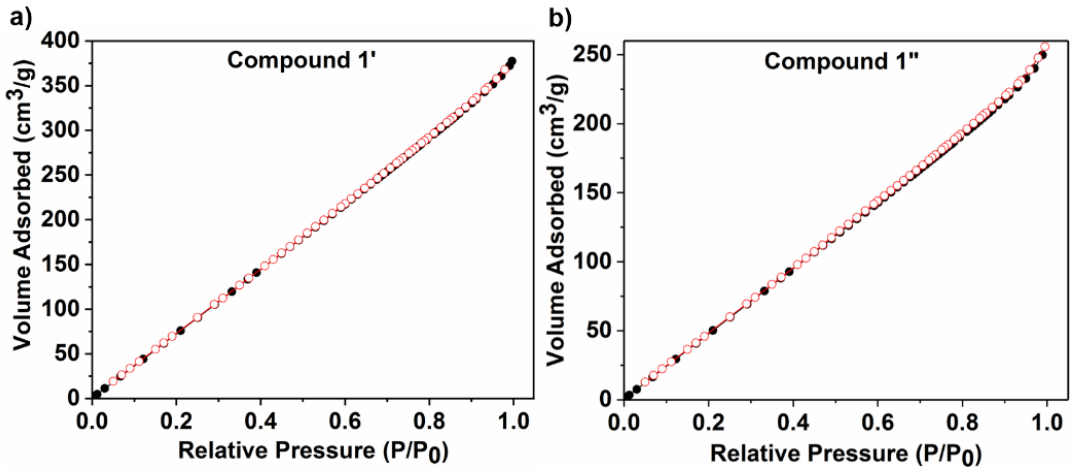

Fig. S7 Nitrogen gas adsorption isotherm of **1′** and **1″**.

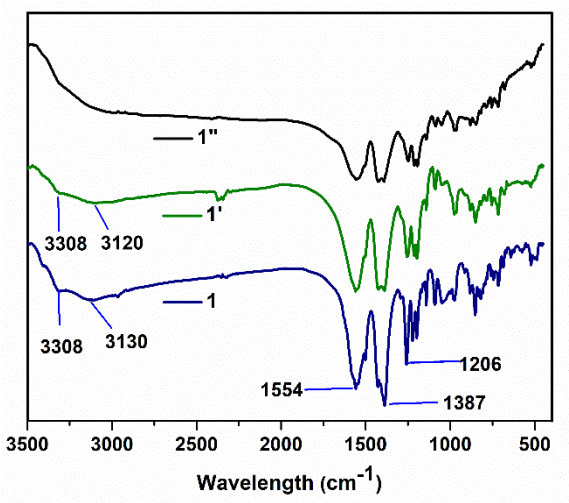

Fig. S8 FT-IR spectra of compounds **1**, **1′** and **1″**.

5.0 Dielectric and electrical conductivity graphs

5.1 Dielectric constant

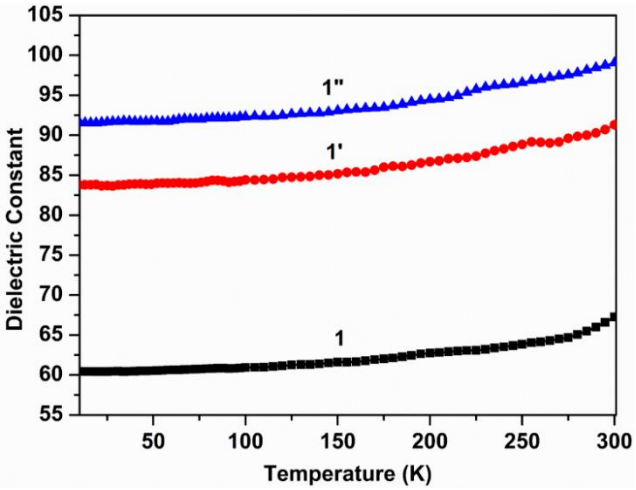

Fig. S9 Temperature dependent dielectric constants of compounds **1**, **1'** and **1"** at 1 kHz.

5.2 Dielectric relaxation

The dielectric relaxation of compounds **1**, **1'**, and **1"** at 300 K and 1 kHz are 67.44, 91.29, and 98.99, respectively, and for 1 MHz are 57.54, 79.18 and 86.20.

