Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

The modulation effect of electron-rich guest on the luminescence of naphthalene diimide-based metal-organic framework

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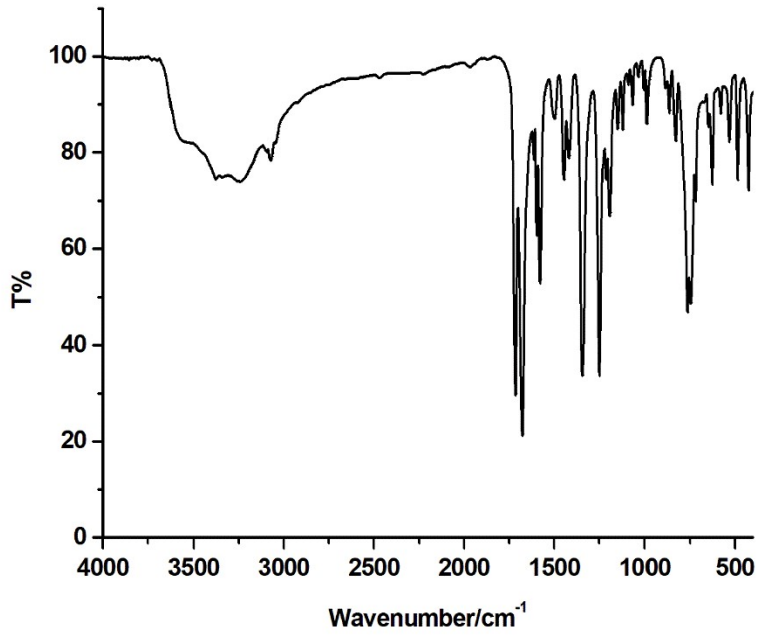

Fig. S1. IR spectra of MOF 1.

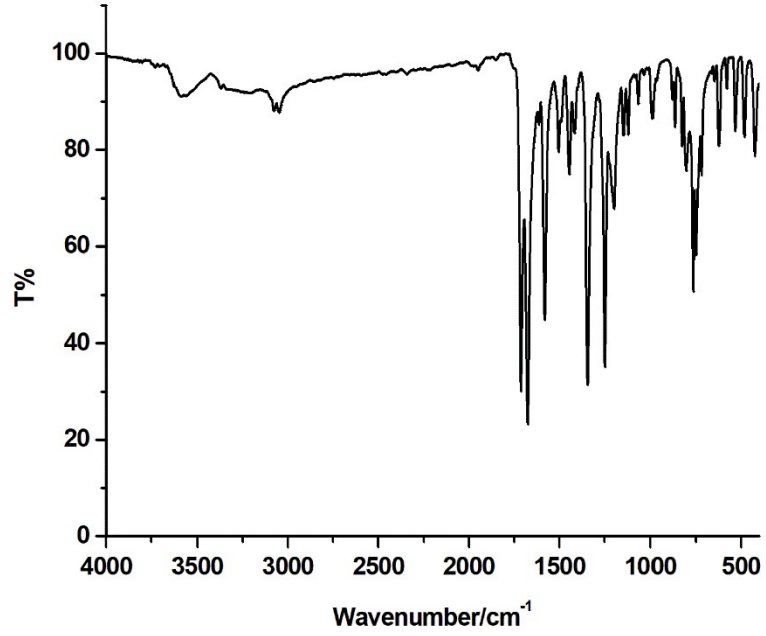

Fig. S2. IR spectra of MOF 2.

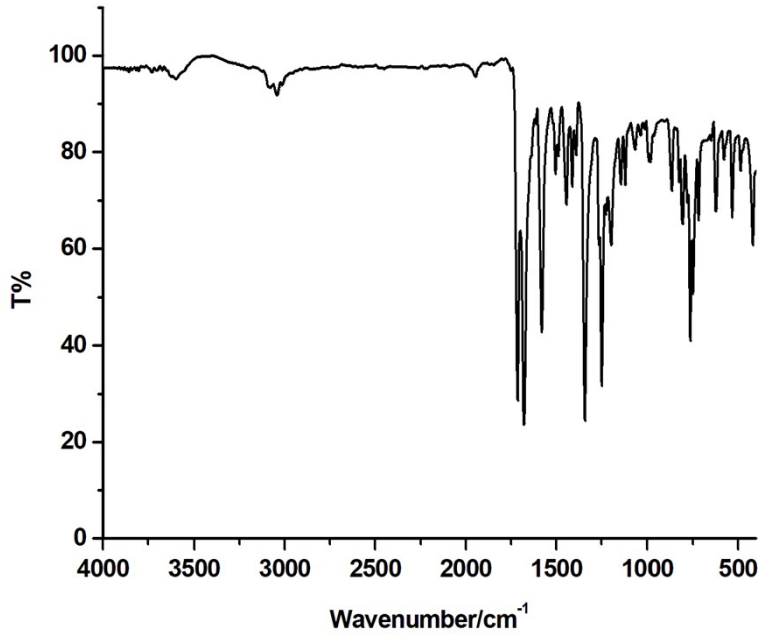

Fig. S3. IR spectra of MOF 3.

