

Electronic Supplementary Information (ESI)

An experimental and computational investigations of photosensitive Schottky barrier diode property of an azobenzene based small organic molecule

Saikat Banerjee,^a Arka Dey,^b Pravat Ghorai,^a Paula Brandão,^c Joaquín Ortega-Castro,^d Antonio Frontera,^{*d} Partha Pratim Ray,^{*b} and Amrita Saha^{*a}

^aDepartment of Chemistry, Jadavpur University, Kolkata- 700032, India.

E-mail: asaha@chemistry.jdvu.ac.in; Tel. +91-33-24572941

^bDepartment of Physics, Jadavpur University, Kolkata- 700032, India.

E-mail: partha@phys.jdvu.ac.in; Tel: +91-9475237259

^cDepartment of Chemistry, CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal.

^dDepartament de Química, Universitat de les Illes Balears, Crta. de Valldemossa km 7.5, 07122 Palma de Mallorca, Balears, Spain. E-mail: toni.frontera@uib.es

Sl. No.	Content	Page No.
1	FTIR spectrum of complex 1	S2
2	¹HNMR Spectrum of compound 1	S3
3	Mass Spectrum of compound 1	S4
4	TGA	S5
5	Powdered X-ray diffraction	S6

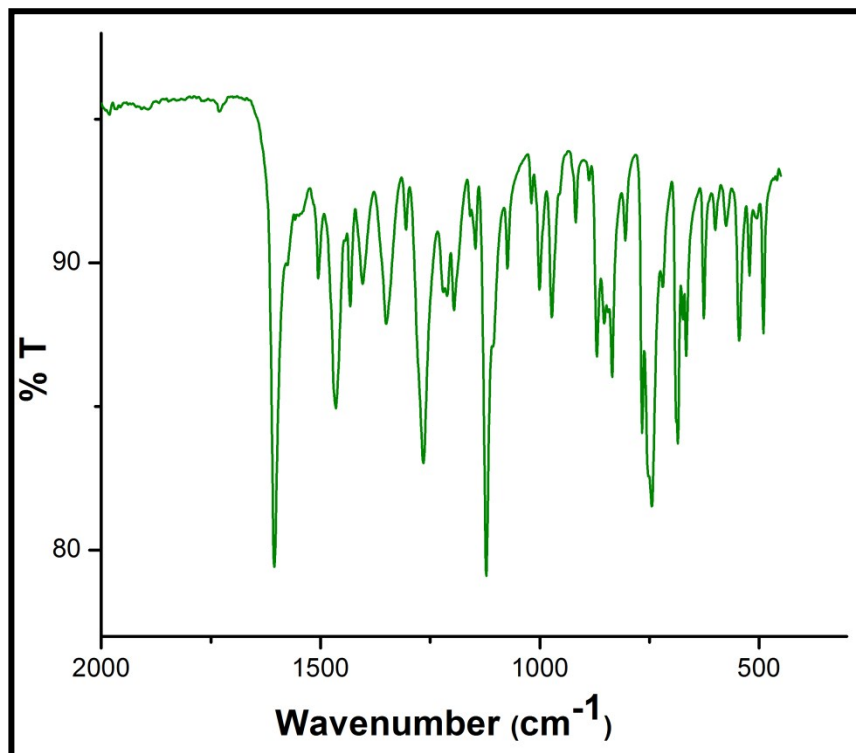


Fig. S1. FTIR spectrum of compound 1.

