

Supporting information

A Versatile Iron [1-(naphthalen-2-ylmethyl)-2-(pyridin-2-yl)-1*H*-benzo[*d*]imidazole]₃ Metal Complex Redox Active Material for Energy Conversion and Storage Systems

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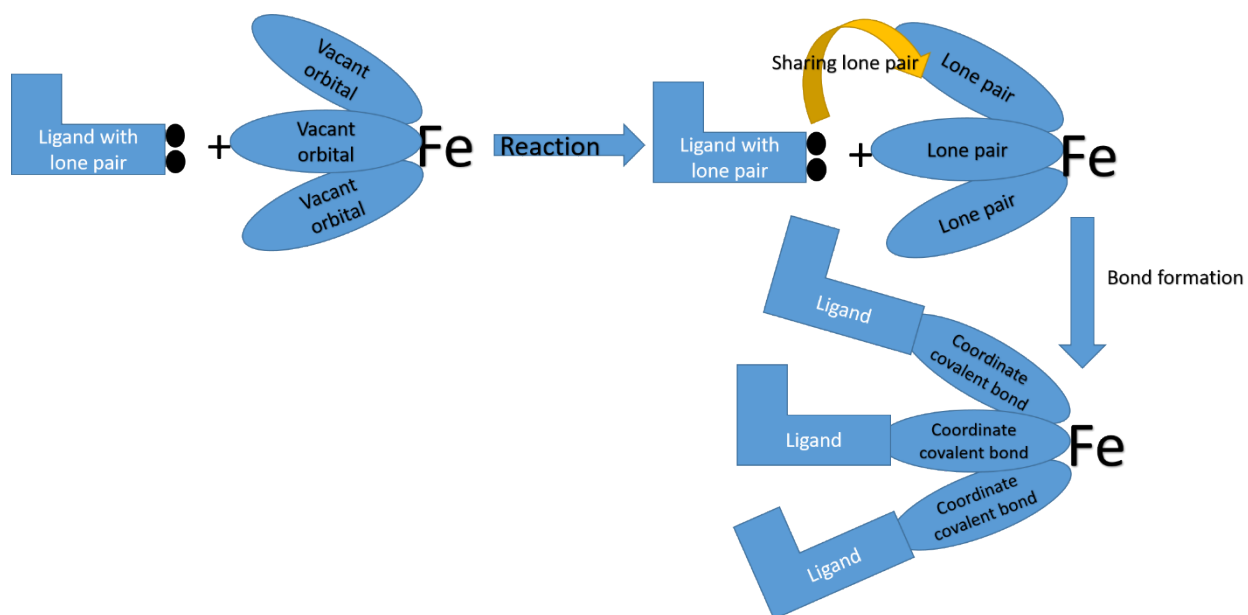
