

Supporting Information

Dinuclear Aluminum Complex as an Active Material for RRAM Switching Device

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Table S1. Crystal data and structure refinement for Complex 1 (CCDC 2426137).

Identification Code	1
Empirical formula	$C_{101}H_{164}Al_2Cl_6N_6O_{21}$
Formula weight	1805.53
Temperature/K	100(2)
Crystal system	triclinic
Space group	P-1
a/Å	16.9763(14)
b/Å	18.1646(18)
c/Å	19.4830(15)
$\alpha/^\circ$	93.121(3)
$\beta/^\circ$	98.030(2)
$\gamma/^\circ$	106.488(3)
Volume/Å³	5676.3(9)
Z	2
$\rho_{\text{calc}}/\text{cm}^3$	1.056
μ/mm^{-1}	0.151
F(000)	1944.0
Crystal size/mm³	$0.28 \times 0.23 \times 0.2$
Radiation	MoK α ($\lambda = 0.71073$)
2θ range for data collection/$^\circ$	4.244 to 50.7
Index ranges	$-20 \leq h \leq 20$, $-21 \leq k \leq 21$, $-23 \leq l \leq 20$
Reflections collected	35913
Independent reflections	20726 [$R_{\text{int}} = 0.0272$, $R_{\text{sigma}} = 0.0557$]
Data/restraints/parameters	20726/0/1238
Goodness-of-fit on F²	1.013
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0966$, $wR_2 = 0.2350$
Final R indexes [all data]	$R_1 = 0.1300$, $wR_2 = 0.2693$
Largest diff. peak/hole / e Å⁻³	0.61/-0.68

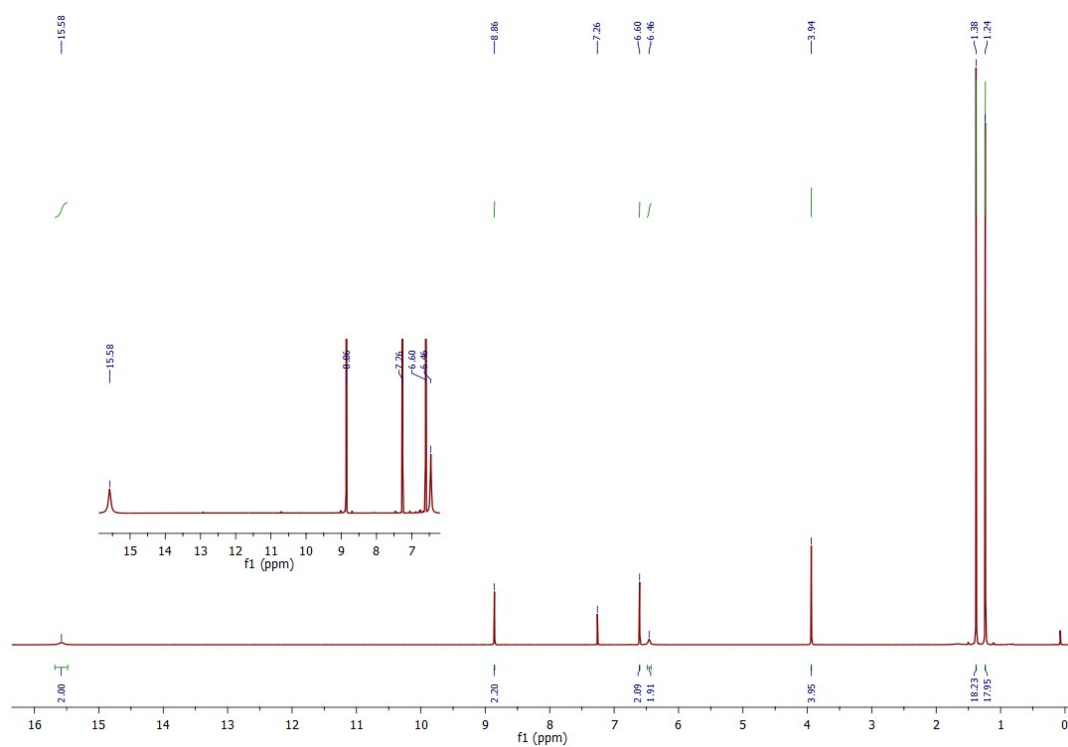


Figure S1. ¹H NMR spectrum of Ligand LH₄ in CDCl₃.