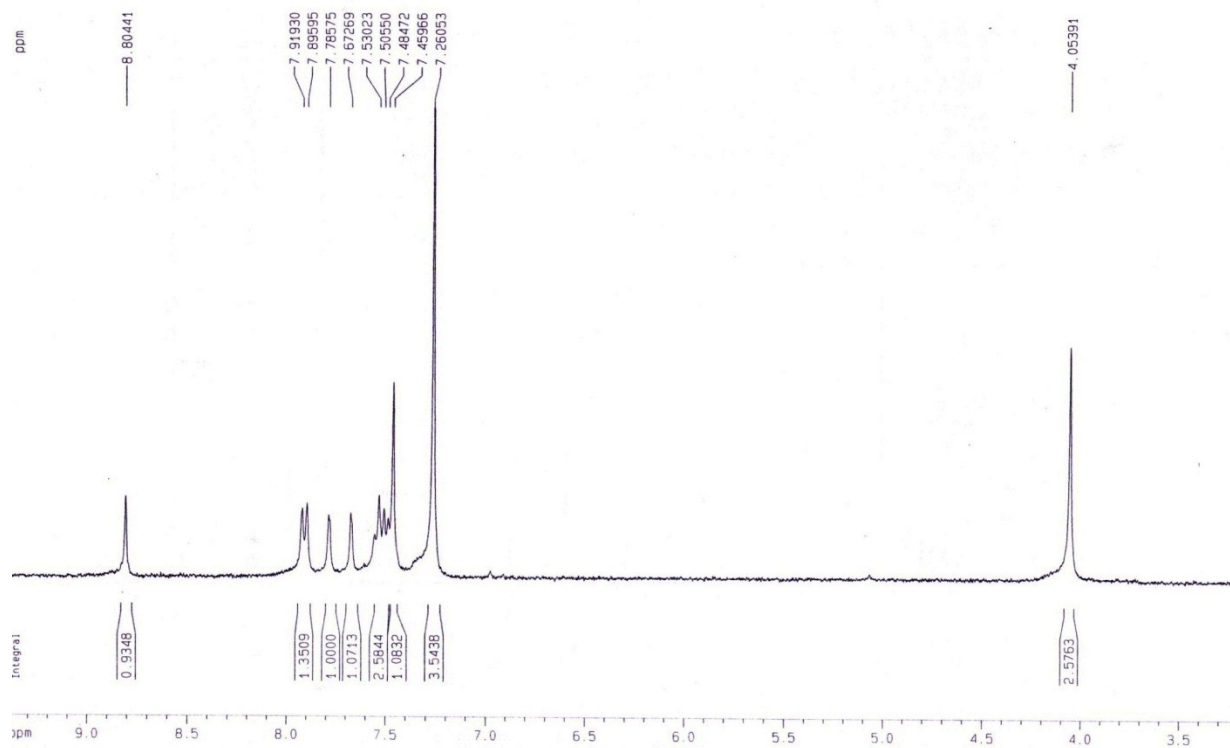


Fig. S2. ^1H NMR(CDCl_3 , 300 MHz) spectrum of compound **1**.

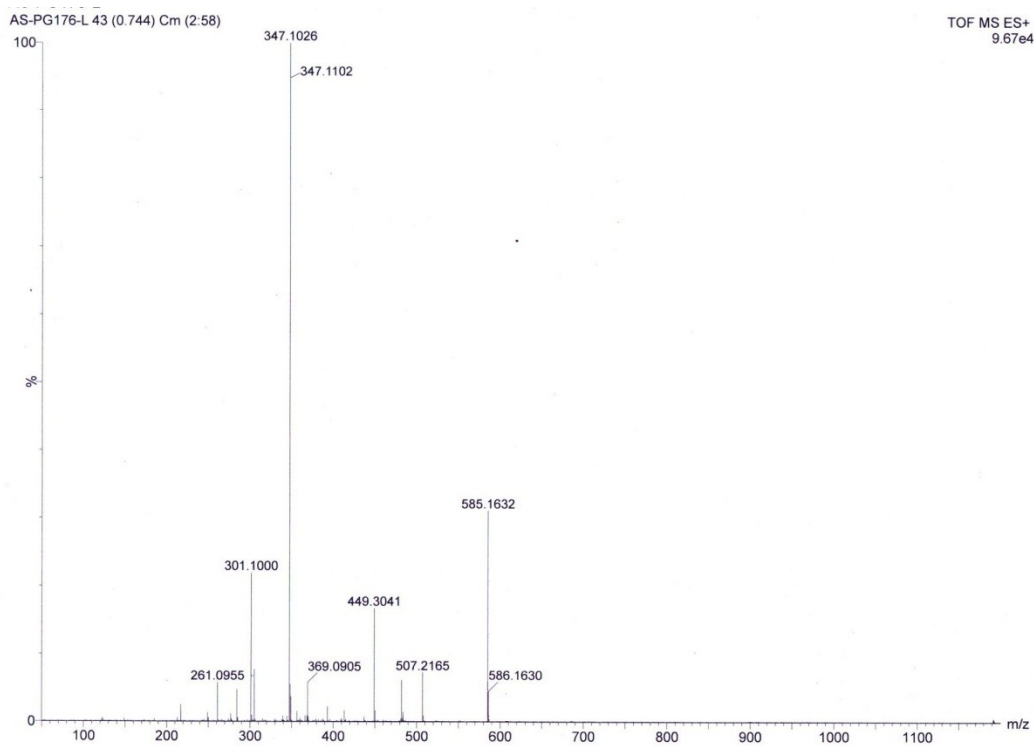


Fig. S3. Mass spectrum of compound **1**.

TGA (Thermo Gravimetric Analysis)

TGA of the compound **1** is measured using Platinum crucible with alpha alumina powder as reference in a PerkinElmer (SINGAPORE) instrument (Model No. - Pyris Diamond TG/DTA).

The result shows good stability of the compound up to 290°C (Figure S4).

