Supporting Information

A highly stable hydrogen-bonded organic framework for hydrogen storage

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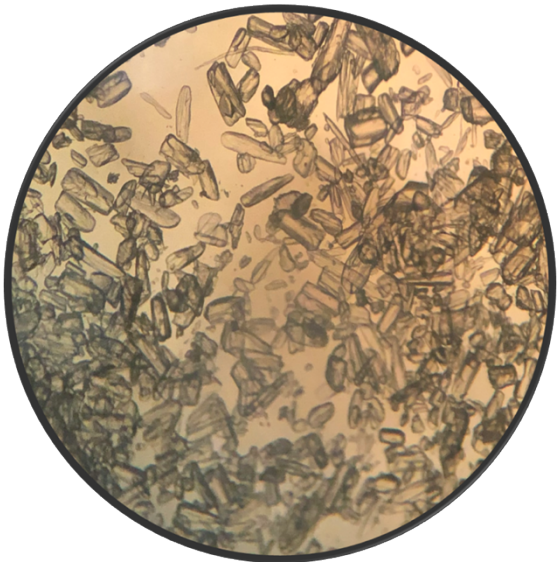


Fig. S1. An optical microscopic image of **1**.

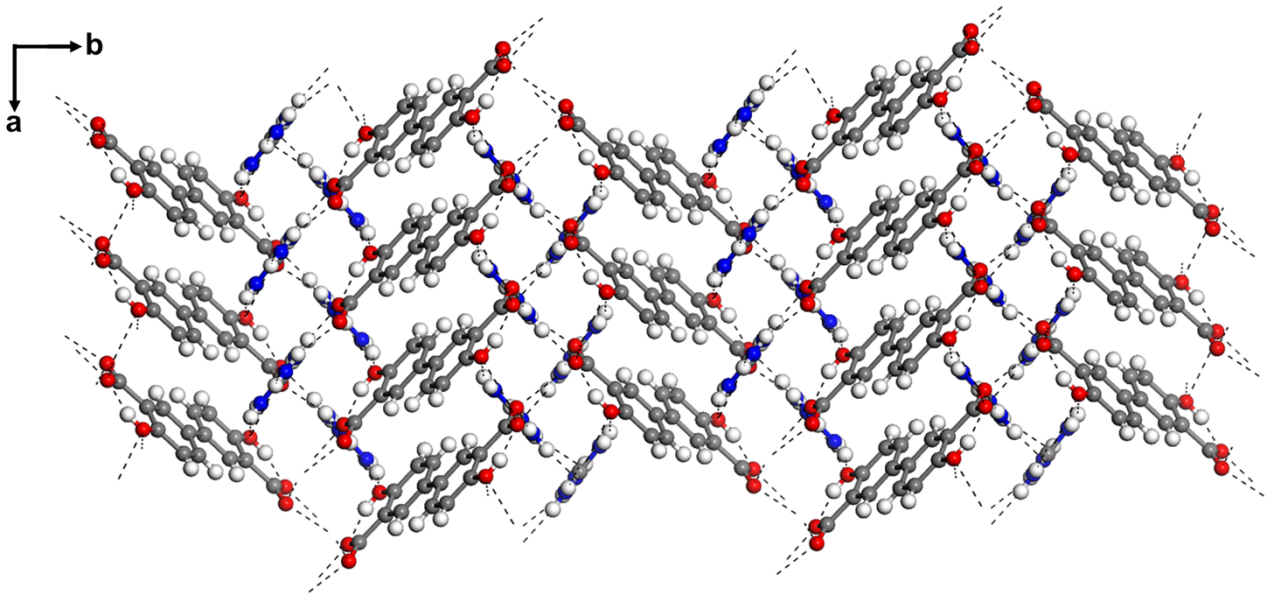


Fig. S2. Crystal structure of 1 along the c-axis. Black lines indicate hydrogen bonds among organic moieties, connecting all entities through hydrogen bonding.