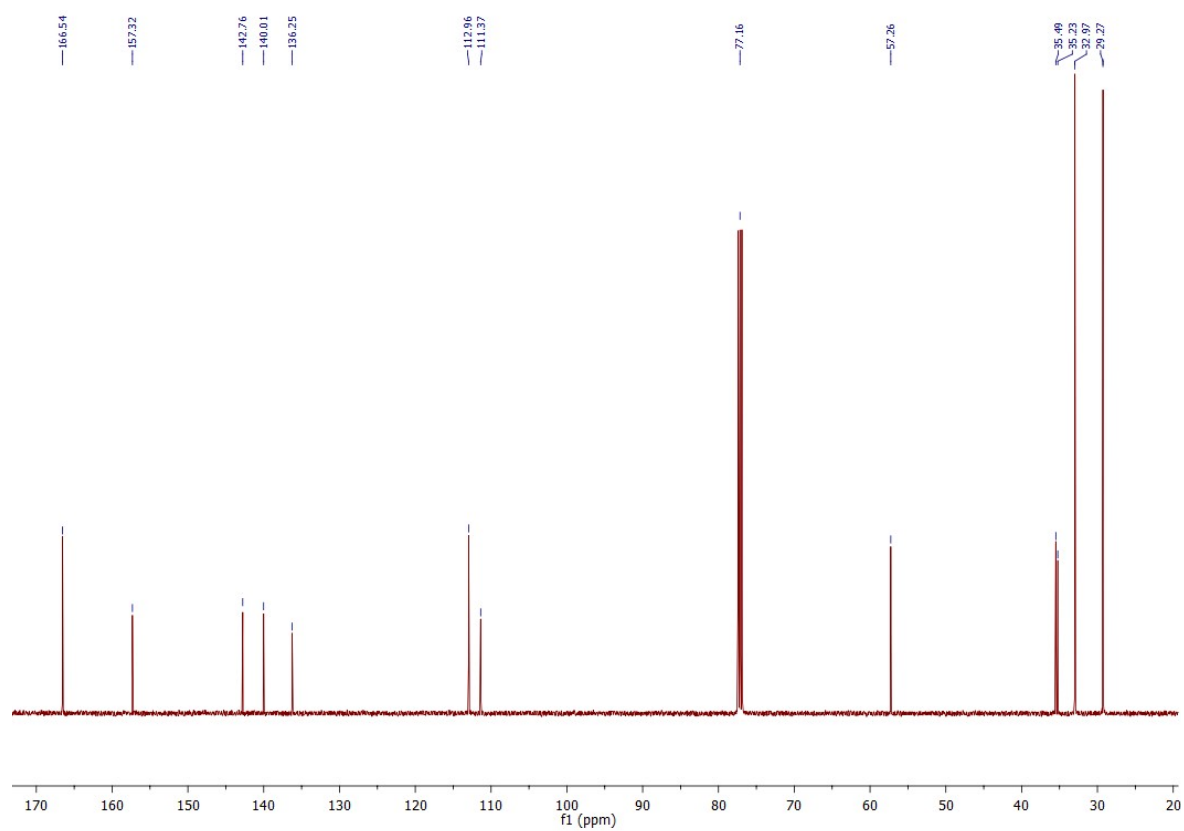
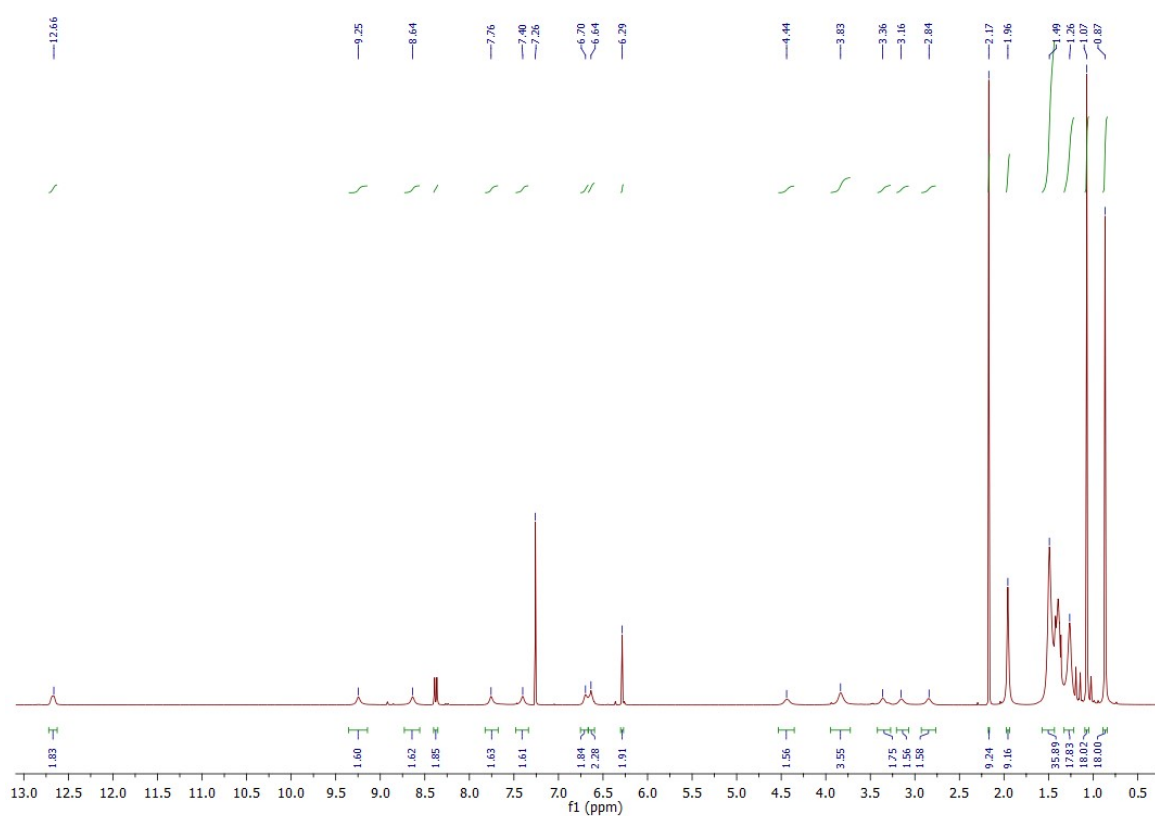