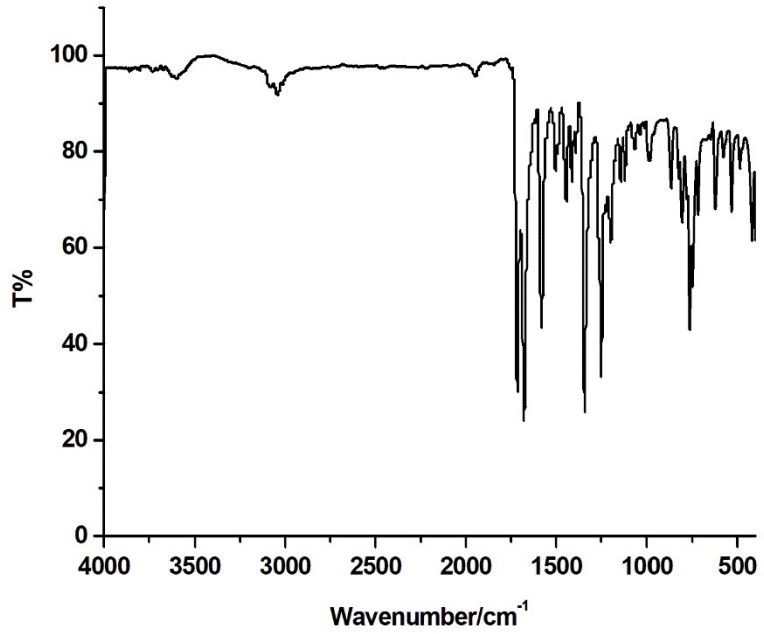

Fig. S4. IR spectra of MOF 4.

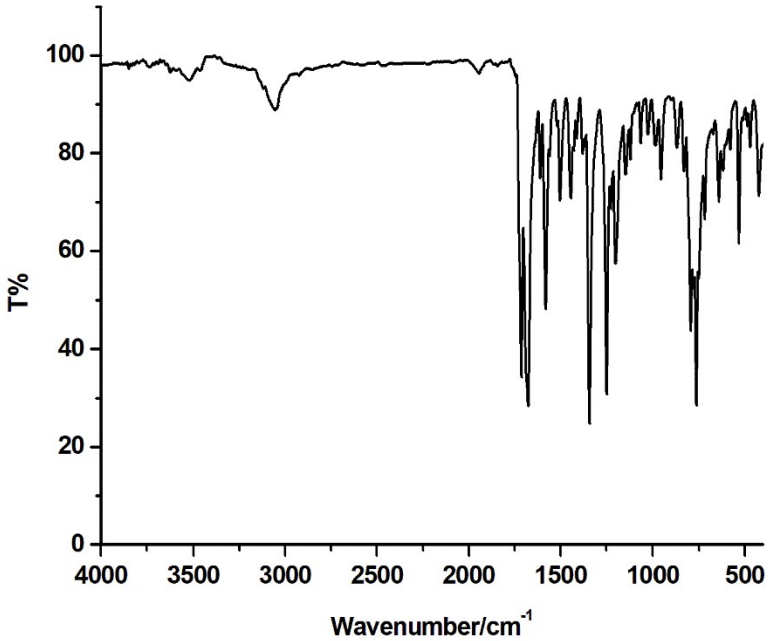

Fig. S5. IR spectra of MOF 5.

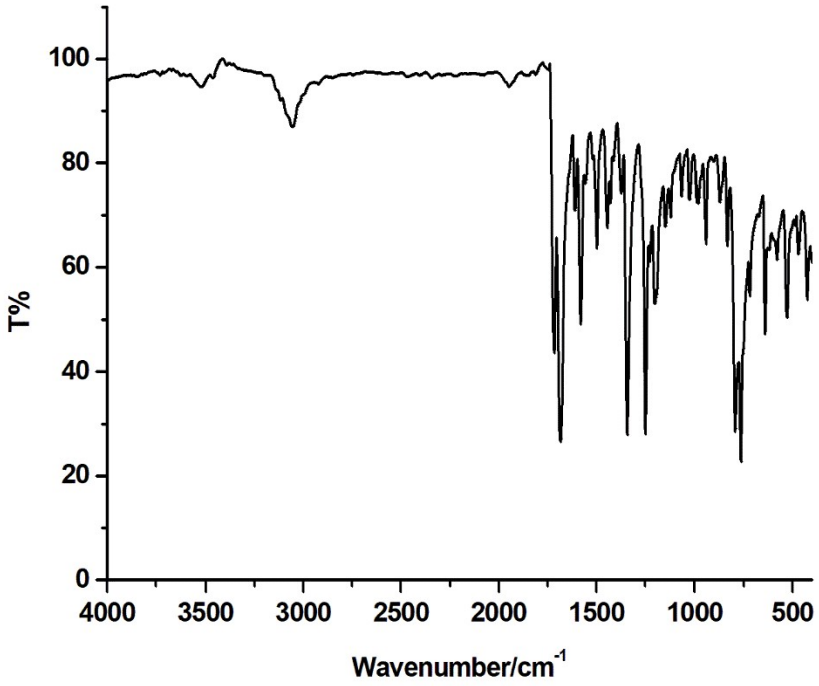

Fig. S6. IR spectra of MOF 6.