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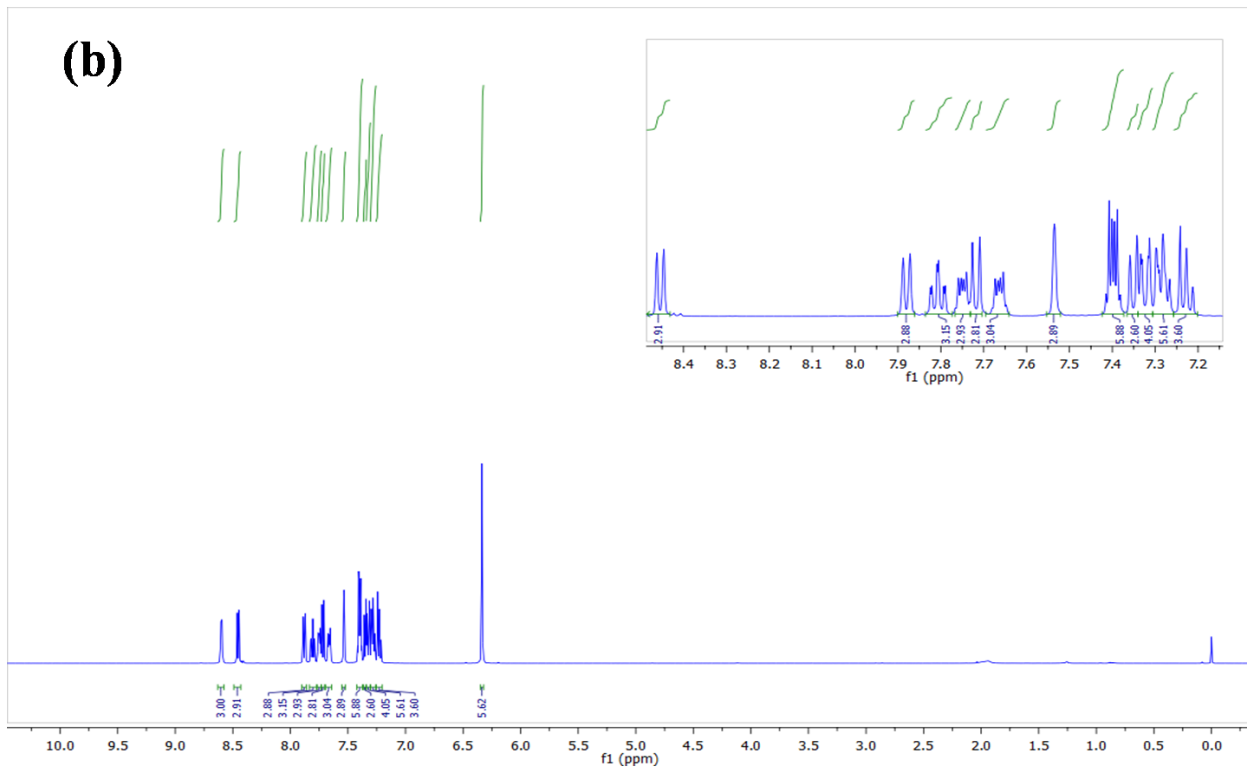
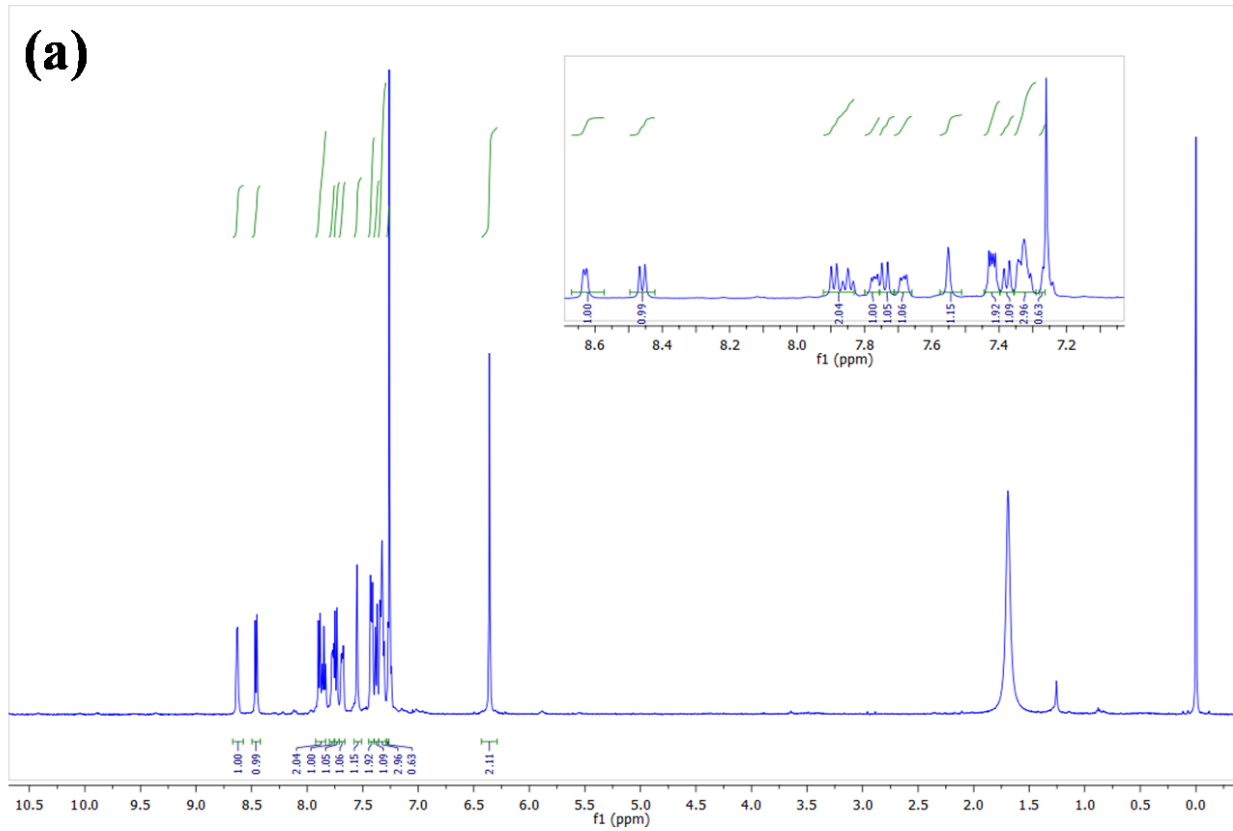
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Scheme S1. Schematic representation of mechanism of iron complex formation.