Figure S2. ¹³C{¹H} NMR spectrum of Ligand LH₄ in CDCl₃.



Fig

ure S3. ¹H NMR spectrum of Complex 1 in CDCl₃.

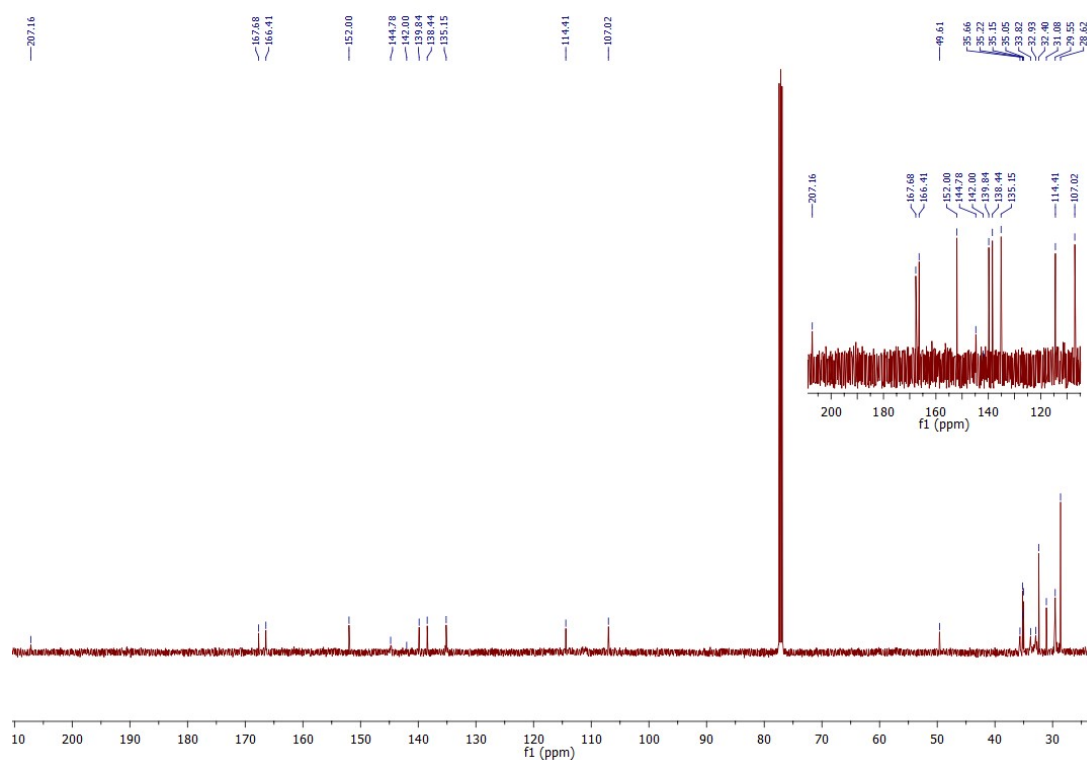


Figure S4. ¹³C {¹H} NMR spectrum of Complex 1 in CDCl₃.

