

Supporting Information for

A flexible metal azolate framework with drastic luminescence response toward solvent vapors and carbon dioxide

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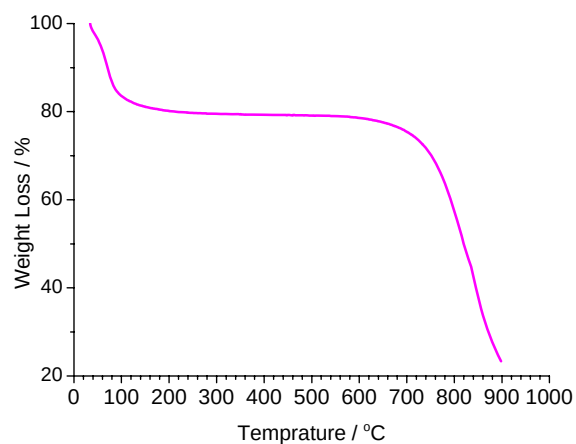


Fig. S1. TGA curve of the as synthesized **1·g**

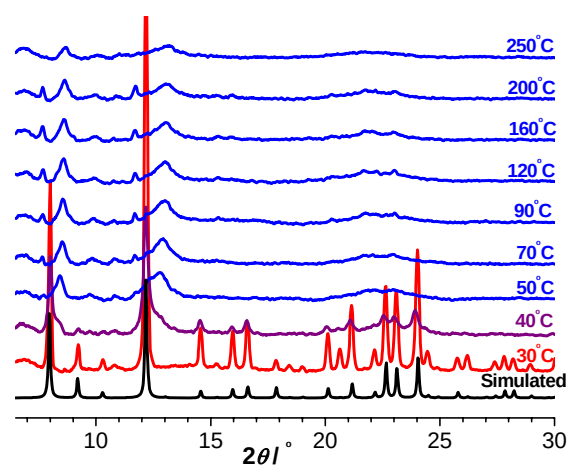


Fig. S2. Variable-temperature PXRD patterns of **1·g**

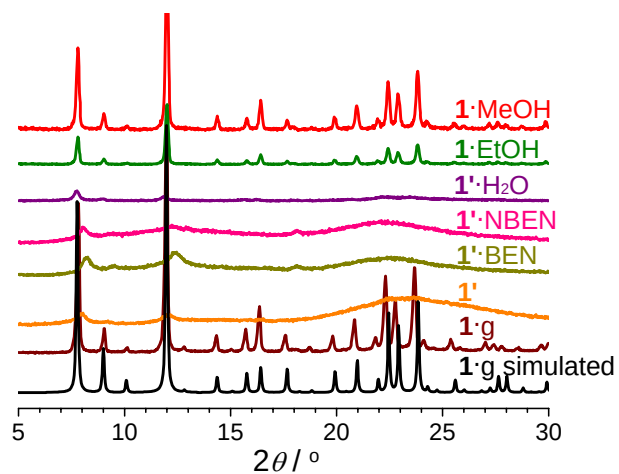


Fig. S3. PXRD patterns of **1·g**, **1'**, **1'·BEN**, **1'·NBEN**, **1'·H₂O**, **1·EtOH**, and **1·MeOH**.

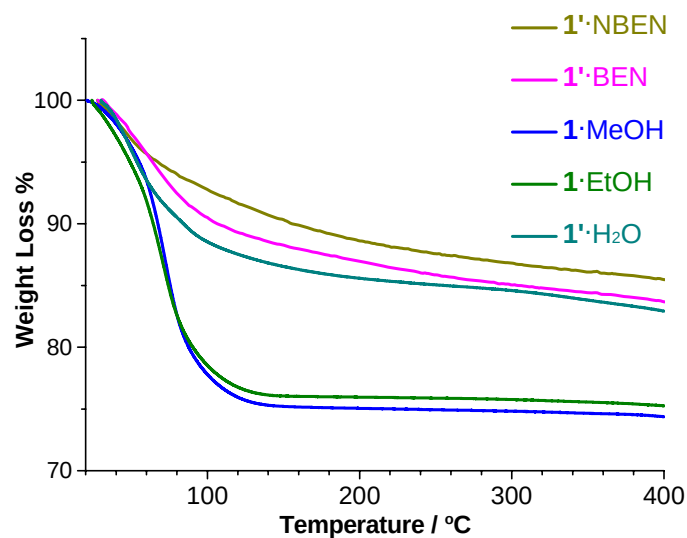


Fig. S4. TGA curve of 1'·NBEN, 1'·BEN, 1·MeOH, 1·EtOH, and 1'·H₂O

Table S1 Summary of guest sorption amounts of 1'