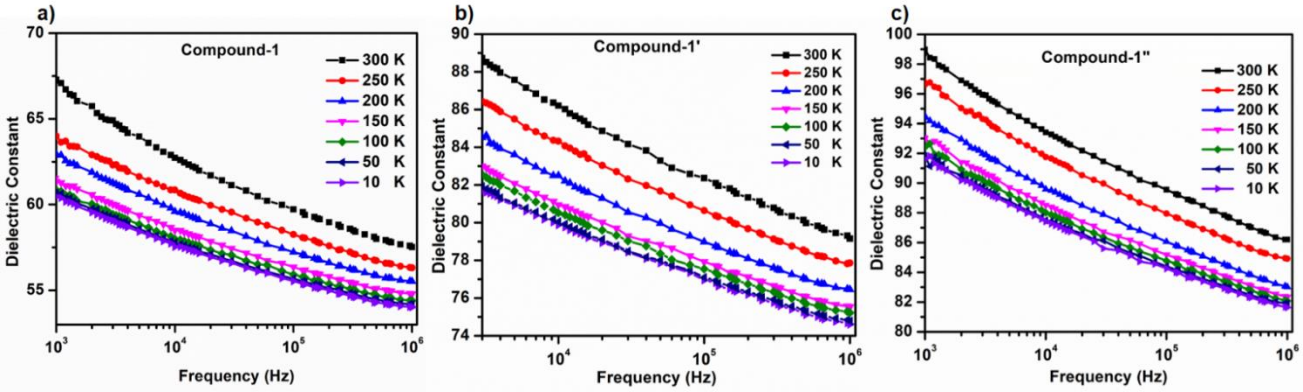

Fig. S10 Frequency dependent dielectric constants of compound **1** (a), **1'** (b) and **1"** (c) at different temperatures.

5.3 Dielectric loss versus temperature

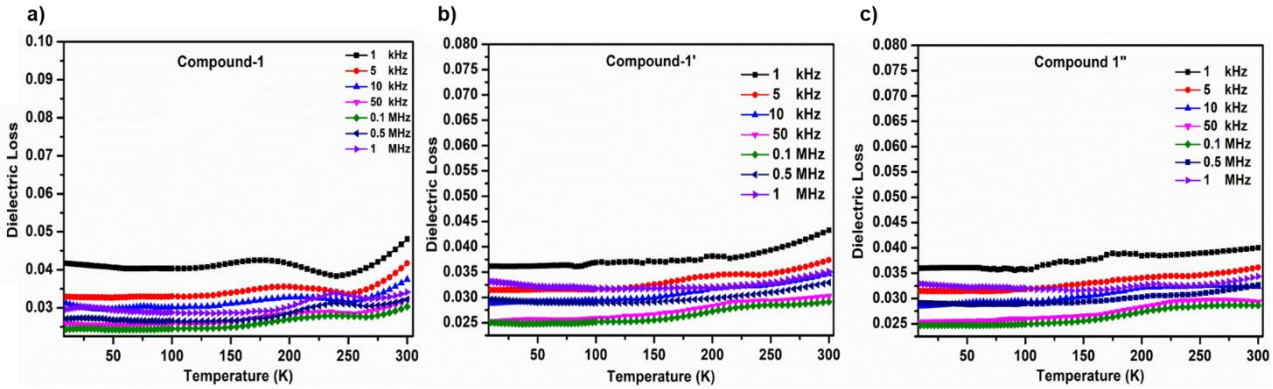

Fig. S11 Temperature dependent dielectric loss of compound **1** (a), **1'** (b), and **1"** (c) at different frequencies.