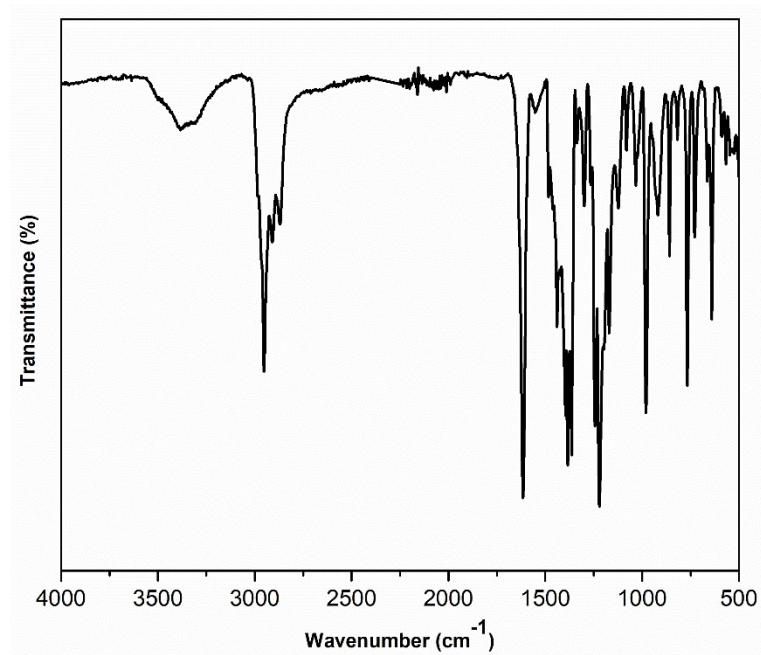


Figure S5. FT-IR Spectrum of Ligand LH₄.

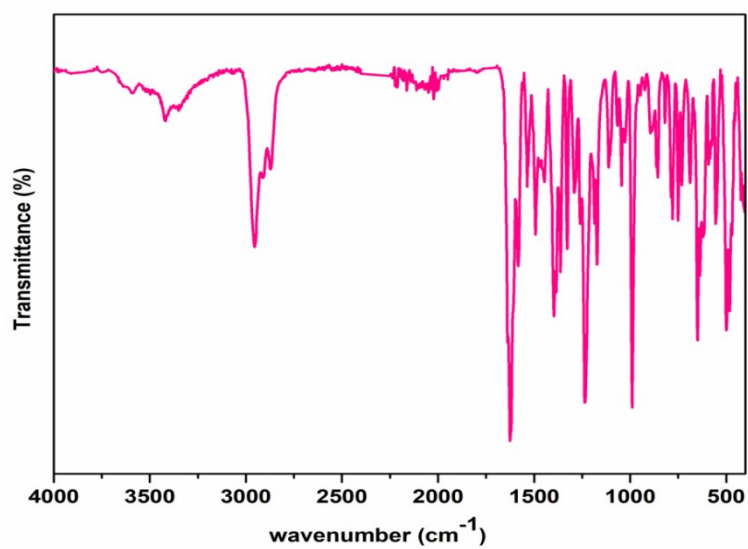


Figure S6. FT-IR Spectrum of Complex 1.

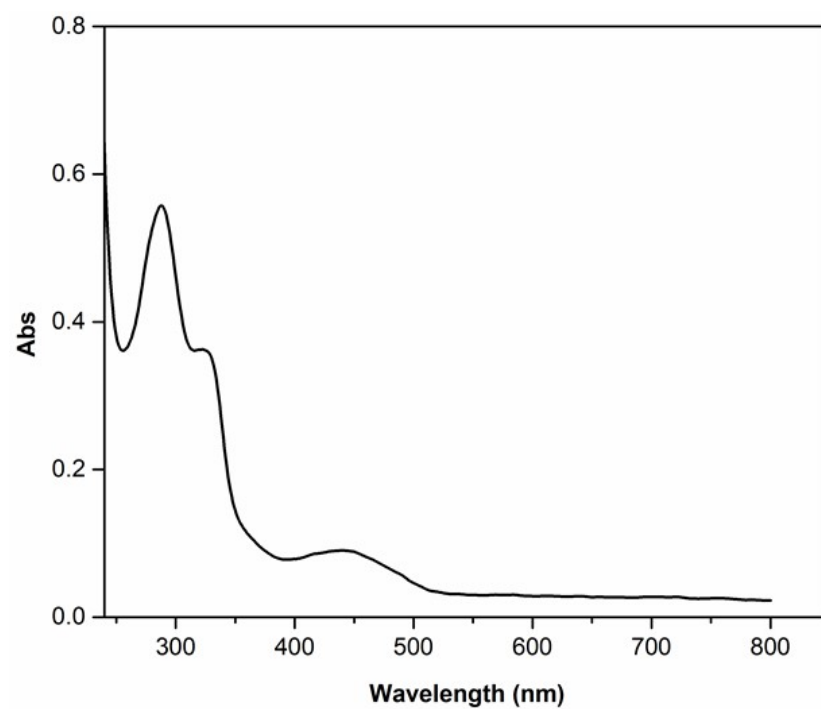


Figure S7. UV-Vis Absorption Spectra of Ligand LH₄ in CH₂Cl₂ (DCM) Solution .