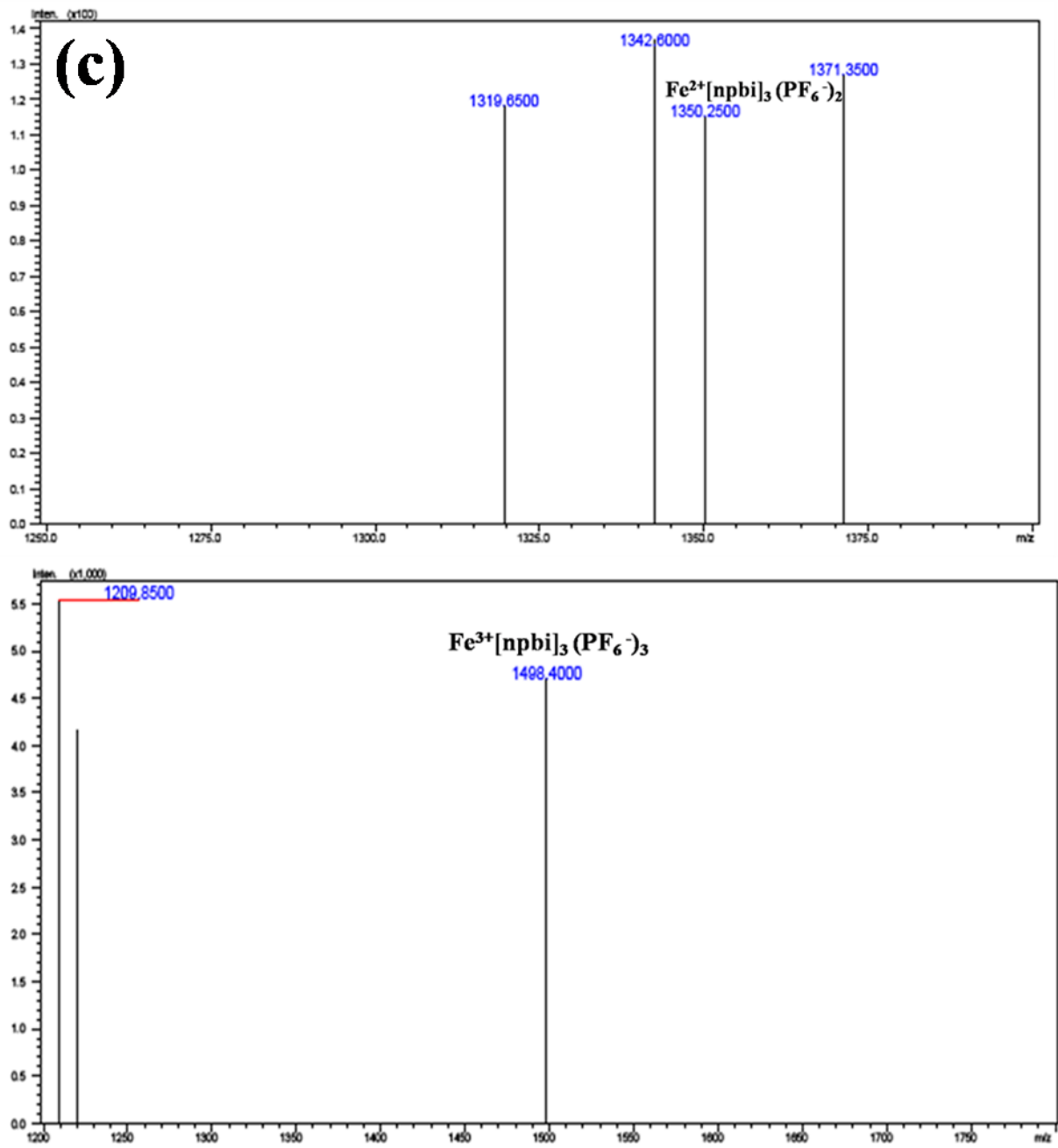


Fig. S1 (a) Proton NMR of npbi ligand (b) Proton NMR of $\text{Fe}^{2+}[\text{npbi}]_3(\text{PF}_6^-)_2$ complex, (c) ESI-MS of $\text{Fe}^{2+}[\text{npbi}]_3(\text{PF}_6^-)_2$ and $\text{Fe}^{3+}[\text{npbi}]_3(\text{PF}_6^-)_3$.

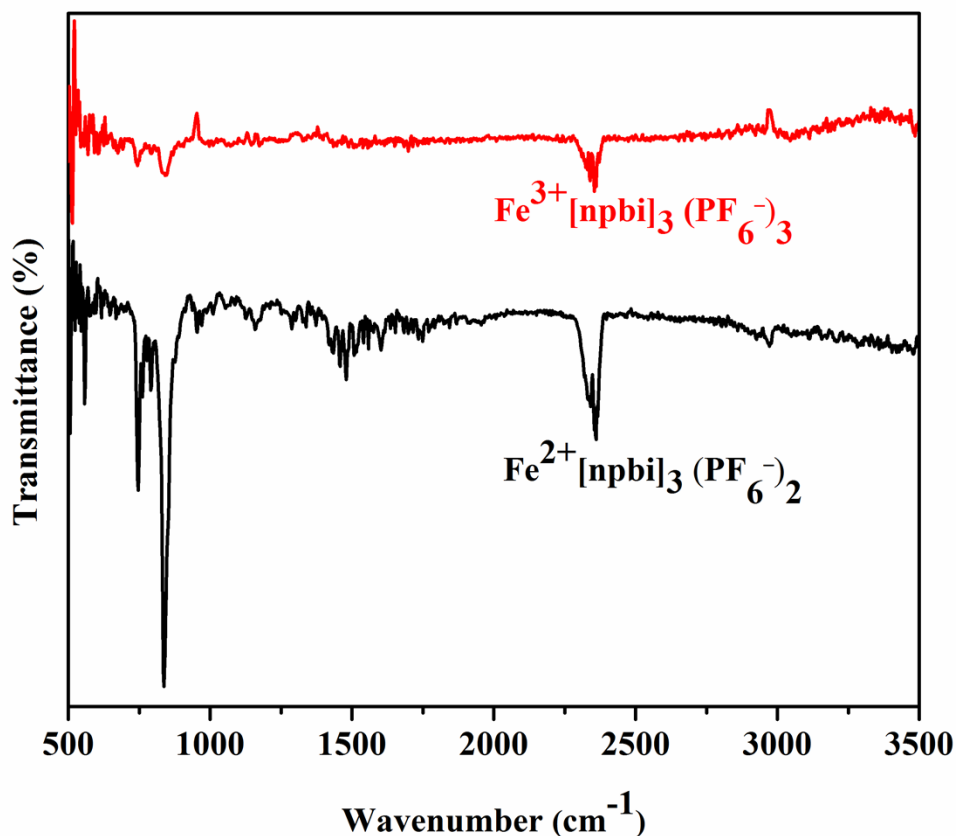


Fig. S2 FTIR spectrum of Fe²⁺[npbi]₃(PF₆⁻)₂ and Fe³⁺[npbi]₃(PF₆⁻)₃.

FTIR and NMR

From our previous report it can be observe that the ligand npbi have some characteristic peaks like C-H stretching at 3047 cm⁻¹, 2871-2920 cm⁻¹ and imine -C=N stretching at 1667 cm⁻¹, aromatic conjugated C=C stretching at 1440, 1510, 1588 cm⁻¹ and -C-N stretching at 1243, 1272, 1328 cm⁻¹.¹ The disappearance and shift of these ligand peaks and formation of new characteristics peaks at 964, 841, 792, 741, 749, 677, 564 cm⁻¹ for the Fe²⁺[npbi]₃(PF₆⁻)₂ and Fe³⁺[npbi]₃(PF₆⁻)₃ complexes proves the formation of complex structures respectively (in Fig. S2).

