

## **Organosilane based magnetic silica nanoparticles for the detection of Al (III) ions and construction of molecular logic gate**

Gurjaspreet Singh<sup>a\*</sup>, Anita Devi<sup>a\*</sup>, Anamika Saini<sup>a</sup>, Diksha<sup>a</sup>, Yamini Thakur<sup>a</sup>, Riddima Singh<sup>b</sup>, Jandeep Singh<sup>b</sup>, Pooja Kalra<sup>c</sup>, Brij Mohan<sup>d\*</sup>

<sup>a</sup>Department of Chemistry, Panjab University, Chandigarh, 160014, India

<sup>b</sup>School of Chemical Engineering and Physical Sciences, Lovely Professional University, Phagwara, 144411, Punjab, India

<sup>c</sup>Department of Chemistry and Biochemistry, School of Basic Sciences and Research, Sharda University, Greater Noida, 201306, U.P., India

<sup>d</sup>Centro de Química Estrutural, Institute of Molecular Sciences, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

\*Corresponding Author

1. Prof. Gurjaspreet Singh

Department of Chemistry & Centre of Advanced Studies

Panjab University, Chandigarh, India

Email: [gjpsingh@pu.ac.in](mailto:gjpsingh@pu.ac.in)

2. Miss Anita Devi

Research Scholar

Department of Chemistry & Centre of Advanced Studies

Panjab University, Chandigarh, India

Email: [anitadevi0025@gmail.com](mailto:anitadevi0025@gmail.com)

3. Brij Mohan

Centro de Química Estrutural, Institute of Molecular Sciences, Instituto Superior Técnico, Universidade de Lisboa, Av. Rovisco Pais, 1049-001 Lisboa, Portugal

Email: [brizharry17@gmail.com](mailto:brizharry17@gmail.com)

## *Table of Contents*

| <b>Entry</b>  | <b>Sr. No.</b> |
|---|----------------|
| <sup>1</sup> H NMR spectrum of compound 3   | (Fig.S1)       |
| <sup>13</sup> C NMR spectrum of compound 3  | (Fig. S2)      |
| Mass spectrum of compound 3   | (Fig. S3)      |
| (a) FT-IR spectrum of Fe <sub>3</sub> O <sub>4</sub> @SiO <sub>2</sub> @silane, (b) EDX analysis,<br>(c) Hysteresis loop of Fe <sub>3</sub> O <sub>4</sub> @SiO <sub>2</sub> @silane  | (Fig. S4)      |
| PXRD patterns of Fe <sub>3</sub> O <sub>4</sub> @SiO <sub>2</sub> @silane with different<br>pH treatments   | (Fig. S5)      |
| (a) FE-SEM images of<br>Fe <sub>3</sub> O <sub>4</sub> @SiO <sub>2</sub> @silane at different magnifications,<br>(b) Thermogravimetric curves of Fe <sub>3</sub> O <sub>4</sub> @SiO <sub>2</sub> ,<br>Fe <sub>3</sub> O <sub>4</sub> @SiO <sub>2</sub> @silane and 3 | (Fig. S6)      |
| UV-Visible absorption changes of sensor Fe <sub>3</sub> O <sub>4</sub> @SiO <sub>2</sub> @silane<br>with various nitro-compounds  | (Fig. S7)      |
| IR spectra of Fe <sub>3</sub> O <sub>4</sub> @SiO <sub>2</sub> @silane-Al (III)   | (Fig. S8)      |

