

Electronic Supplementary Information

Ni-MOF based luminescent sensor for selective and rapid sensing of Fe (II) and Fe(III) ions

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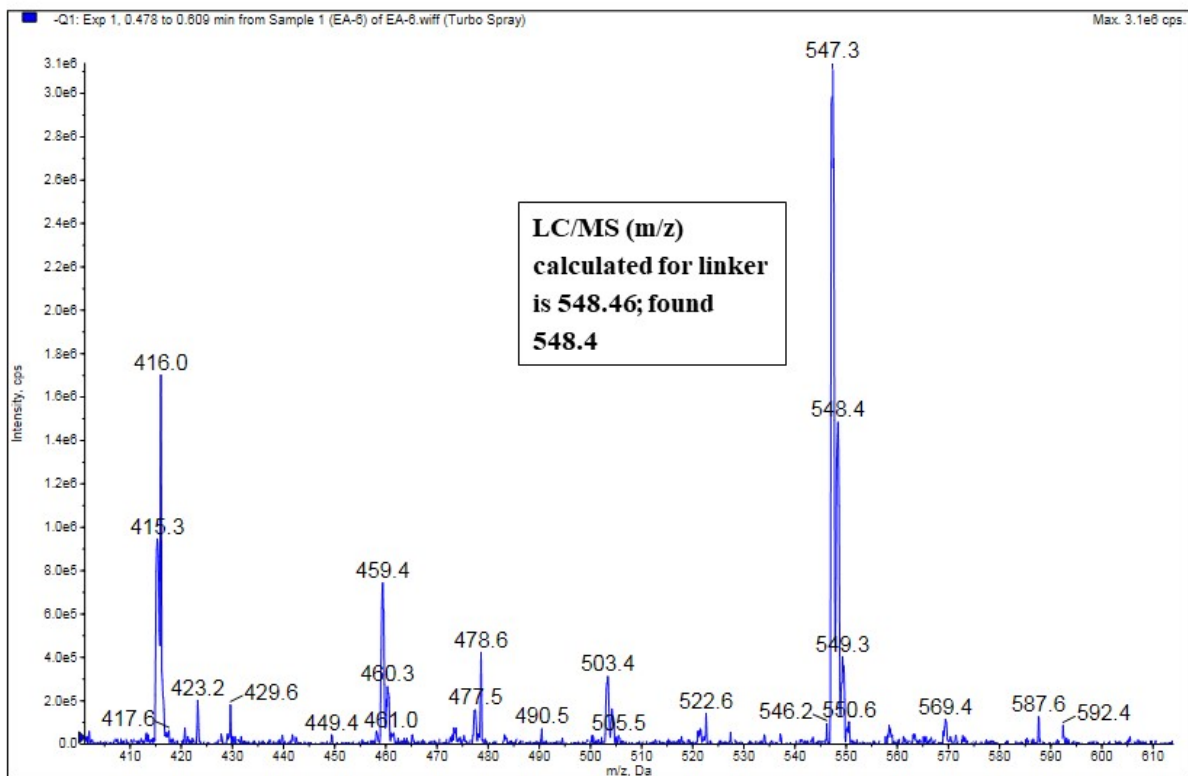


Fig. S1 LC-MS (m/z) of linkerbis (N, N-trimellitoyl)-4,4'-oxydianiline.