	MeOH	EtOH	H ₂ O	Ben	Nben
Weight loss	25%	24%	15.5%	15%	13.5%
Formula	1·32.5MeOH	1·21.4EtOH	1·31.8H ₂ O	1'·7.0Ben	1'·4.0Nben

[a] 1 and 1' refers to Zn₇(ip)₁₂(OH)₂

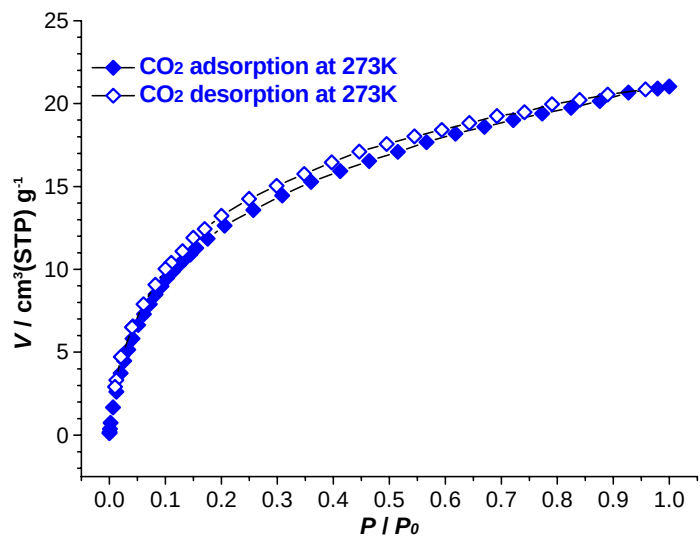


Fig. S5 CO₂ sorption isotherms of 1' at 273 K

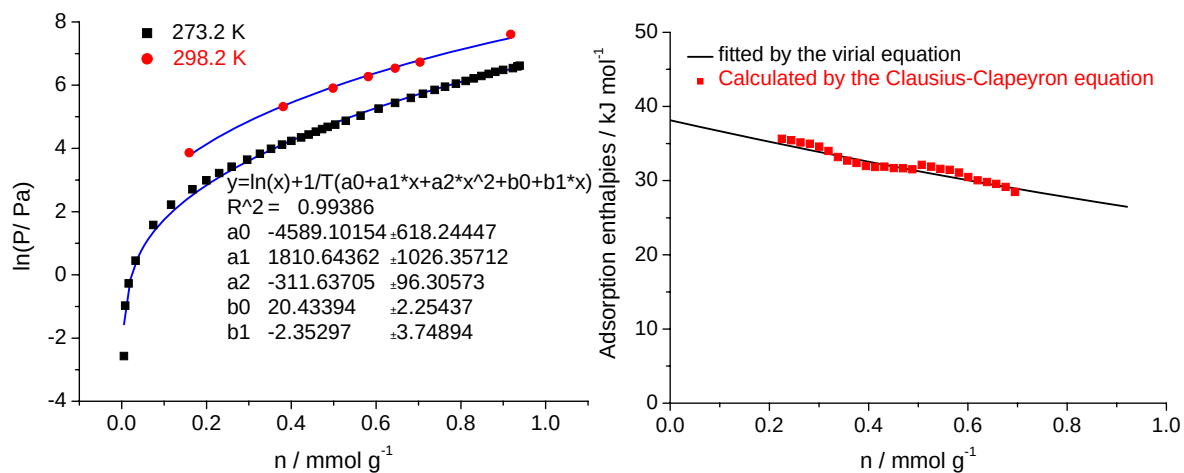


Fig. S6 Adsorption enthalpies of CO_2 fitted by the virial equation from adsorption isotherms measured at 273 and 298 K and calculated by the Clausius-Clapeyron equation.