5.4 Dielectric loss versus frequency

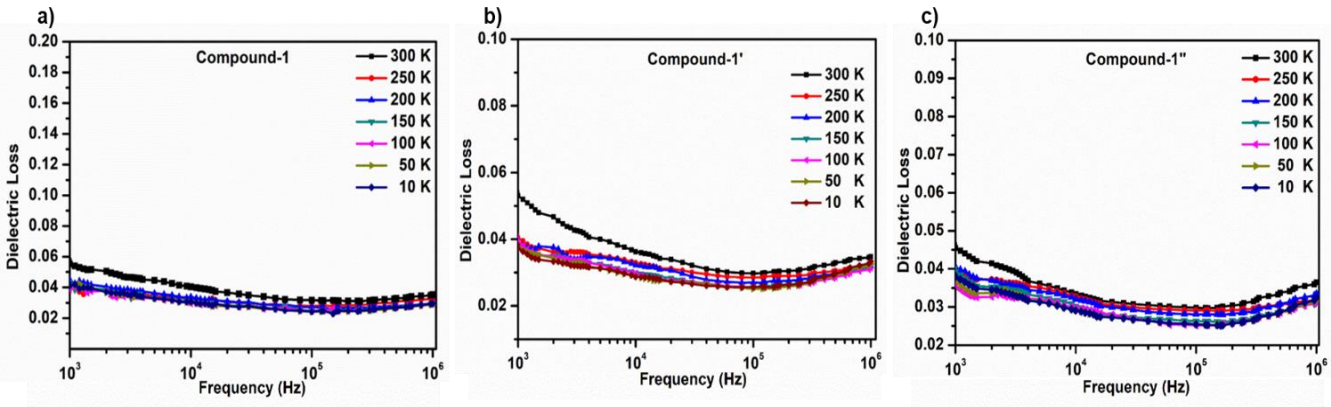

Fig. S12 Frequency dependent dielectric loss of compound **1** (a), **1'** (b), and **1"** (c) at different temperatures.

5.5 Electrical conductivity versus temperature

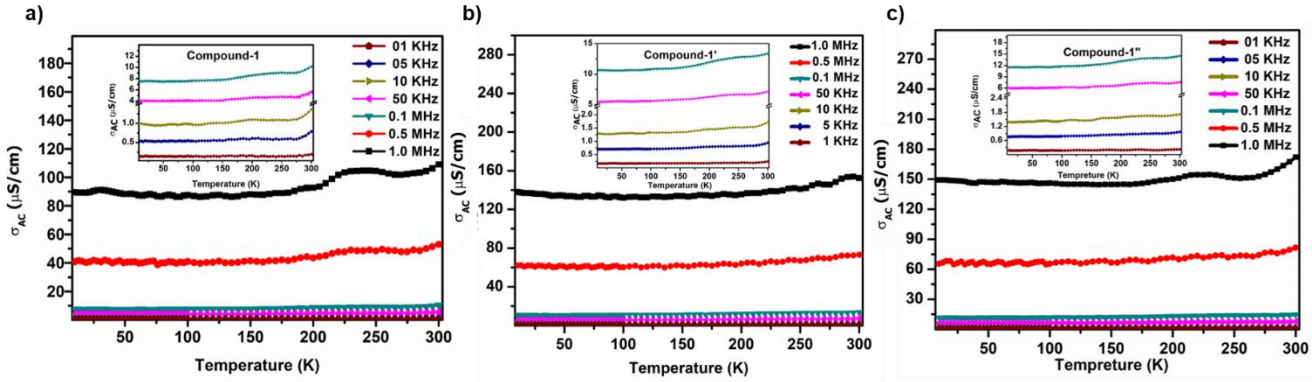

Fig.S13 Temperature dependent electrical conductivities of compound **1** (a), **1'** (b), and **1"** (c) at different frequencies.