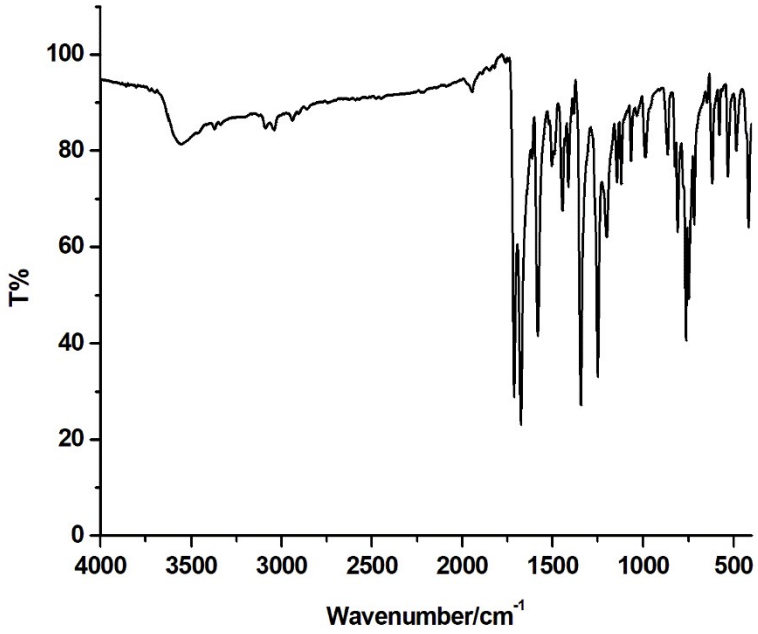

Fig. S7. IR spectra of MOF 7.

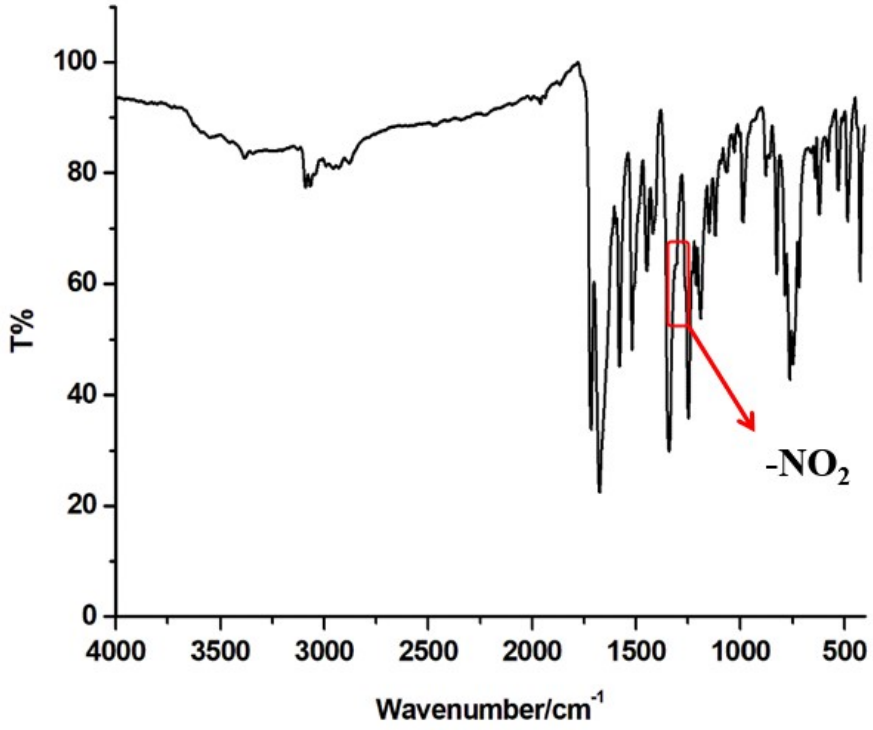

Fig. S8. IR spectra of MOF 8.

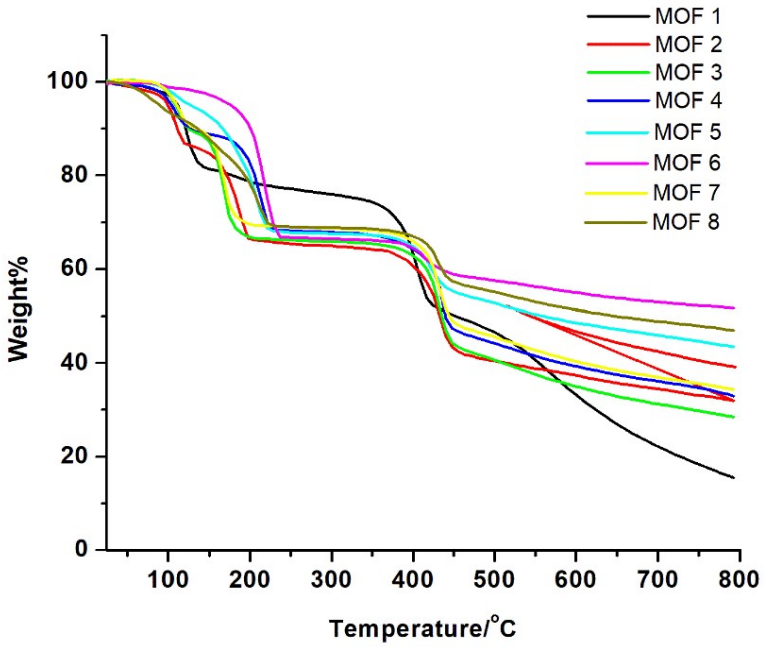

Fig. S9. TGA curves of MOFs 1-8.

Table S1. Weight loss and Calculated formula of MOFs 2-8.