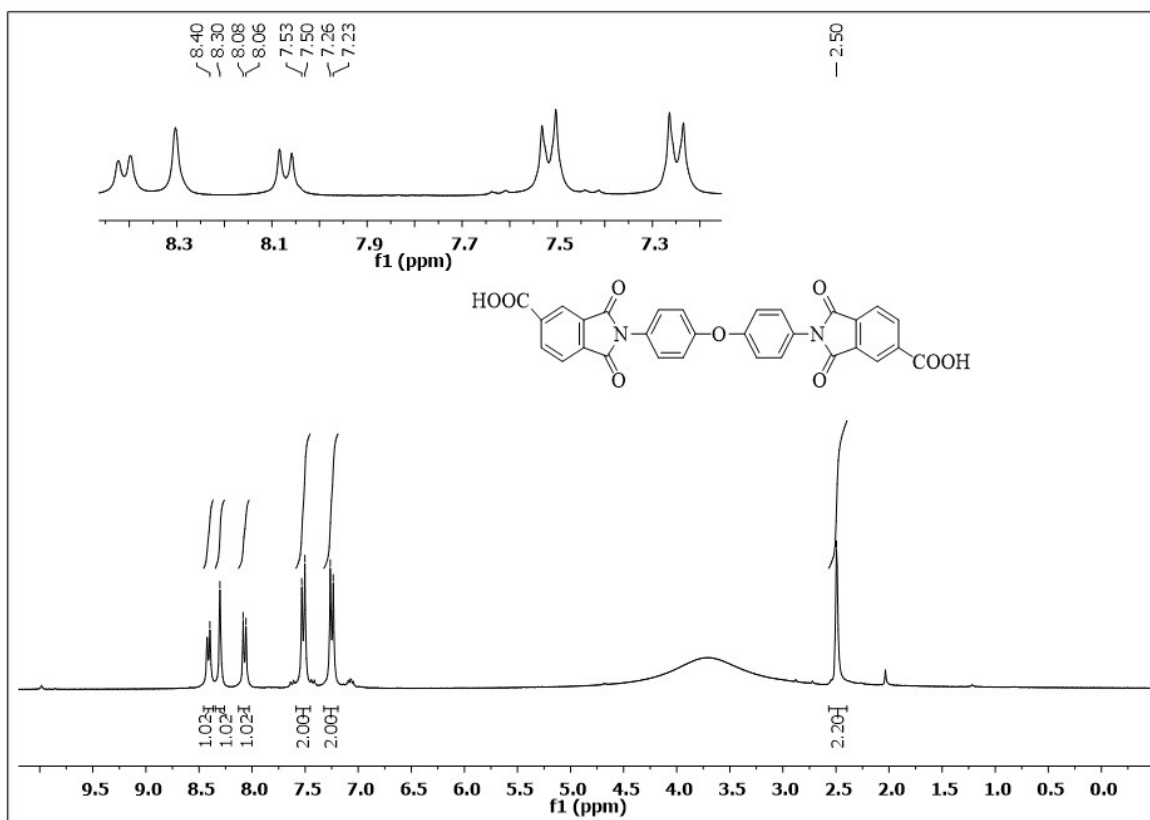


Fig. S2 $^1\text{H-NMR}$ of linker bis(N,N-trimellitoyl)-4,4'-oxydianiline.

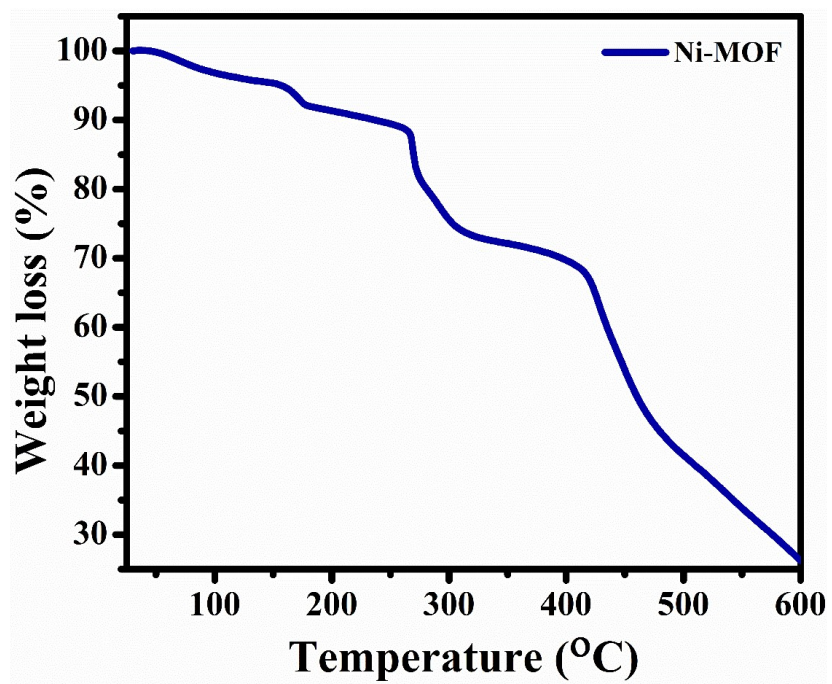


Fig. S3 Thermogravimetry (TGA) analysis of Ni-MOF.