5.6 Electrical conductivity versus frequency

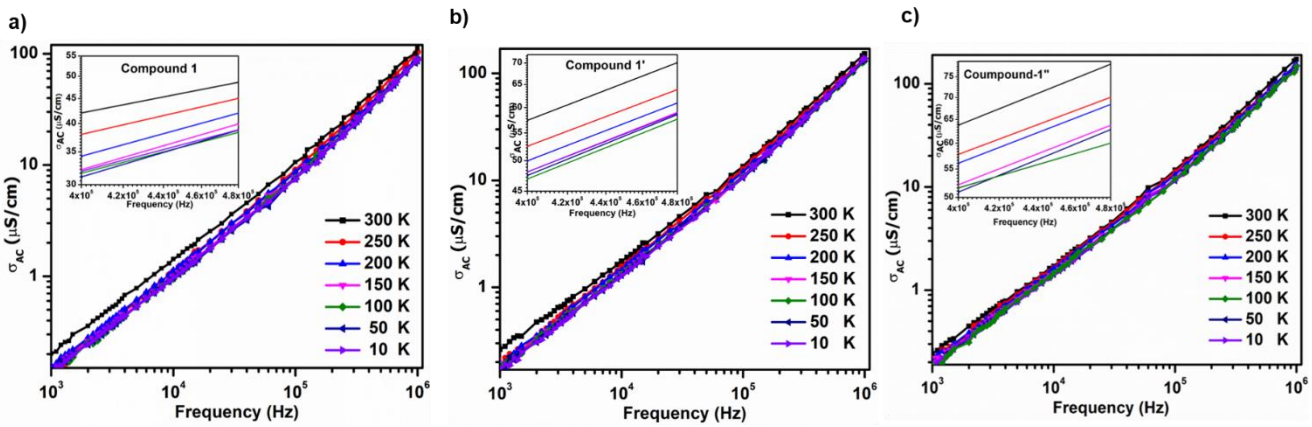

Fig. S14 Frequency dependent electrical conductivities of compound **1** (a), **1'** (b), and **1"** (c) at different temperatures.

6.0 Crystal Data of Compound 1 (CCDC 1840045)

Table S1. Crystal and structure refinement data for compound **1**

Empirical formula	C38 H28 Cu6 F12 O28
Formula weight	1541.84
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 7.1011(2) Å
	b = 29.2707(9) Å
	c = 12.1221(3) Å
	β = 96.8380(10)°
Volume	2501.71(12) $Å^3$
Z	2
Density (calculated)	2.047 Mg/m^3
Absorption coefficient	2.643 mm^{-1}
F(000)	1524
Crystal size	0.14 × 0.12 × 0.02 mm^3
Theta range for data collection	2.19 to 25.06°
Index ranges	−8<=h<=8, −34<=k<=34, −14<=l<=14
Reflections collected	50821
Independent reflections	4436 [R(int) = 0.0465]
Completeness to theta = 25.06°	99.6%
Absorption correction	multi-scan
Max. and min. transmission	0.9490 and 0.7085
R_1, wR_2 [$I > 2\sigma(I)$] [a]	R_1 = 0.0307, wR_2 = 0.0699
R_1, wR_2 (all data) [a]	R_1 = 0.0433, wR_2 = 0.0790

[a] $R_1 = \Sigma||F_0| - |F_c||/\Sigma|F_0|$; $wR_2 = [\Sigma w(F_0^2 - Fc^2)_2/\Sigma w(F_0^2)_2]^{1/2}$

7.0 Crystal Data of HFDPA Ligand (CCDC 1955564)

Table S2. Crystal and structure refinement data for hydrolysed HFDPA ligand

Empirical formula	$C_{19}H_{16}F_6O_{11}$
Formula weight	534.32
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	*C2/c*
Unit cell dimensions	a = 39.860(4) Å
	b = 17.4023(18) Å
	c = 13.4692(14) Å
	β =100.218(3)°
Volume	9194.8(17) $Å^3$
Z	16
Density (calculated)	1.544 Mg/m^3
Absorption coefficient	0.156 mm^{-1}
F(000)	4352
Crystal size	0.20 x 0.18 x 0.02 mm^3
Theta range for data collection	2.30 to 25.04°
Index ranges	-47<=h<=46, 20<=k<=19, -16<=l<=16
Reflections collected	60896
Independent reflections	8095 [R(int) = 0.1158]
Completeness to theta = 25.06°	99.5%
Absorption correction	multi-scan
Max. and min. transmission	0.9969 and 0.9695
R_1, wR_2 [$I > 2\sigma(I)$] [a]	R_1 = 0.0650, wR_2 = 0.1557
R_1, wR_2 (all data) [a]	R_1 = 0.1297, wR_2 = 0.1809

[a] $R_1 = \Sigma||F_0| - |F_c||/\Sigma|F_0|$; $wR_2 = [\Sigma w(F_0^2 - Fc^2)_2/\Sigma w(F_0^2)_2]^{1/2}$

References

S1. L. J. Farrugia. *J. Appl. Cryst*. 1999, **32**, 837–838.

S2. G. M. Sheldrick. *Acta Cryst.* 2015, **C71**, 3–8.

S3. G. M. Sheldrick. *Acta Cryst.* 2008, **A64**, 112–122.

S4. A. L. Spek. *Acta Cryst.* 2015, **C71**, 9–18.