Sample	Weight loss in the 125-250 °C	Calculated formula
MOF 2	19.3%	$ZnSiF_6(DPNDI)_2 \cdot 1.95$(naphthalene)
MOF 3	20.5%	$ZnSiF_6(DPNDI)_2 \cdot 1.85$(1-fluoronaphthalene)
MOF 4	22.6%	$ZnSiF_6(DPNDI)_2 \cdot 1.58$(1-chloronaphthalene)
MOF 5	23.3%	$ZnSiF_6(DPNDI)_2 \cdot 1.53$(1-bromonaphthalene)
MOF 6	26.7%	$ZnSiF_6(DPNDI)_2 \cdot 1.50$(1-iodonaphthalene)
MOF 7	20.6%	$ZnSiF_6(DPNDI)_2 \cdot 1.91$(1-methylnaphthalene)
MOF 8	23.8%	$ZnSiF_6(DPNDI)_2 \cdot 1.86$(1-nitronaphthalene)

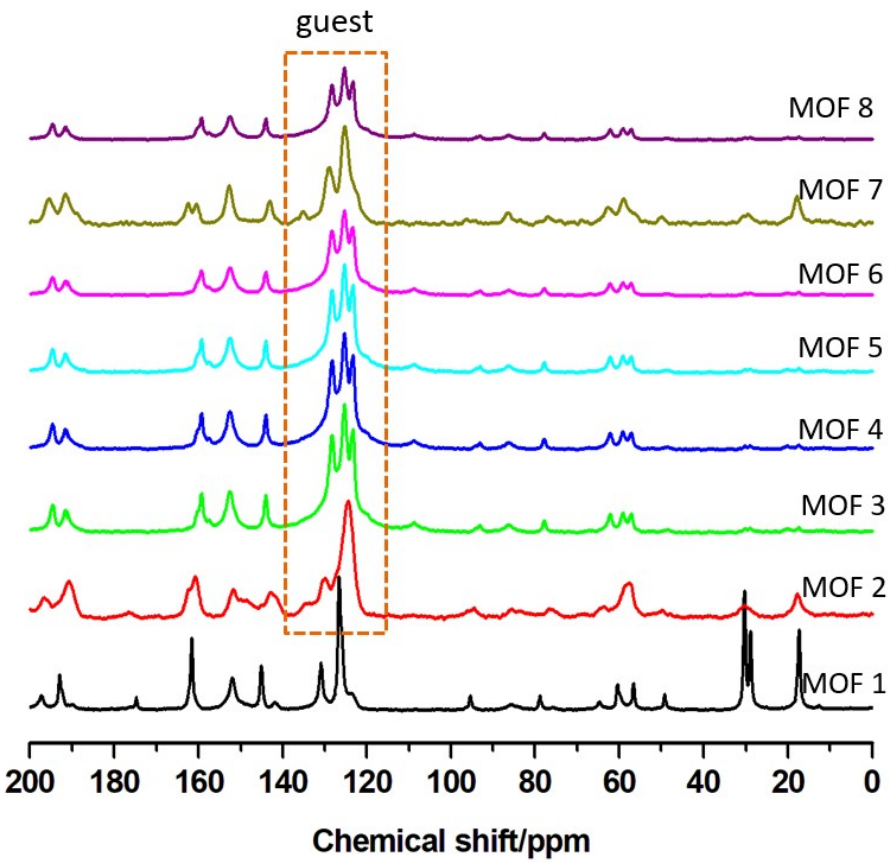

Figure S10. Solid-state ^{13}C NMR spectra of MOF 1-8.

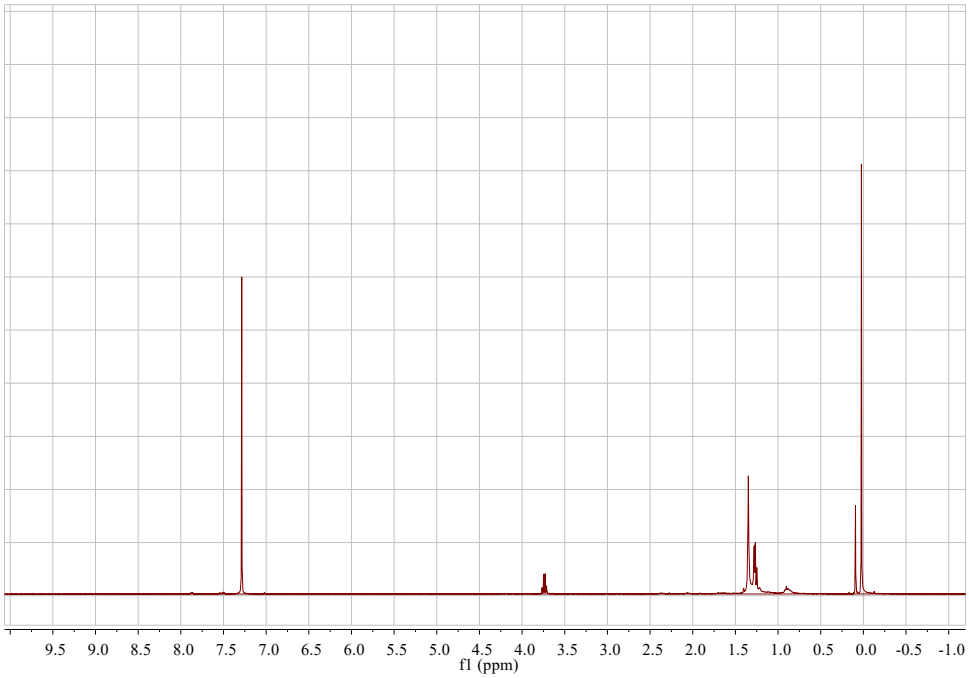

Fig. S11. ^{1}H NMR spectra of the deuterated chloroform extract of MOF 7.