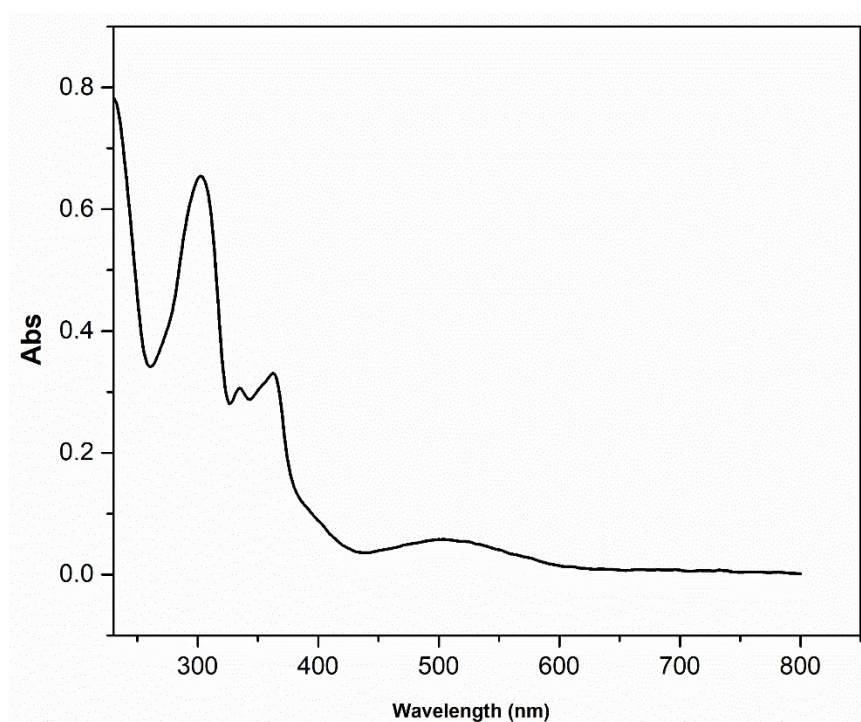


Figure S8. UV-Vis Absorption Spectra of Complex 1 in CH₂Cl₂ (DCM) Solution .

Calculation of Optical band gap E_{opt} using UV-Vis spectrum of complex 1:

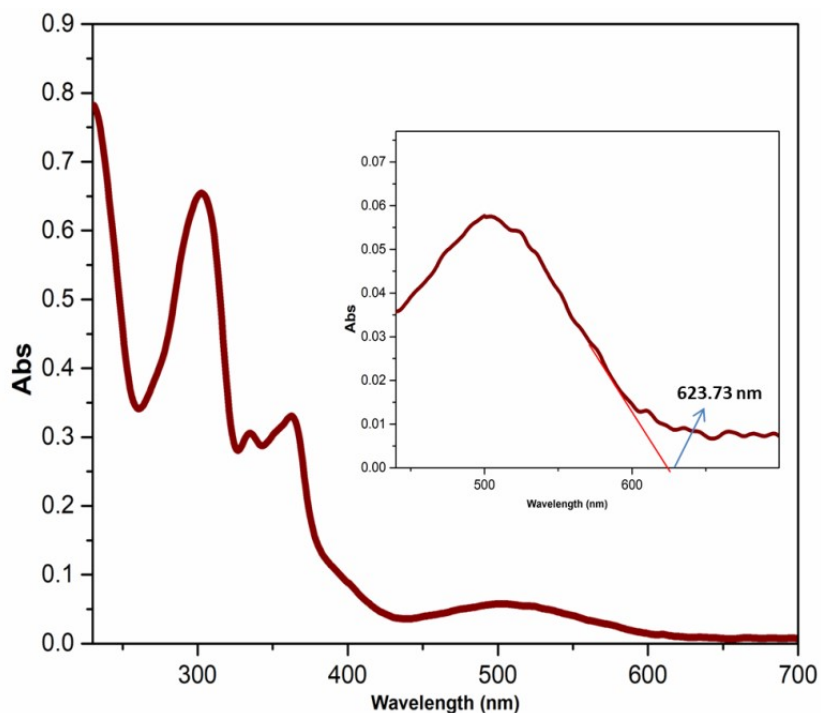


Figure S9. UV-Vis absorption spectrum for the Complex **1** in CH_2Cl_2 (DCM) Solution exhibiting onset optical absorbance.

$$E_{\text{opt}} = hc/\lambda_{\text{onset}}$$

Where, E_{opt} is the optical band gap of the complex **1**, h is the Planck constant ($6.63 \times 10^{-34} \text{ m}^2\text{kg/s}$), c is the speed of light ($3 \times 10^8 \text{ m/s}$), λ_{onset} is the onset optical absorbance wavelength.

$$E_{\text{opt}} (\text{eV}) = 1240/\lambda_{\text{onset}} (\text{nm}) = 1240/623.73 = 1.98 \text{ eV}$$