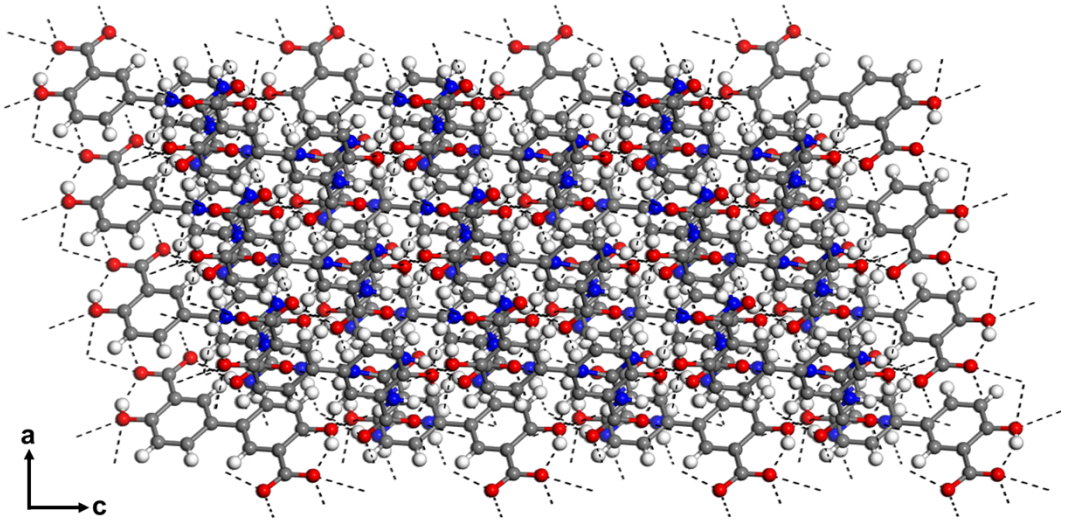


Fig. S3. Crystal structure of 1 along the b-axis. Black lines indicate hydrogen bonds among organic moieties, connecting all entities through hydrogen bonding.

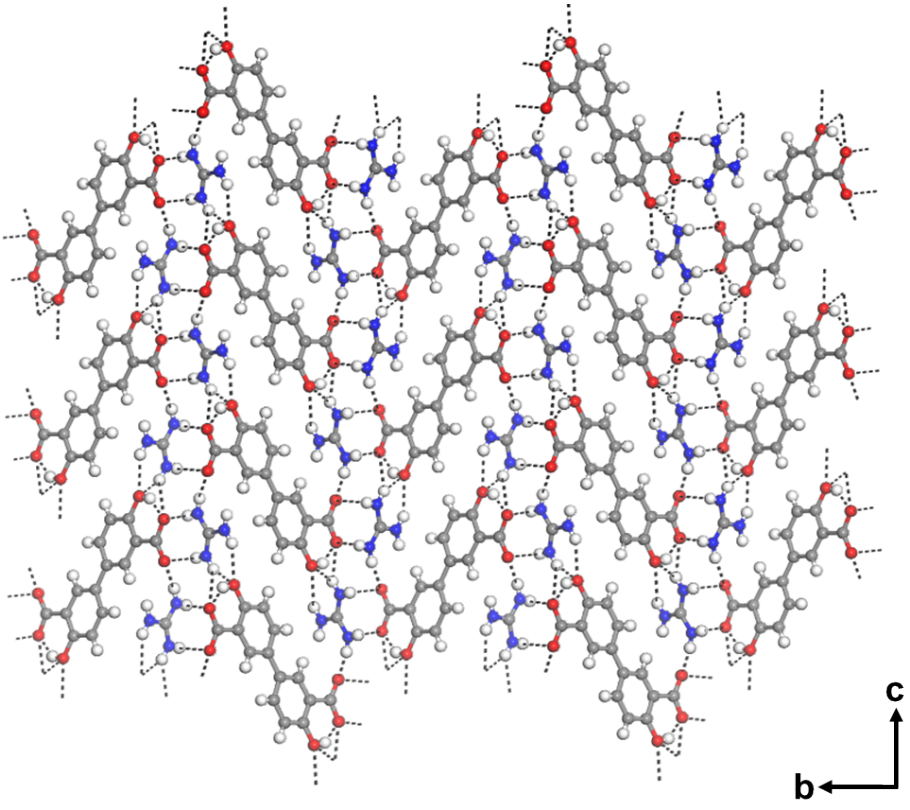
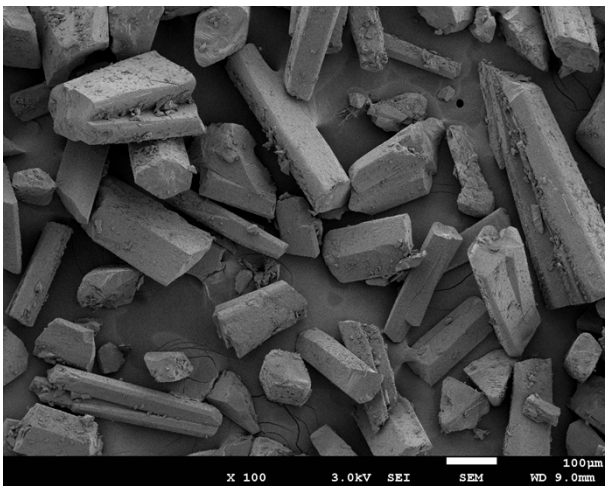
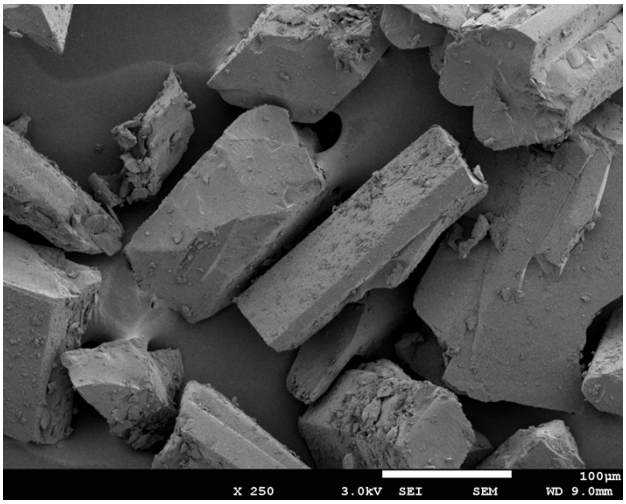