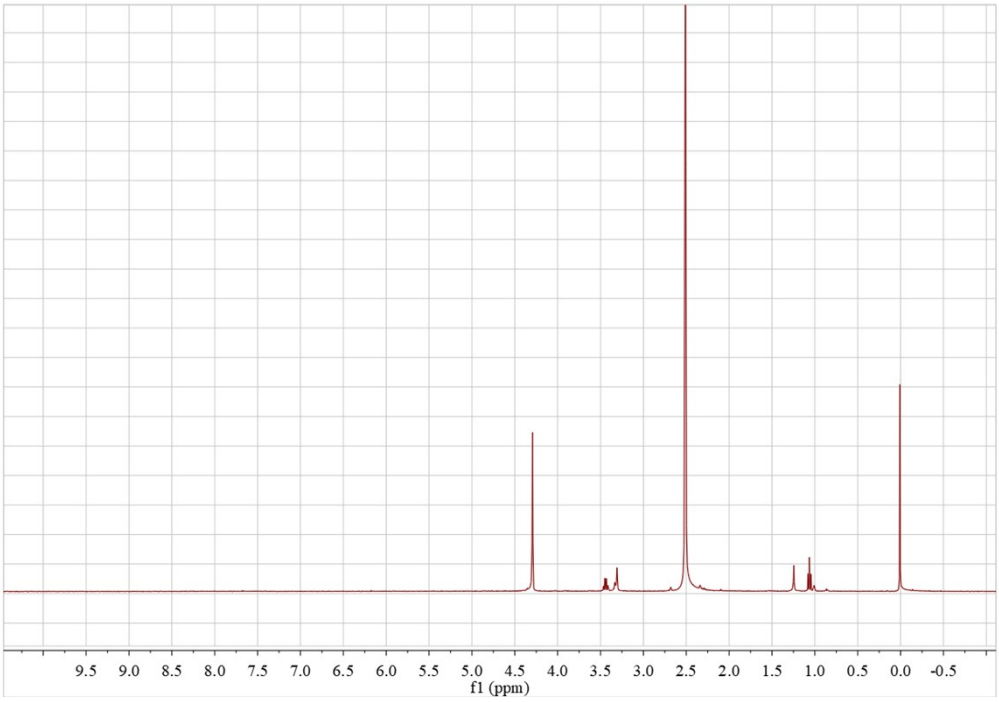

Fig. S12. ^{1}H NMR spectra of the deuterated DMSO extract of MOF 7.

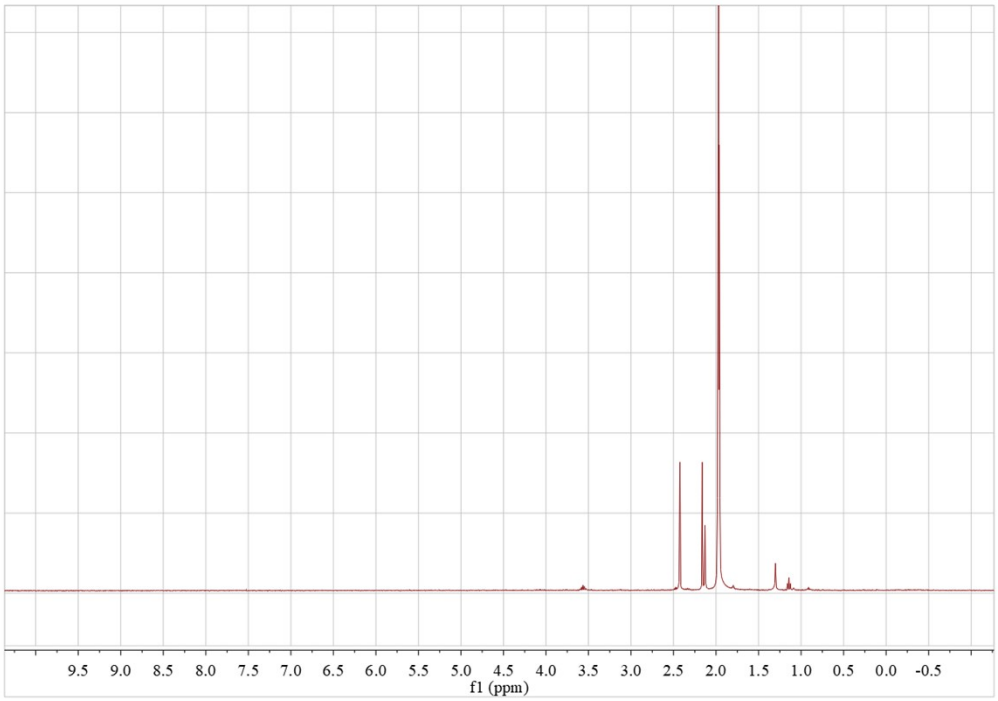

Fig. S13. ^{1}H NMR spectra of the deuterated acetonitrile extract of MOF 7.

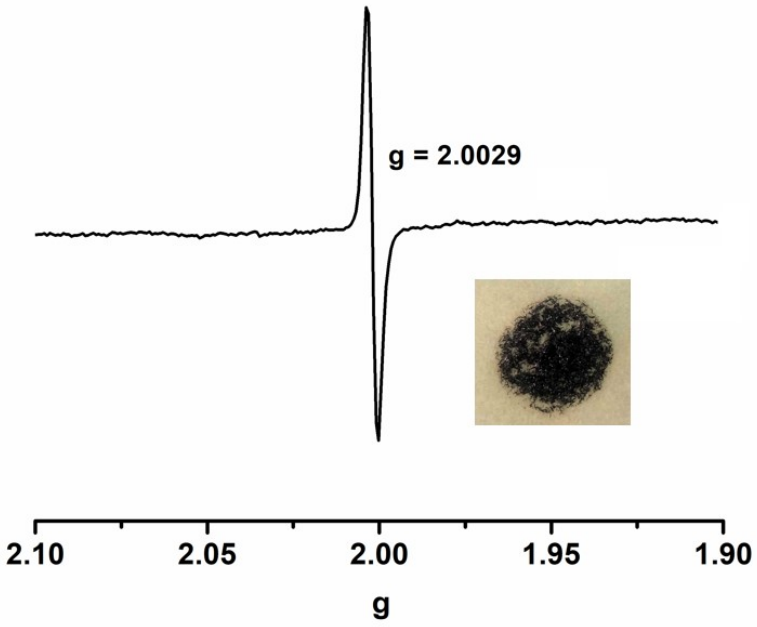

Fig. S14. ESR spectrum of MOF 1 ⊃ 1-naphthylamine (inset show the photographs of sample).