**Calculation of molecular orbital energy levels using electrochemical studies and E_{opt} ,
optical band gap of complex 1:**

$$E_{\text{HOMO}} = -[E_{\text{ox, onset}} - E_{\text{ox, Fc}}] - 4.8 \text{ eV}$$

$$E_{\text{LUMO}} = E_{\text{HOMO}} + E_{\text{opt}}$$

Where E_{opt} is the optical band gap of the complex 1, E_{HOMO} and E_{LUMO} are the HOMO and LUMO energy levels, $E_{\text{ox, onset}}$ is the onset oxidation potential for the complex 1, 4.8 eV is the ferrocene reference energy level and $E_{\text{ox, Fc}}$ is the potential when ferrocene starts to oxidize (0.40 eV vs. Ag/AgCl).

$$E_{\text{HOMO}} = -[-0.13 - 0.40] - 4.8$$

$$= -4.27 \text{ eV}$$

$$E_{\text{LUMO}} = -4.27 + 1.98 = -2.29 \text{ eV}$$

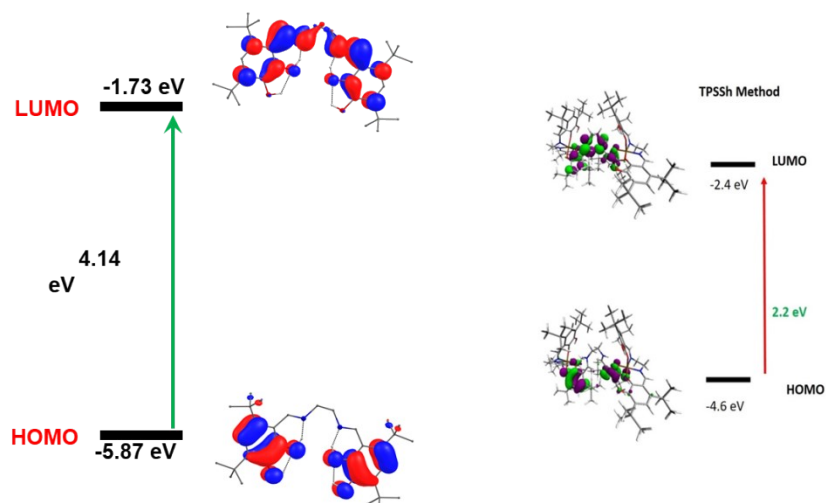


Figure S10. HOMO-LUMO energy gap of the complex 1 and uncoordinated Bis catecholaldimine ligand (LH_4) calculated by DFT.

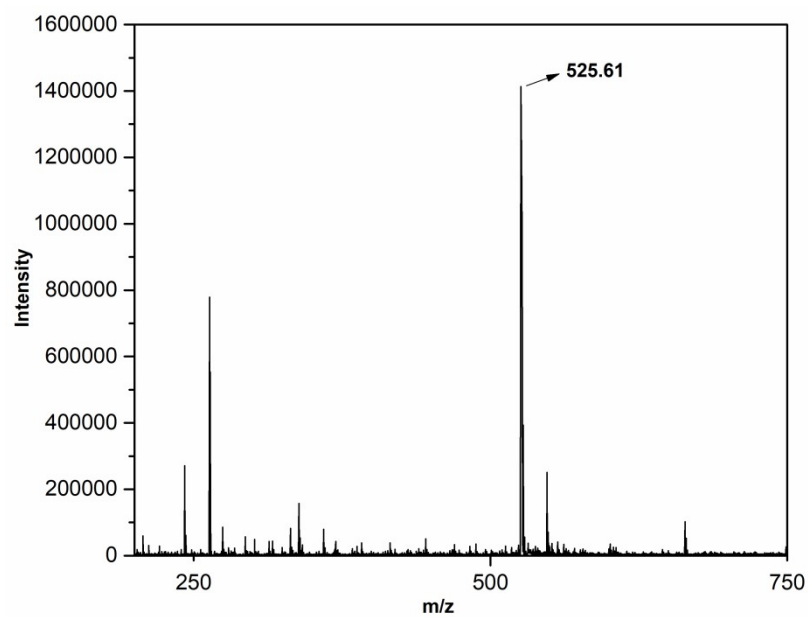


Figure S11. ESI-MS spectrum for LH₄.