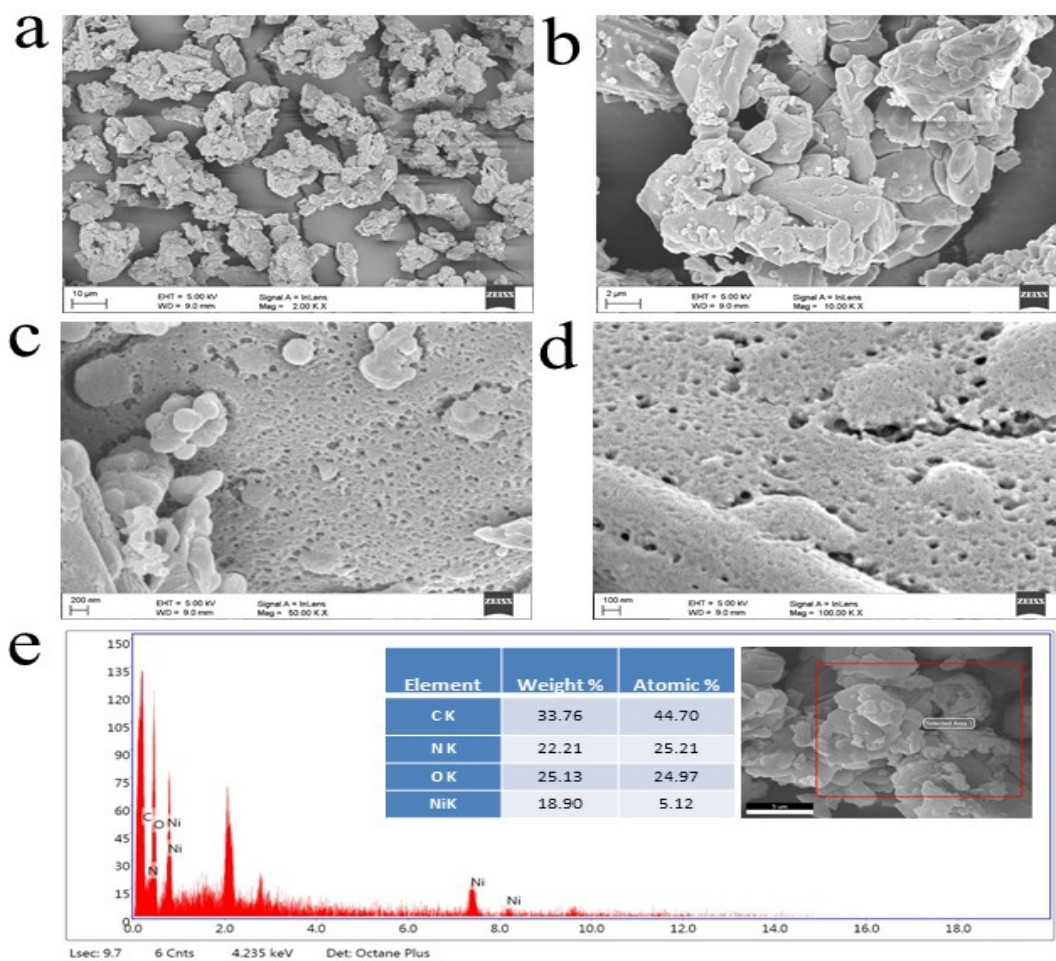


Fig. S4 (a), (b), (c), (d) FE-SEM images of Ni-MOF at different magnification of 10 μm, 2 μm, 200nm, 100nm respectively and; (e) EDAX spectrum of Ni-MOF.