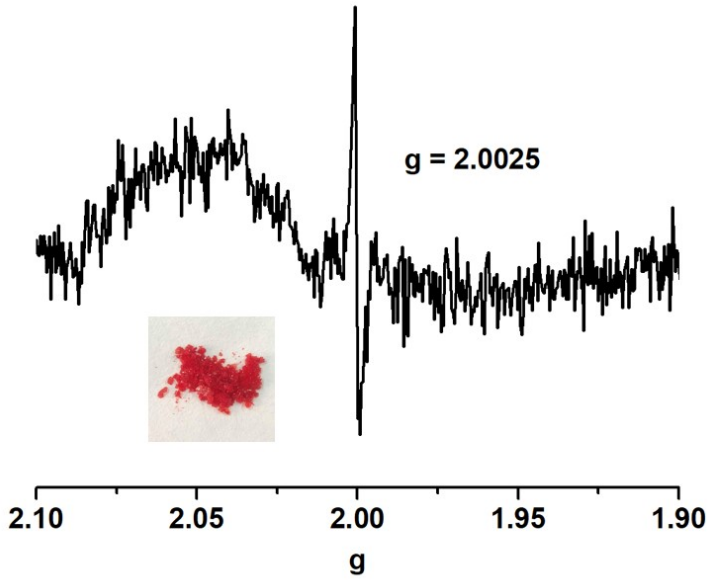

Fig. S15. ESR spectrum of MOF 1 ⊃ 1-naphthol (inset show the photographs of sample).

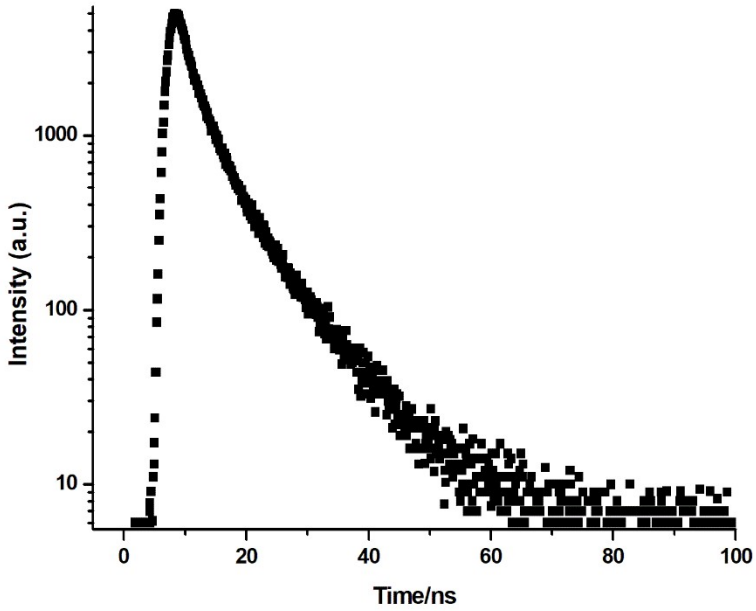

Fig. S16. Fluorescent decay curve of MOF 1 in solid state at room temperature.

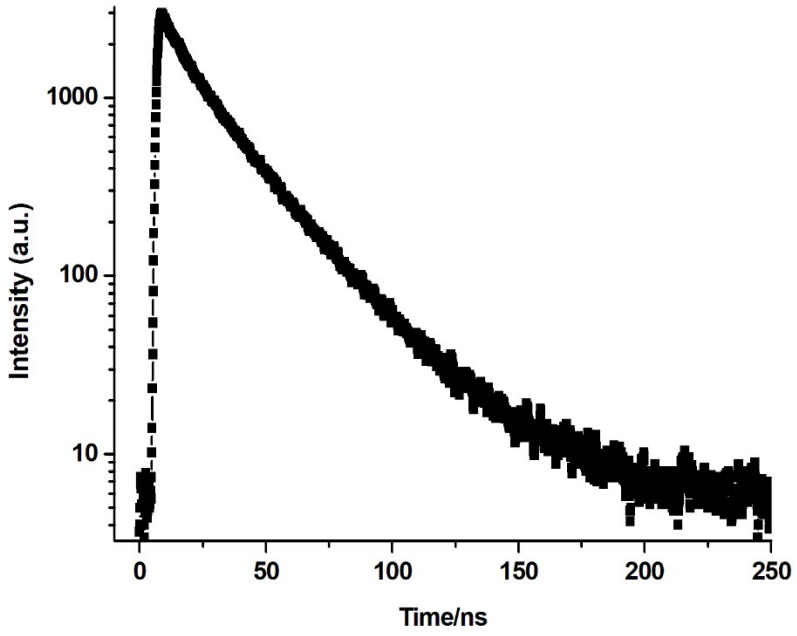

Fig. S17. Fluorescent decay curve of MOF 2 in solid state at room temperature.