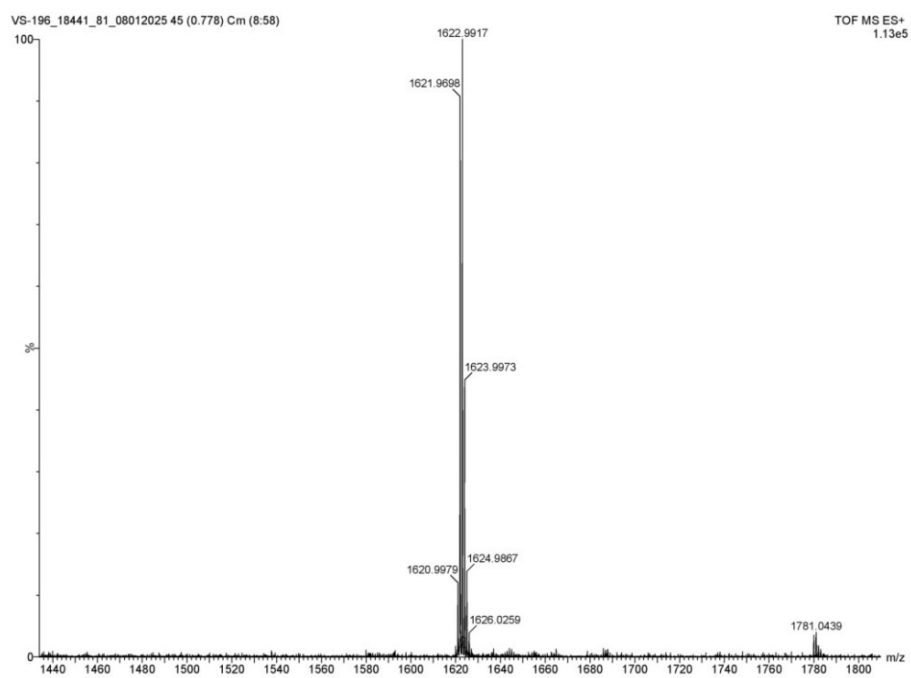
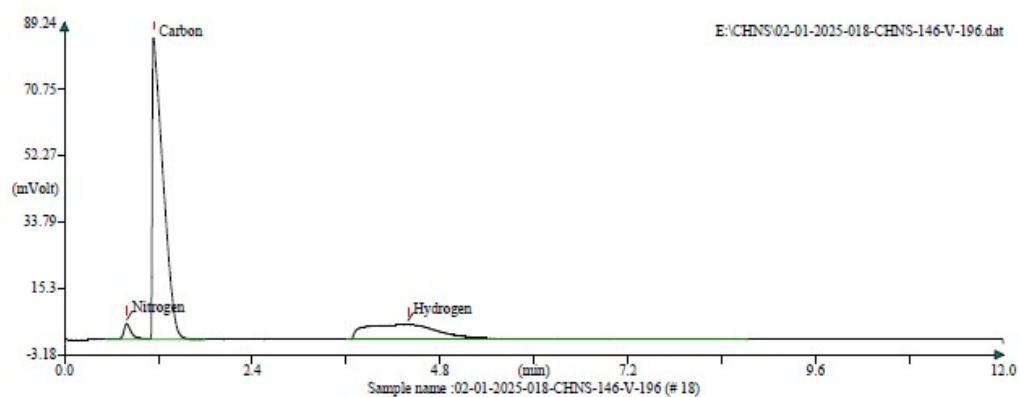


Figure S12. ESI-MS spectrum of Complex 1.



Peak Number (#)	Retention Time (min)	Area (.1* μ V*sec)	Element %	Component Name
1	0.800	296259	4.776	Nitrogen
2	1.142	8031119	59.382	Carbon
3	4.392	2927007	7.631	Hydrogen
		11254380	71.788	

Figure S13: CHN Analysis of Complex 1.

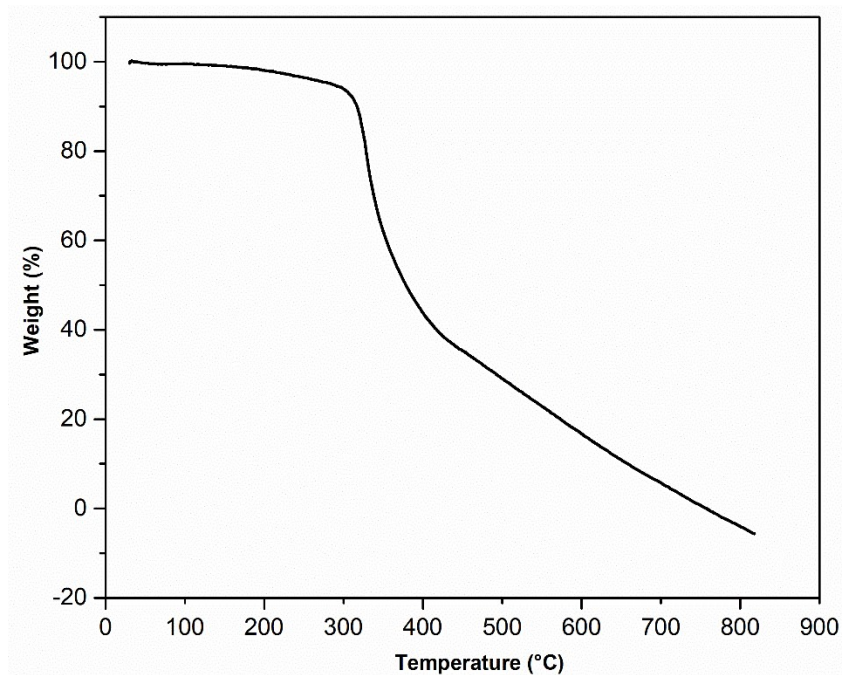


Figure S14: TGA Analysis of Complex 1. Heating rate = 5°C min⁻¹ under a nitrogen atmosphere.