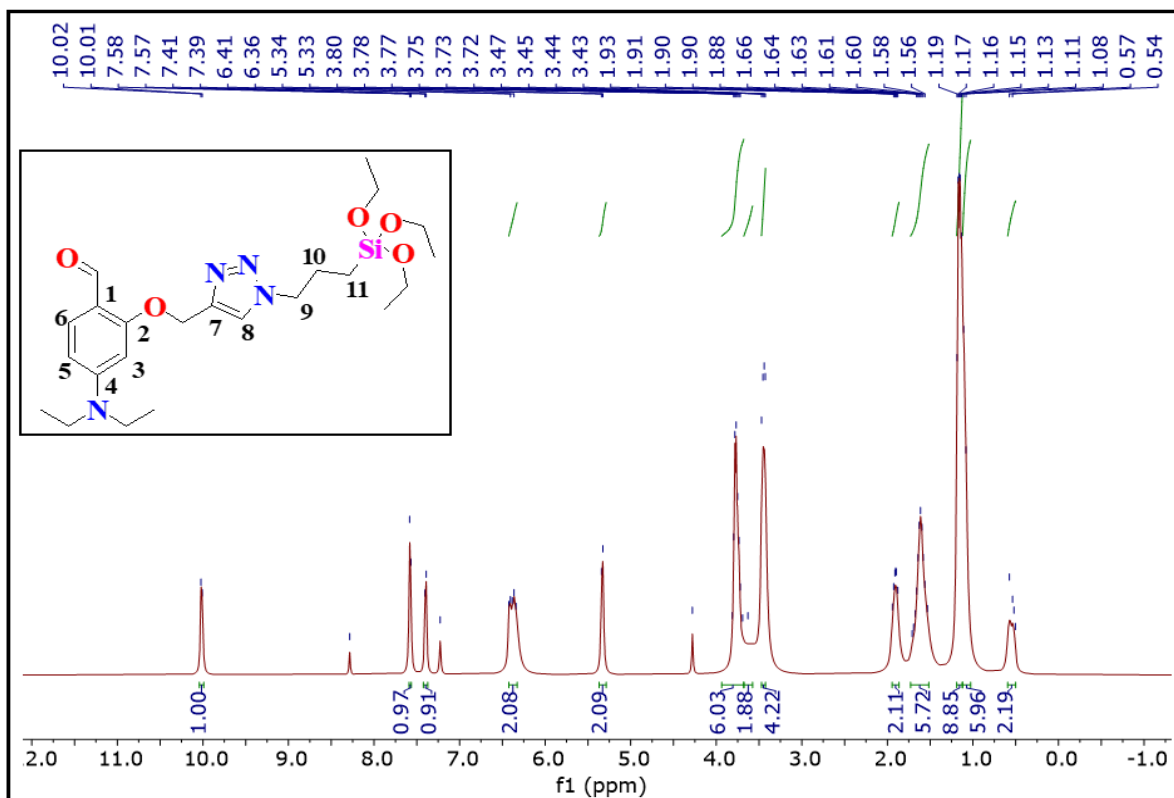


Fig. S1. <sup>1</sup>H NMR