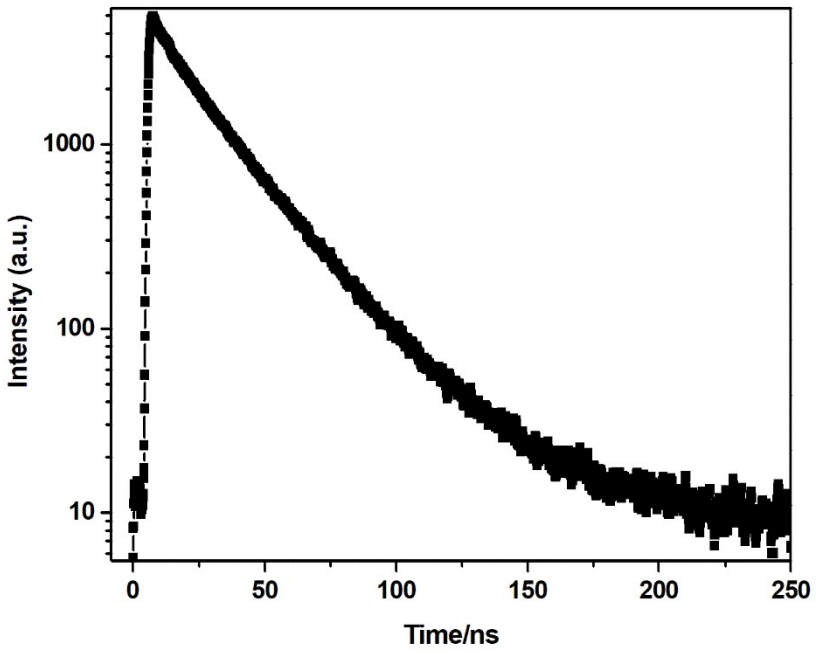

Fig. S18. Fluorescent decay curve of MOF 3 in solid state at room temperature.

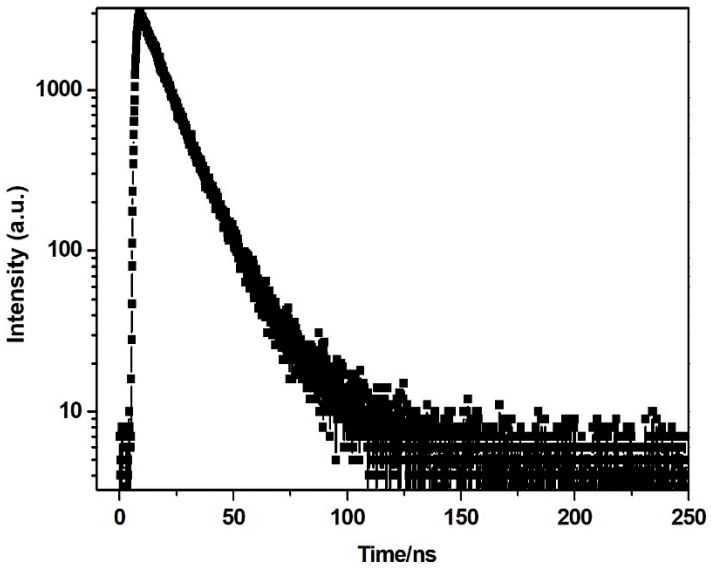

Fig. S19. Fluorescent decay curve of MOF 4 in solid state at room temperature.

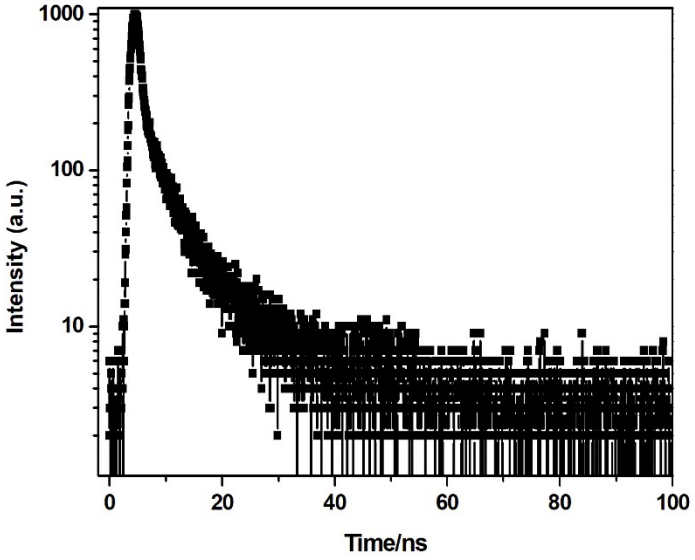

Fig. S20. Fluorescent decay curve of MOF 5 in solid state at room temperature.

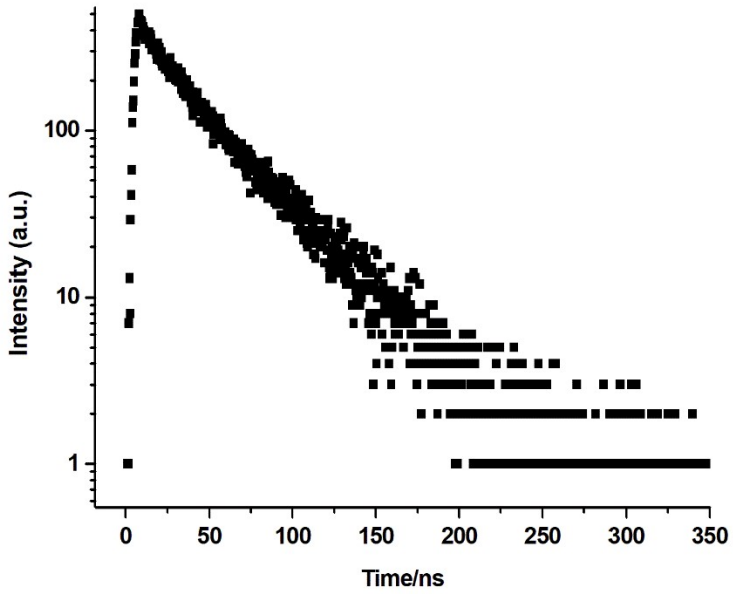

Fig. S21. Fluorescent decay curve of MOF 6 in solid state at room temperature.