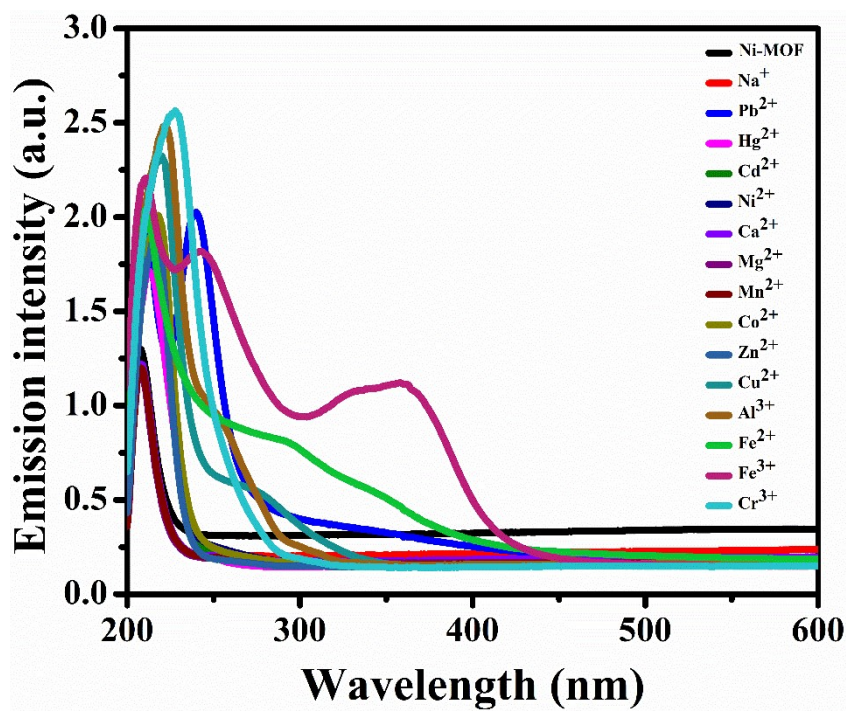


Fig. S5 UV-vis spectra of Ni-MOF and Ni-MOF with different metal ions.

Limit of Detection (LOD)

The detection limit was calculated by titrating increasing concentration of Fe (II)/Fe (III) (0-500 μ M) with Ni-MOF. The readings of blank (Ni-MOF) were recorded to calculate standard deviation.

The LOD was calculated by using the formula;

$$LOD = \frac{3\sigma}{k}$$

Where, σ = standard deviation of Ni-MOF,

k = slope of the linear regression line between the plots of emission intensity vs. concentration of Fe(II)/Fe(III).

Table S1: The results of linear regression line:

| | σ | $3 \times \sigma$ | k | R^2 |
|-----------|----------|-------------------|--------|--------|
| Fe^{2+} | 7.414916 | 22.24475 | -0.889 | 0.9105 |
| Fe^{3+} | | | -1.440 | 0.9567 |

Table S2: Sensing capabilities of some reported MOFs towards Fe²⁺ and Fe³⁺ in terms of limit of detection (LOD):

| MOF | Analytes | LOD (μM) | Medium | References |
|--------------------------------------------------------------------------------------------------------|--------------------------------------|----------------|---------|------------------|
| 534-MOF-Tb | Fe ³⁺ | 130 | Water | S1 |
| FJI-C8 (Zn-MOF) | Fe ³⁺ | 23.3 | DMF | S2 |
| [(CH ₃) ₂ NH ₂] ₂ [Tb(bptc)]·0.4DMF·3.6H ₂ O. | Fe ³⁺ | 180 | Ethanol | S3 |
| NNU-1 (Zn-MOF) | Fe ³⁺ | 200 | Water | S4 |
| Eu(C ₃₃ H ₂₄ O ₁₂)(H ₂ NMe)(H ₂ O) | Fe ³⁺ | 200 | Water | S5 |
| Ni-MOF | Fe ²⁺ Fe ³⁺ | 25.03 15.44 | Ethanol | This work |

Table S3: N₂ adsorption parameters of the Ni-MOF

| PARAMETERS | VALUE |
|------------------------------------------------------------------------------------------|-----------------------------|
| Surface Area | |
| Single point surface area at P/Po = 0.110030026: | 2.2238 m ² /g |
| BET Surface Area: | 2.2669 m ² /g |
| Langmuir Surface Area: | 0.7629 m ² /g |
| t-Plot Micropore Area: | 6.8160 m ² /g |
| t-Plot external surface area: | -4.5491 m ² /g |
| BJH Adsorption cumulative surface area of pores between 10.000 Å and 500.000 Å diameter: | 4.9384 m ² /g |
| Pore Volume | |
| t-Plot micropore volume: | 0.002638 cm ³ /g |
| BJH Adsorption cumulative volume of pores between 10.000 Å and 500.000 Å diameter: | 0.001282 cm ³ /g |
| Pore Size | |
| BJH Adsorption average pore diameter (4V/A): | 10.388 Å |

References

- S1** M. Chen, W. M. Xu, J. Y. Tian, H. Cui, J. X. Zhang, C. Sen Liu and M. Du, *Journal of Materials Chemistry C*, 2017, **5**, 2015.
- S2** C. H. Chen, X. S. Wang, L. Li, Y. B. Huang and R. Cao, *Dalton Transactions*, 2018, **47**, 3452.
- S3** X. L. Zhao, D. Tian, Q. Gao, H. W. Sun, J. Xu and X. H. Bu, *Dalton Transactions*, 2016, **45**, 1040.
- S4B**. L. Hou, D. Tian, J. Liu, L. Z. Dong, S. L. Li, D. S. Li and Y. Q. Lan, *Inorganic Chemistry*, 2016, **55**, 10580.
- S5S**. Dang, E. Ma, Z. M. Sun and H. Zhang, *Journal of Materials Chemistry*, 2012, **22**, 16920.