spectrum of compound 3

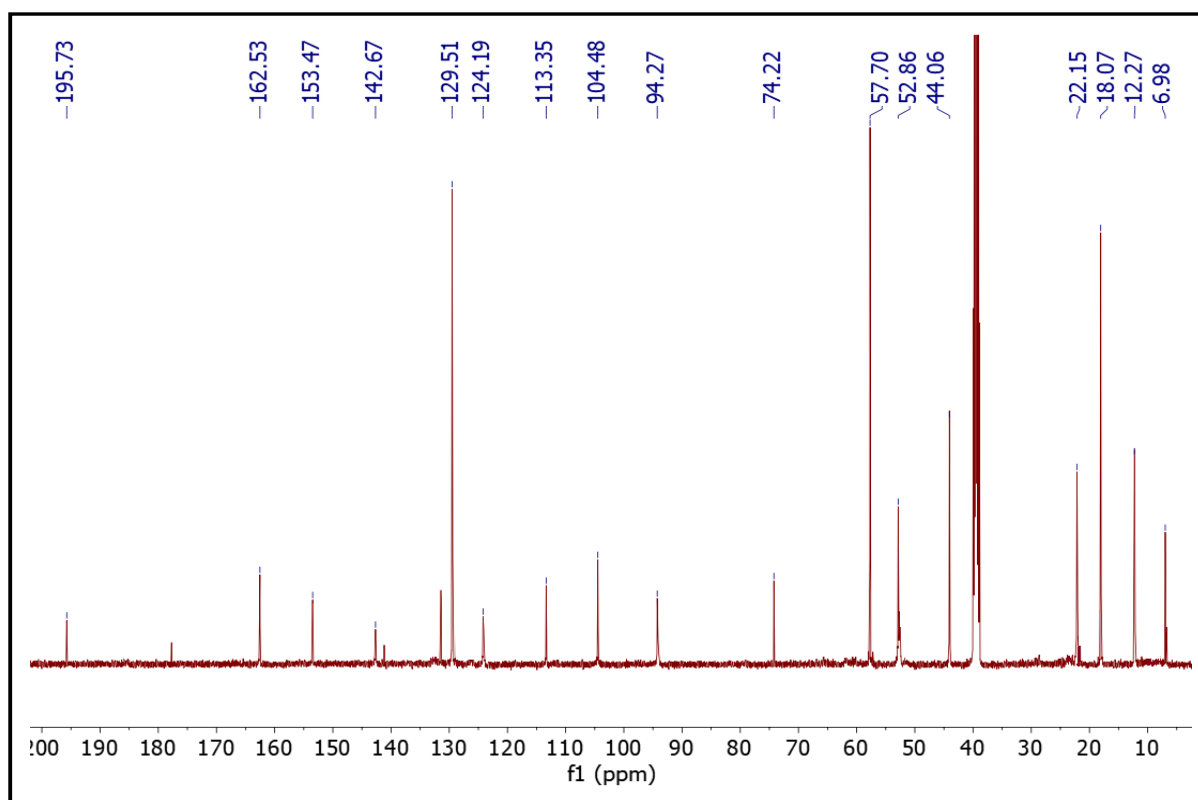