NMR Spectrum (in Fig S1) revealed that number of proton and exact structures of the ligand and the complex. The Fig S1a showed the NMR of npbi confirm that presence of -CH₂- by a singlet peak at δ=6.36 ppm with two protons. All aromatic protons of naphthalene ring, pyridine ring and benzimidazole ring were appeared as multiplet peaks at the range of δ=7.28-8.62

ppm with 15 protons. At the same instance, Fig S1b showed the NMR of $\text{Fe}^{2+} [\text{npbi}]_3 (\text{PF}_6^-)_2$ confirm that presence of three $-\text{CH}_2-$ by a singlet peak (lower intensity) at $\delta=6.36$ ppm with six protons. All aromatic protons of naphthalene rings, pyridine rings and benzimidazole rings were seemed as multiplet peaks (lower intensity) at the range of $\delta=7.23-8.59$ ppm with 45 protons. From these above results it was confirmed that the formation of iron complex.

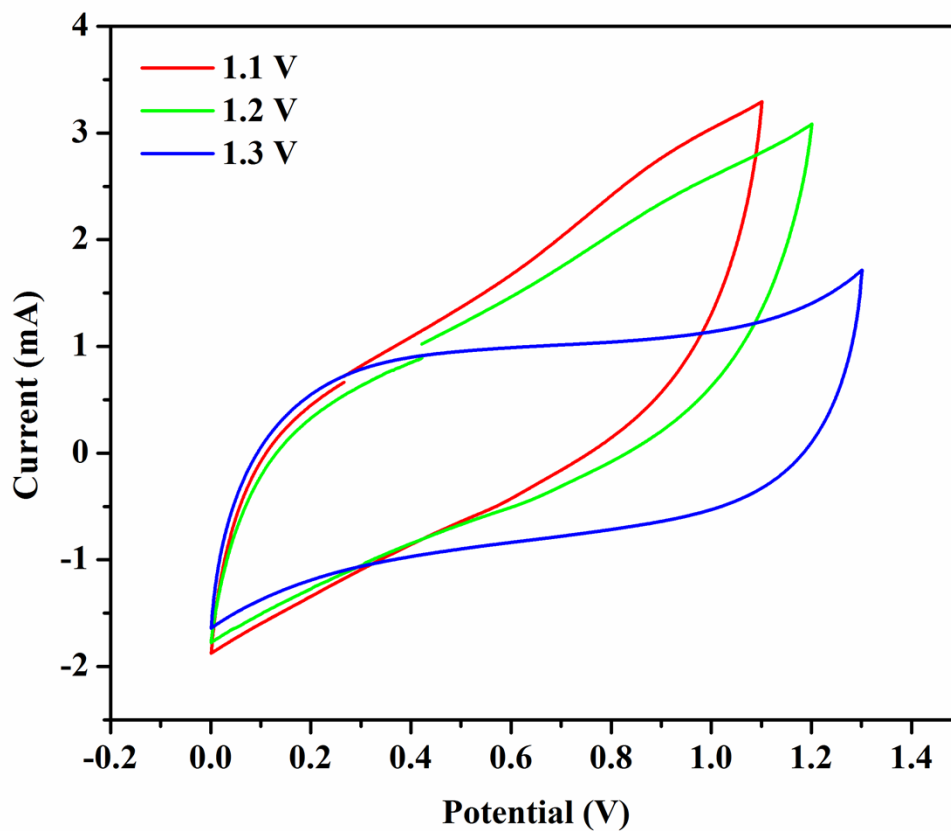


Fig. S3 Potential window setting plots of $\text{H}_2\text{SO}_4 + \text{Fe}^{2+/3+} [\text{npbi}]_3$ electrolytes.

Table S1 J-V results of DSC devices with Fe^{2+/3+} [npbi]₃ electrolyte and DTTCY dye under 1 sun illumination.

Device	Voc (V)	Jsc (mA/cm ²)	FF	Efficiency (%)
Device 1	0.72	6.34	0.66	3.0127
Device 2	0.73	6.46	0.64	3.0181
Device 3	0.72	6.72	0.59	2.8546
Average	0.72333333	6.50666666	0.63	2.9618
SD values	0.006	0.1942506	0.030655	0.0928
PCE result	0.72 ± 0.006	6.5 ± 0.194	0.63 ± 0.306	2.96 ± 0.09

Reference

- 1) S. Balamurugan, S. Ganesan *Electrochim. Acta*, 2020, **329**, 135169.