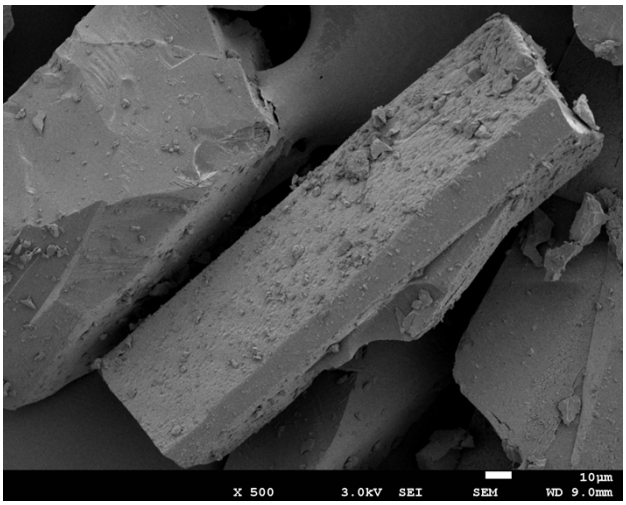
Fig. S4. Crystal structure of 1 along the a-axis. Black lines indicate hydrogen bonds among organic moieties, connecting all entities through hydrogen bonding.



(a)



(b)



(c)

Fig. S5. SEM images for **1** with magnification: (a) x 100, (b) x 250, and (c) x 500.

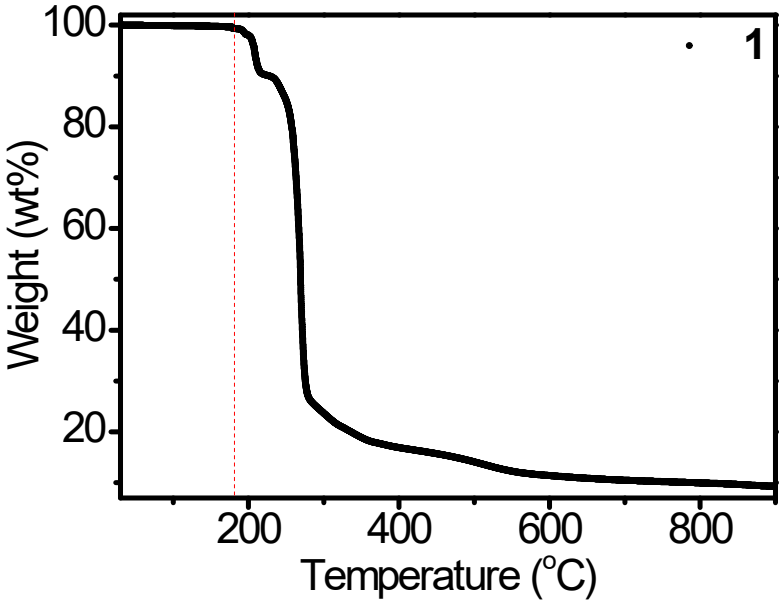


Fig. S6. Thermogravimetric analysis data for **1**.