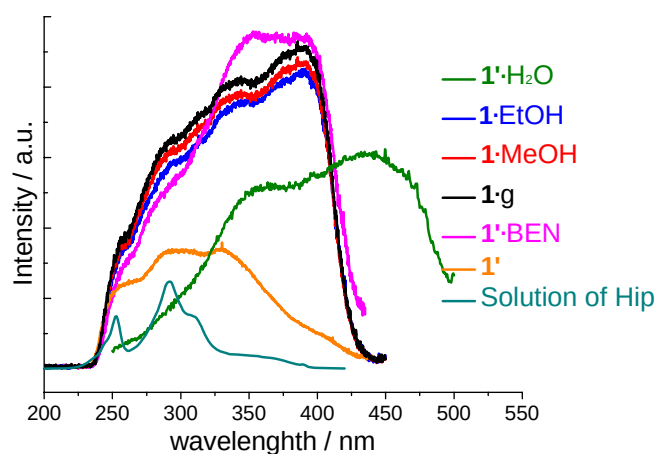


Fig. S7. Photoluminescence excitation spectra of $1 \cdot \text{g}$, $1'$, $1 \cdot \text{BEN}$, $1 \cdot \text{MeOH}$, $1 \cdot \text{EtOH}$, $1 \cdot \text{H}_2\text{O}$, and methanol solution of Hip (10^{-6} M).

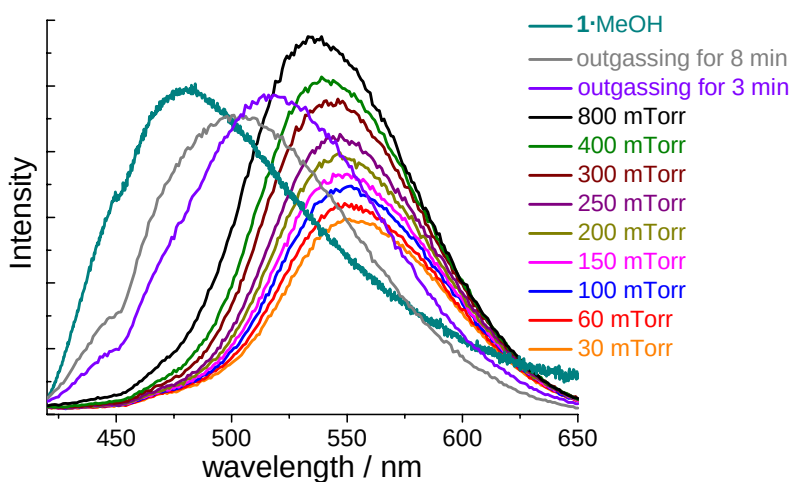


Fig. S8. Photoluminescence emission profiles of **1**·MeOH under dynamic vacuum (at the beginning, pressure above 1000 mTorr cannot be read by the low-pressure sensor). Loading MeOH increases the emission intensity of both the crystalline and quasi-amorphous phases. The phase transition from crystalline to quasi-amorphous also increases the emission intensity, which surpasses the effect of MeOH desorption.

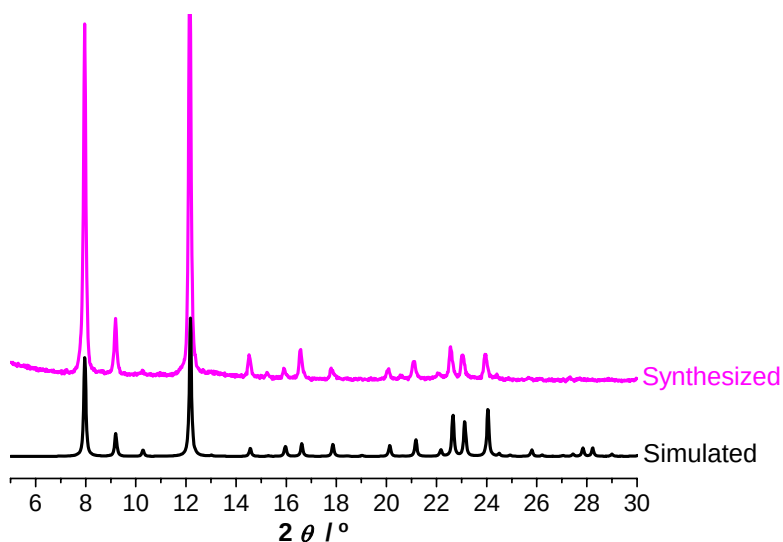


Fig. S9 PXRD patterns of film of **1**·g thin film grown on a zinc plate.