Figure S15: Vacuum probe station

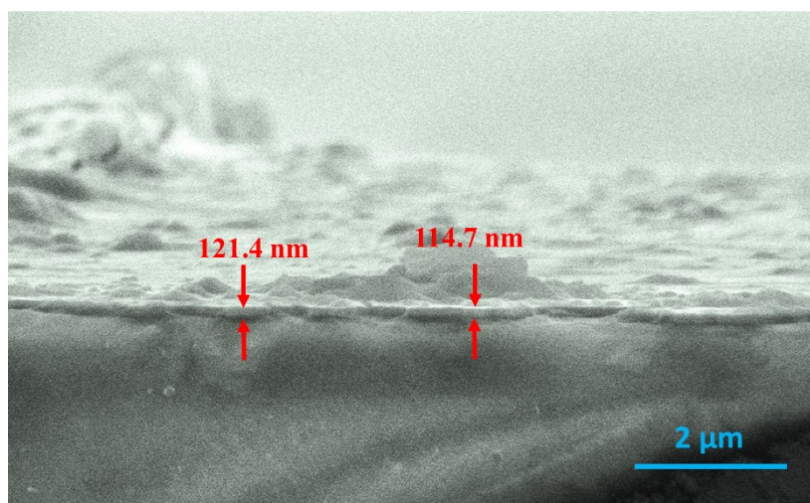


Figure S16. Cross-sectional SEM image of the device ITO/Complex **1**/Ag showing uniformity of the spin coated active layer mentioning thickness in different places of the device which showed 121.4 and 114.7 nm.

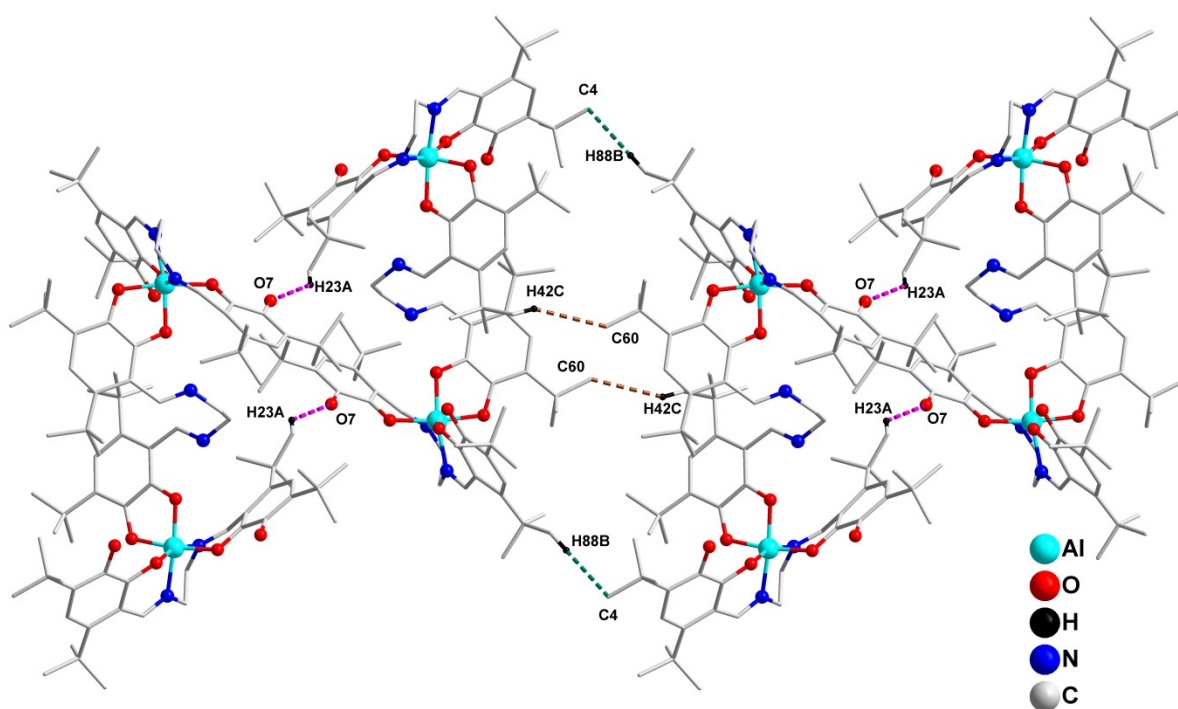


Figure S17: Supramolecular hydrogen bonded C–H...O interactions and C–H...C interactions present together throughout the crystal structure of Complex 1.