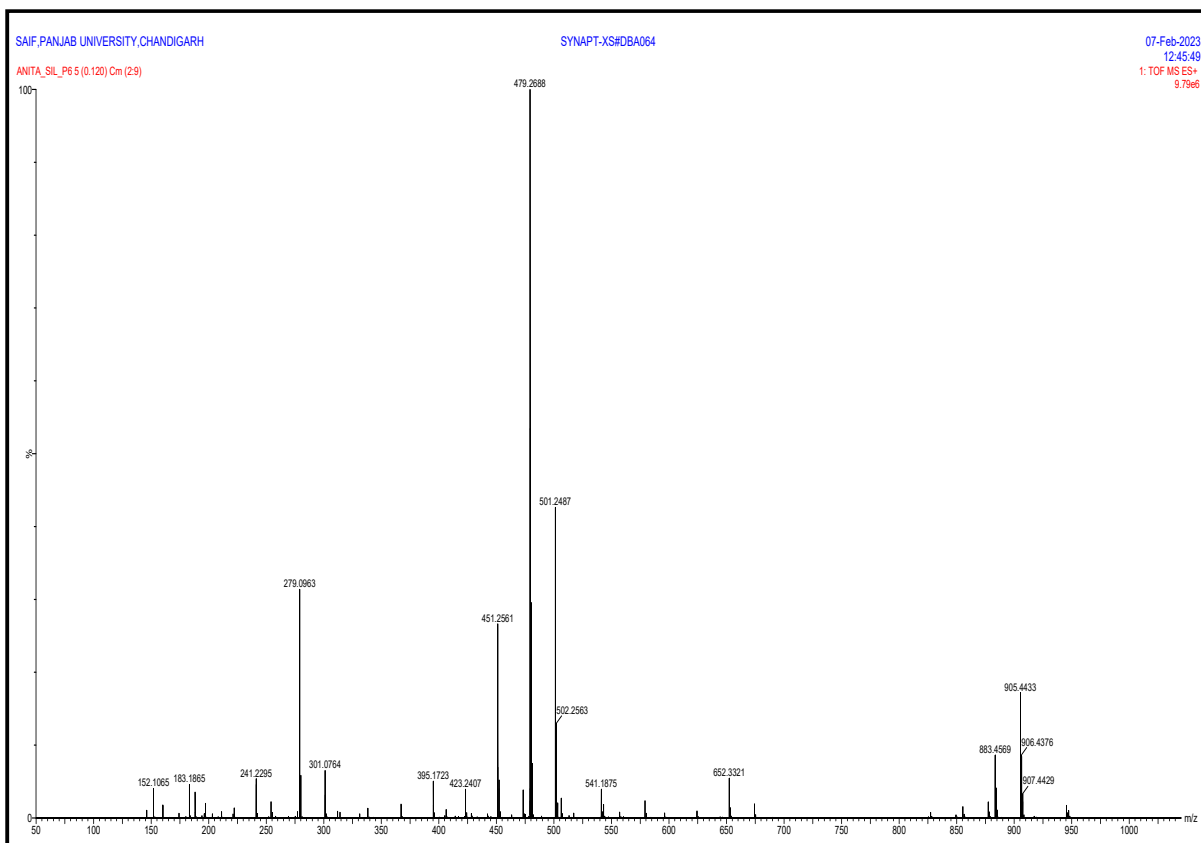
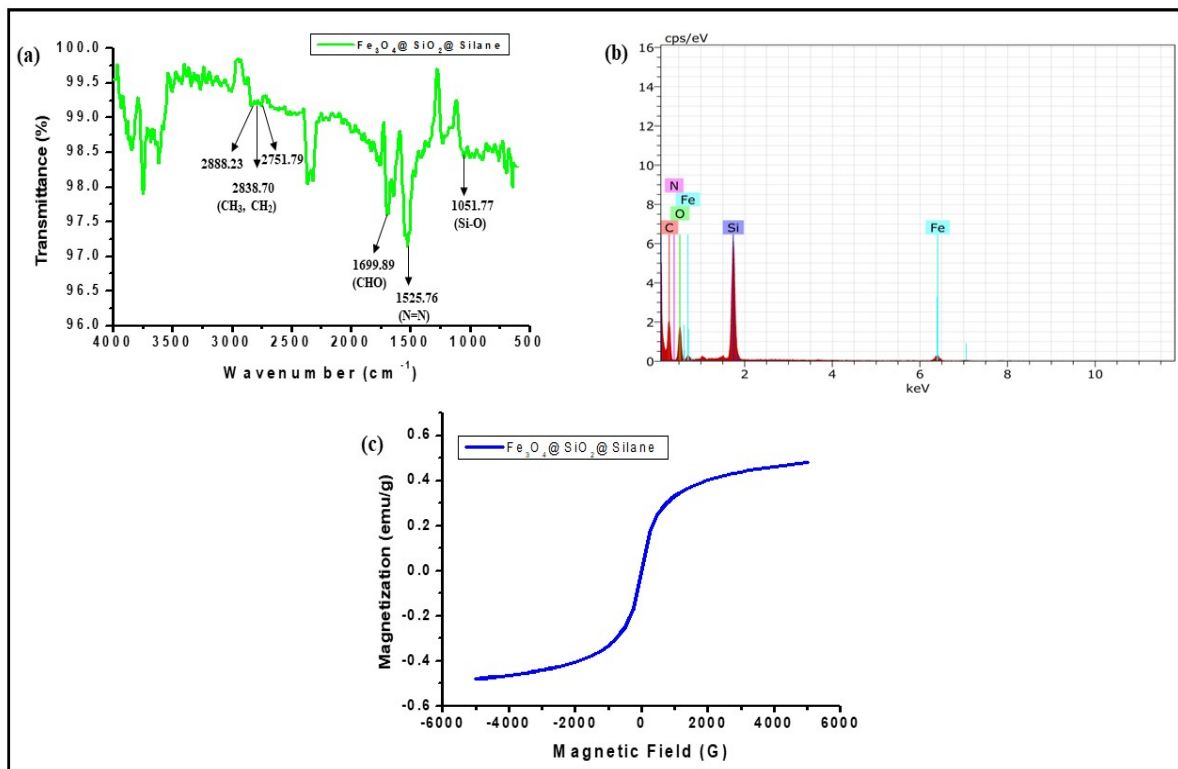