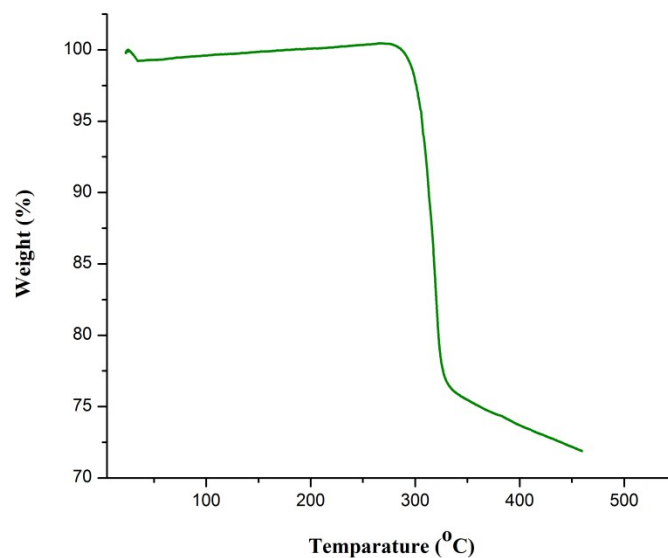


Fig. S4. Thermo Gravimetric Analysis of compound **1** showing stability of the compound is very appreciable up to 290°C.

Powdered X-ray diffraction

The bulk purity of the complex **1** has been confirmed. It is shown in [Figure S5](#). The simulated pattern (A) is obtained from cif file of the complex and experimental pattern (B) is collected from powdered XRD.

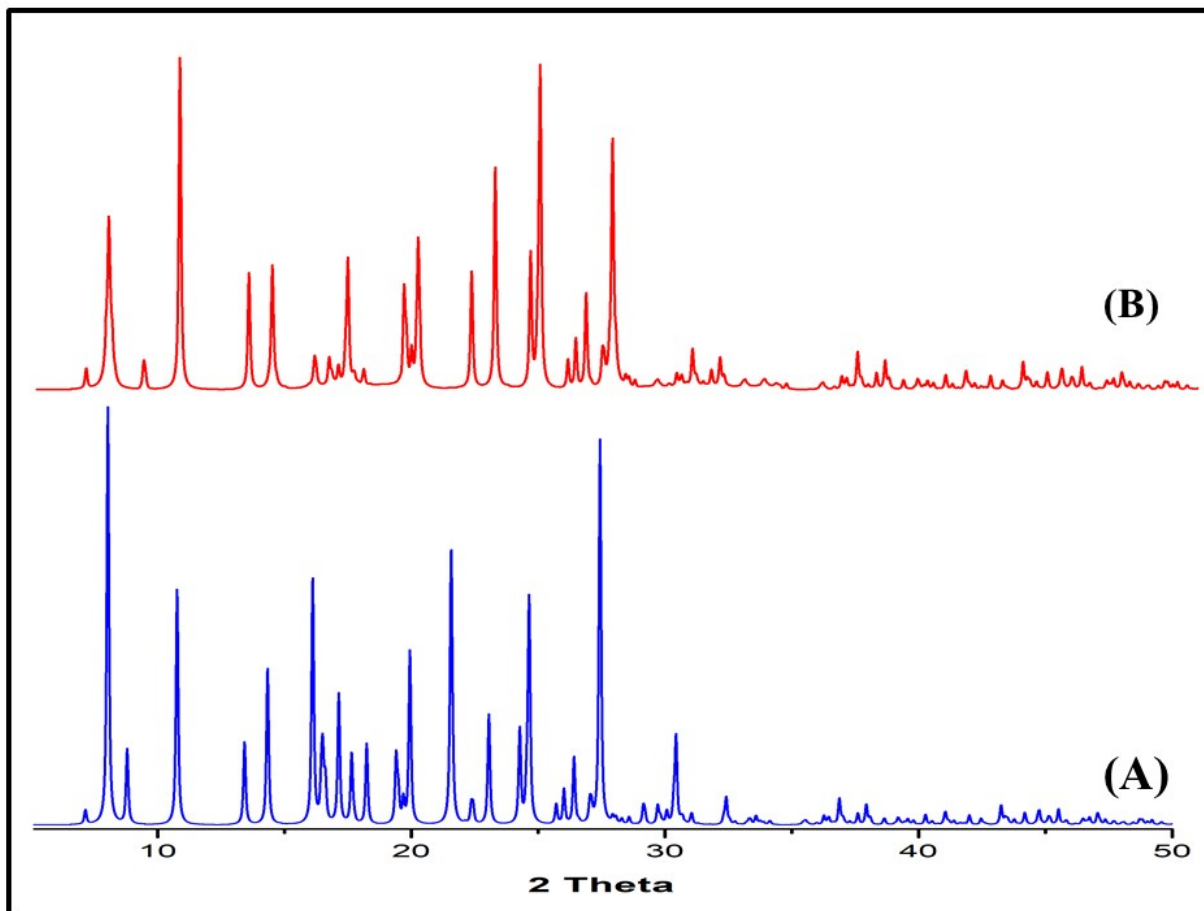


Fig. S5. Simulated (A) and experimental (B) powdered XRD pattern indicating the purity of the bulk materials of compound **1**.