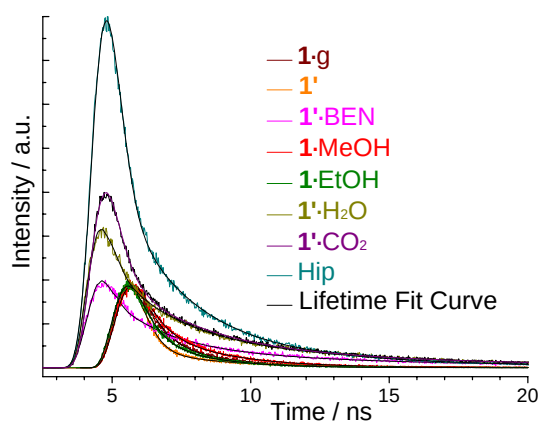


Fig. S10 Luminescence decay profiles of **1**, **1'**, **1·EtOH**, **1·MeOH**, **1'·BEN**, **1'·H₂O** and methanol solution of Hip (10^{-6} M).

Table S2 Fitted lifetimes corresponding to Fig. S11.

	$\tau_1(\text{ns})$	Rel%	τ_2	Rel%	τ_3	Rel%	χ^2	weighted- average lifetime (ns)
1·g	0.84(1)	64.06(1)	2.91(4)	35.94(1)	—	—	1.006	1.58
1'	0.39(1)	69.51(5)	2.1(2)	25.66(1)	5.2(5)	14.83(2)	0.996	1.58
1'·BEN	0.24(3)	9.6(5)	2.47(6)	36.94(3)	10.47(10)	53.44(1)	1.000	6.53
1'·H₂O	0.12(2)	14.(1)	2.14(4)	35.52(2)	8.12(6)	50.64(1)	1.004	4.88
1·MeOH	0.69(2)	37.53(2)	2.52(2)	62.47(2)	—	—	0.998	1.83
1·EtOH	0.54(1)	45.46(3)	1.90(2)	54.54(2)	—	—	1.006	1.28
1'·CO₂	0.37(1)	22.(1)	2.62(6)	36.45(2)	9.1(1)	40.86(1)	0.996	4.79

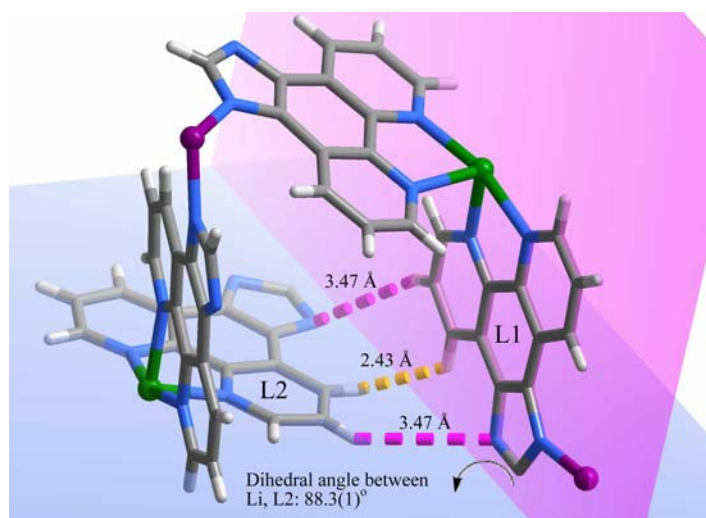


Fig. S11 Perspective view of the contact of adjacent ip⁻ ligands in **1.g**.