Fig. S2. <sup>13</sup>C NMR spectrum of compound 3



**Fig. S3.** Mass spectrum of compound 3



**Fig. S4.** (a) FT-IR spectrum of  $\text{Fe}_3\text{O}_4@SiO_2@silane$ , (b) EDX analysis, (c) Hysteresis loop of  $\text{Fe}_3\text{O}_4@SiO_2@silane$

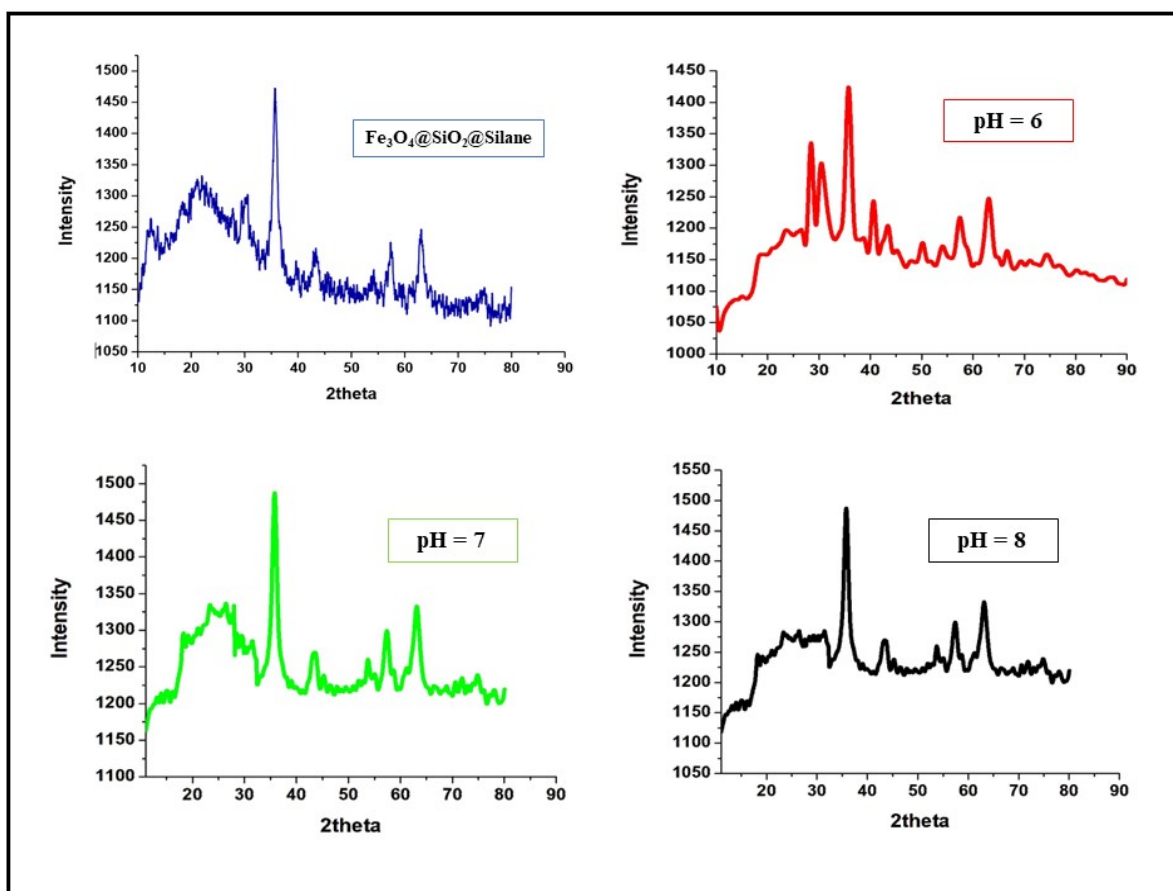


Fig. S5. PXRD patterns of  $\text{Fe}_3\text{O}_4@SiO_2@silane$  with different pH treatments

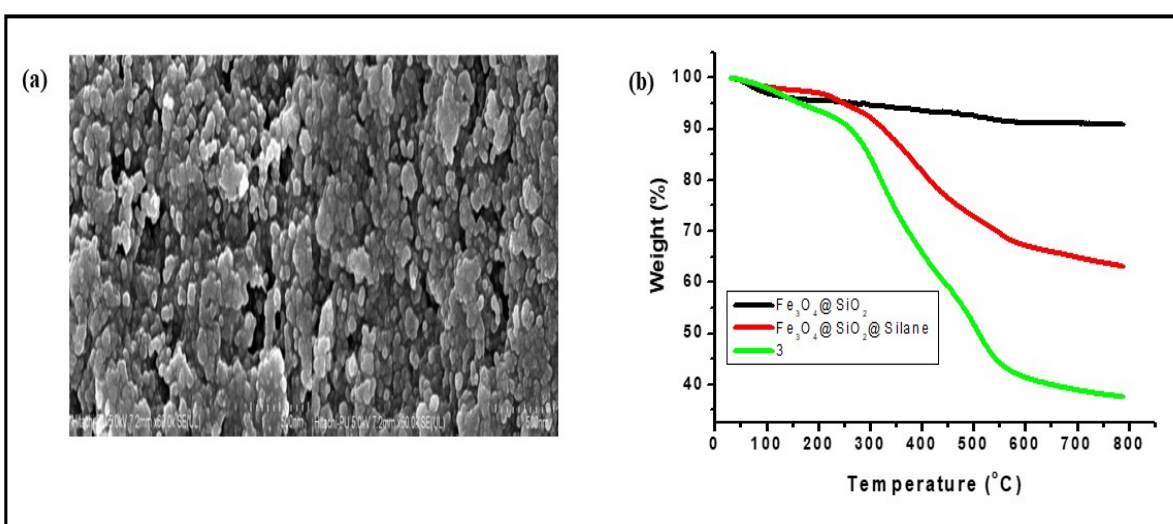


Fig. S6. (a) FE-SEM images of  $\text{Fe}_3\text{O}_4@SiO_2@silane$  at different magnifications, (b) Thermogravimetric curves of  $\text{Fe}_3\text{O}_4@SiO_2$ ,  $\text{Fe}_3\text{O}_4@SiO_2@silane$  and 3