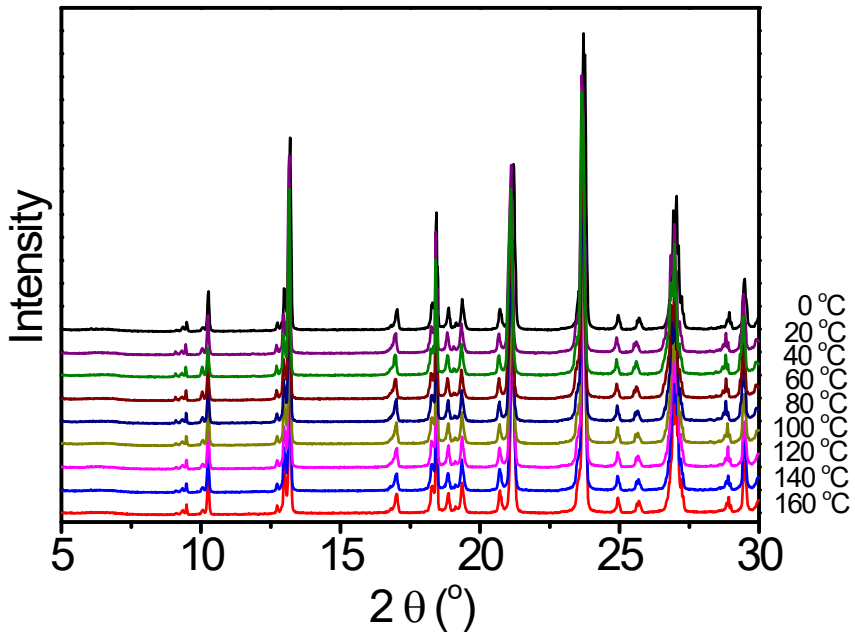


Fig. S7. Variable-temperature PXRD profiles of **1**.

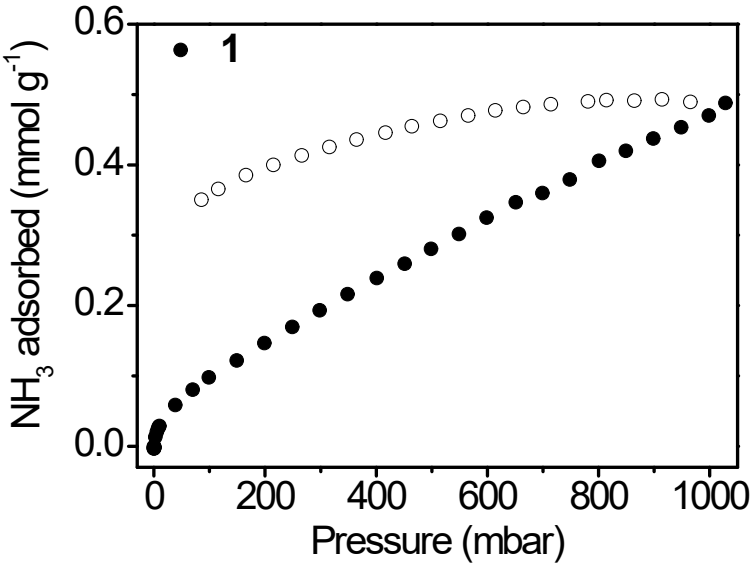


Fig. S8. NH_3 isotherms of **1** at 298 K.