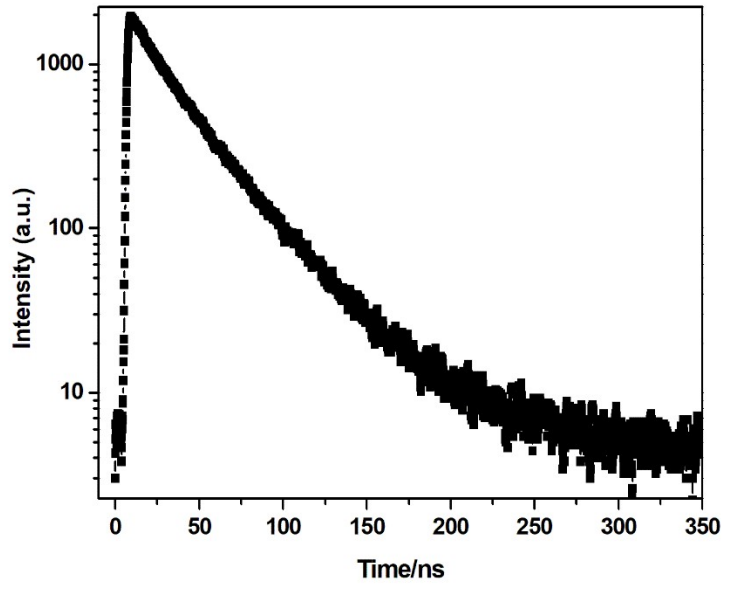

Fig. S22. Fluorescent decay curve of MOF 7 in solid state at room temperature.

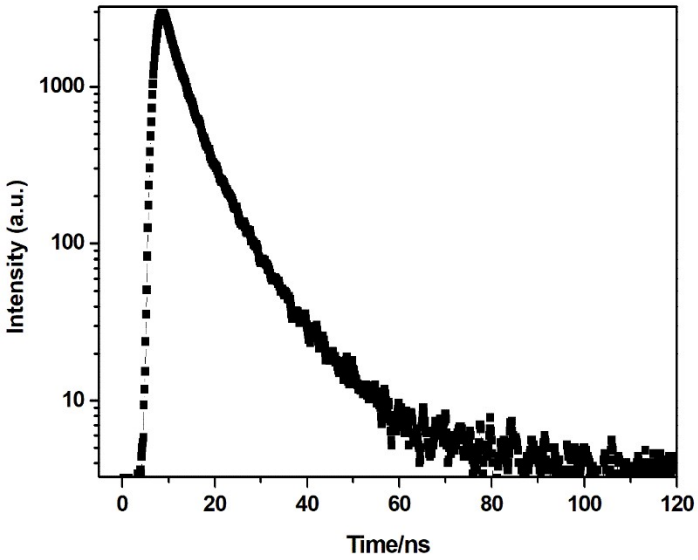

Fig. S23. Fluorescent decay curve of MOF 8 in solid state at room temperature.

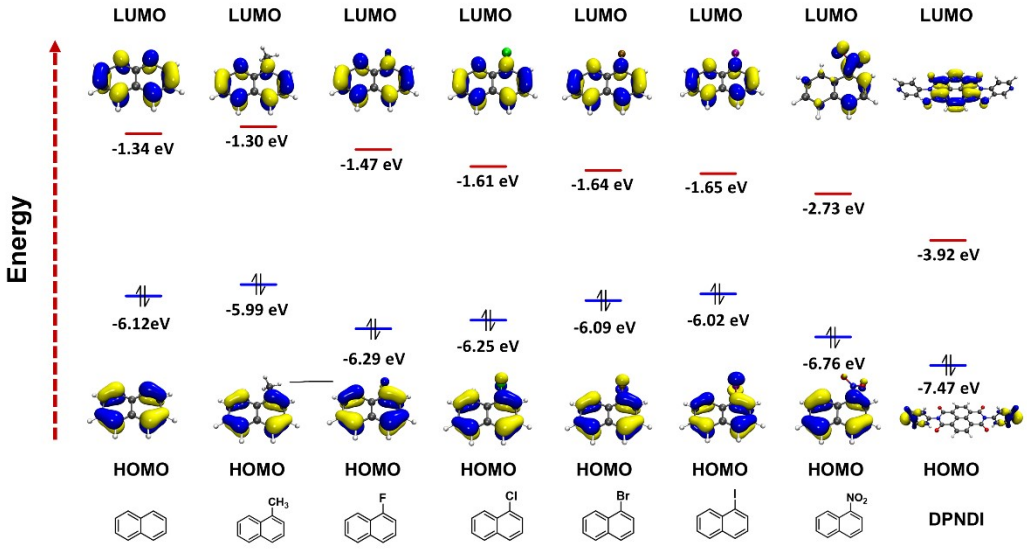

Fig. 24. HOMO and LUMO energy levels of naphthalene derivatives and DPNDI. Molecular orbital energy was evaluated with density functional theory (DFT) computations using the Gaussian 16 suite of programs. A hybrid functional, B3LYP, was used for all calculations.