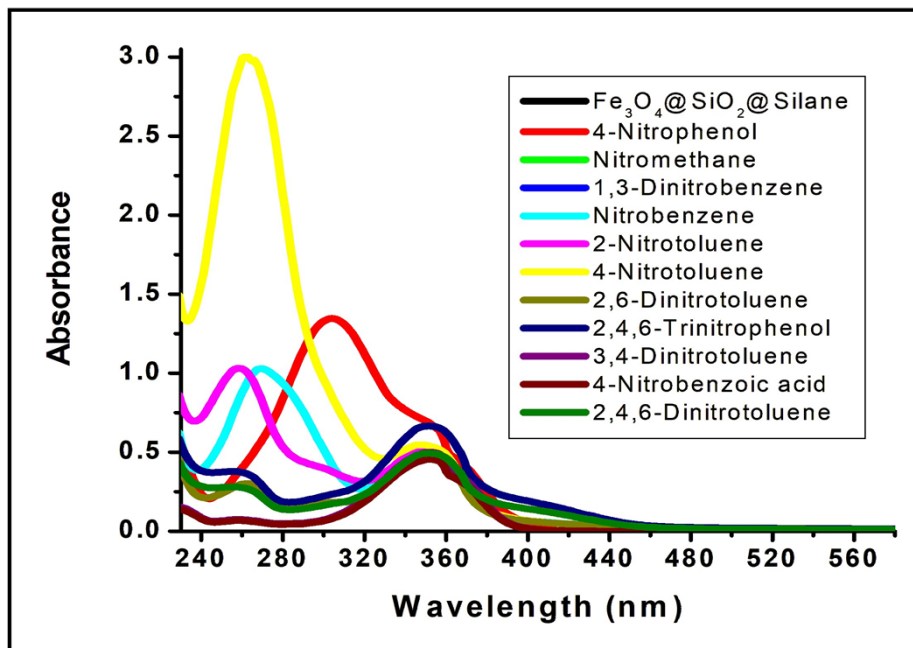


Fig. S7. UV-Visible absorption changes of sensor  $\text{Fe}_3\text{O}_4@\text{SiO}_2@\text{silane}$  with various nitro-compounds

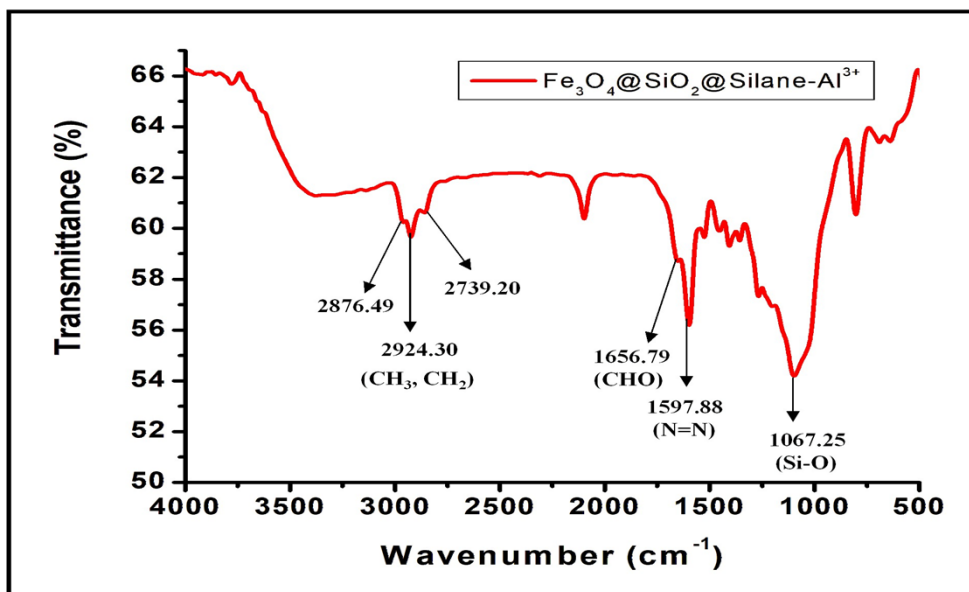


Fig. S8. IR spectra of  $\text{Fe}_3\text{O}_4@\text{SiO}_2@\text{silane-Al(III)}$