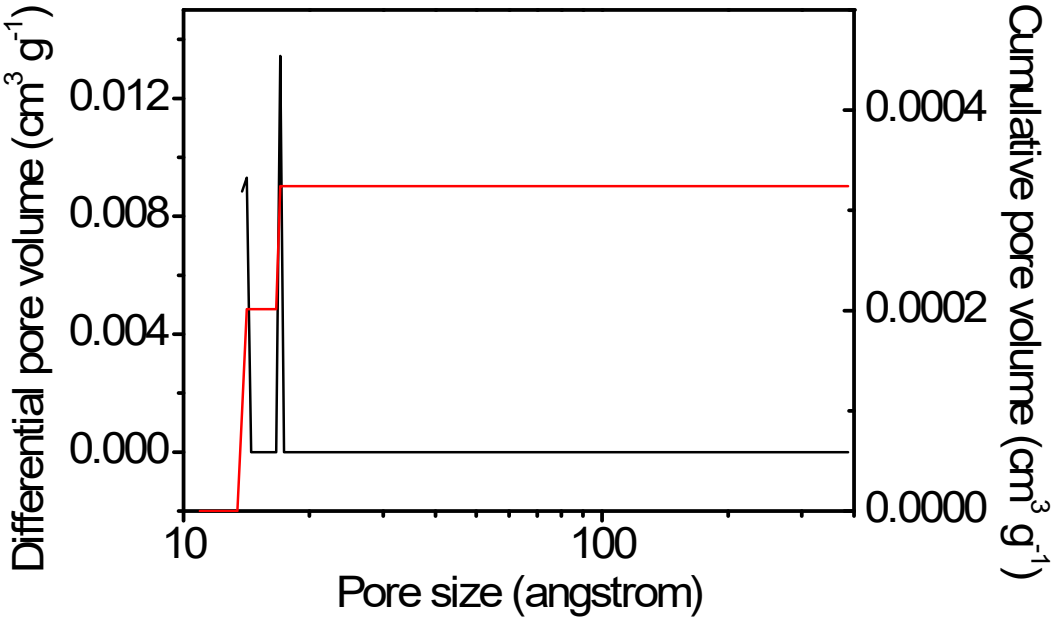


Fig. S9. Pore size distribution of **1** from N_2 isotherm data. The total pore volume is calculated to be 0.00032 $cm^3\ g^{-1}$

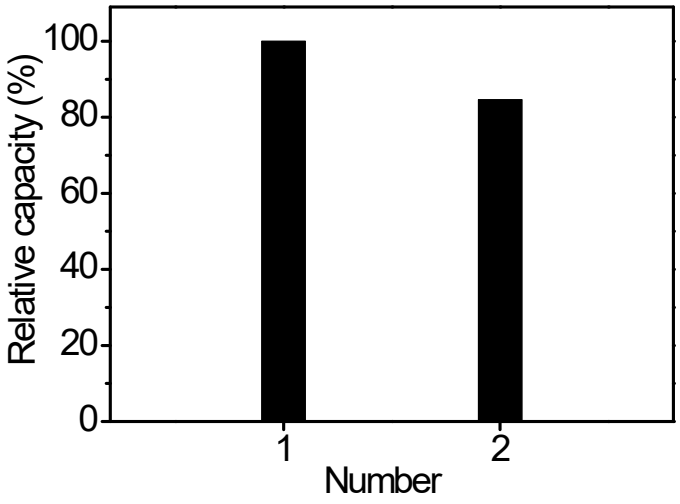


Fig. S10. Recyclability test of H_2 storage using **1**.

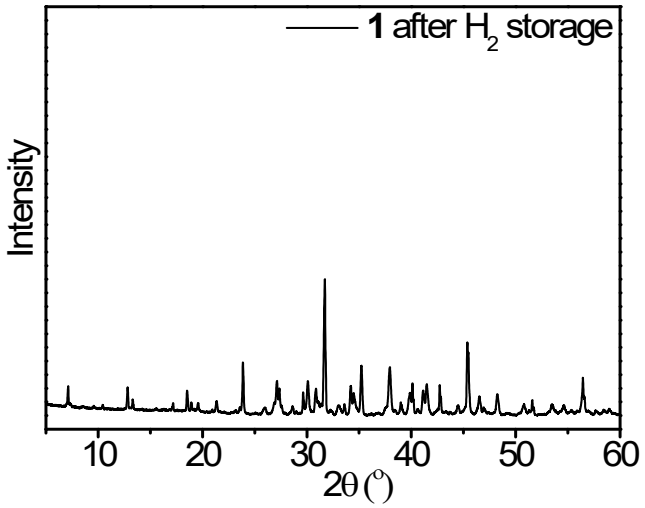


Fig. S11. The PXRD pattern of **1** after hydrogen storage.

Table S1. Crystal data and structure refinement for **1**. (CCDC number: 2336974)

Empirical formula	$C_{16}H_{20}N_6O_6$
Formula weight	392.38
Temperature (K)	100(2)
Wavelength (Å)	0.700 Å
Crystal system, space group	Monoclinic, $P2_1/n$
Unit cell dimensions (Å)	a = 4.8040(10), b = 18.247(4), c = 9.818(2) Å
Unit cell dimensions (°)	α = 90.00, β = 104.00(3), γ = 90.00
Volume (A^3)	835.1(3) $Å^3$
Z	2
Calculated density (Mg/m^3)	1.561
F(000)	412
Theta range for data collection (deg)	2.199 to 33.446
Reflections collected	7449 [R(int) = 0.0883]
Completeness to theta	98.2%
Data / restraints / parameters	2859 / 0 / 128
Goodness-of-fit on F^2	1.142
Final R indices [I>2sigma(I)]	R1 = 0.0806, wR2 = 0.2449
R indices (all data)	R1 = 0.0818, wR2 = 0.2481
Largest diff. peak and hole ($e.A^{-3}$)	0.673 and -0.615 $e.Å^{-3}$