Electronic Supplementary Material (ESI) for CrystEngComm

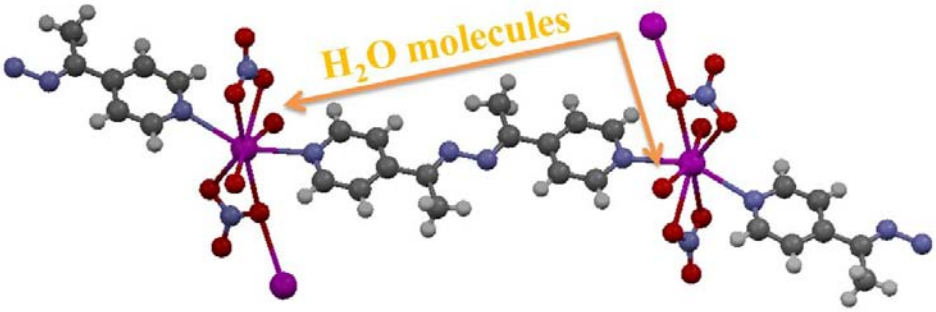
Electronic Supplementary Information for MS:

Reversible Crystal-to-Crystal Transformation in Nano-porous Three-dimensional Lead(II) MOFs; Study of Solvent Attendance on Iodide Adsorption Affinity

Lida Hashemi, Ali Morsali*

[a]Department of Chemistry, Faculty of Sciences, Tarbiat Modares University, P.O. Box 14115-175, Tehran, Islamic Republic of Iran

a)



b)

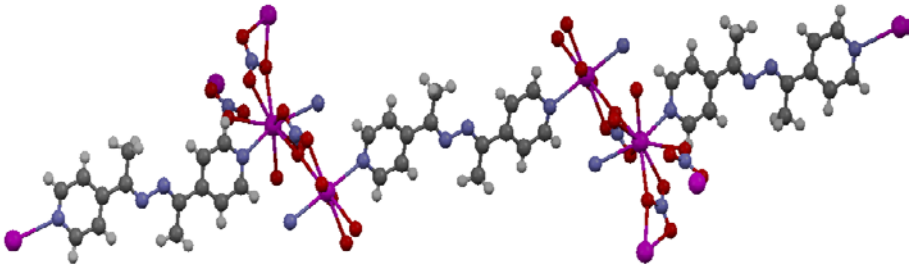


Figure S1. ORTEP diagram of the **a**) compound $[Pb(4\text{-bpdh})(NO_3)_2(H_2O)]_n$ (**HMTI-1**) and **b**) compound $[Pb(4\text{-bpdh})(NO_3)_2]_n$ (**HMTI-2**)

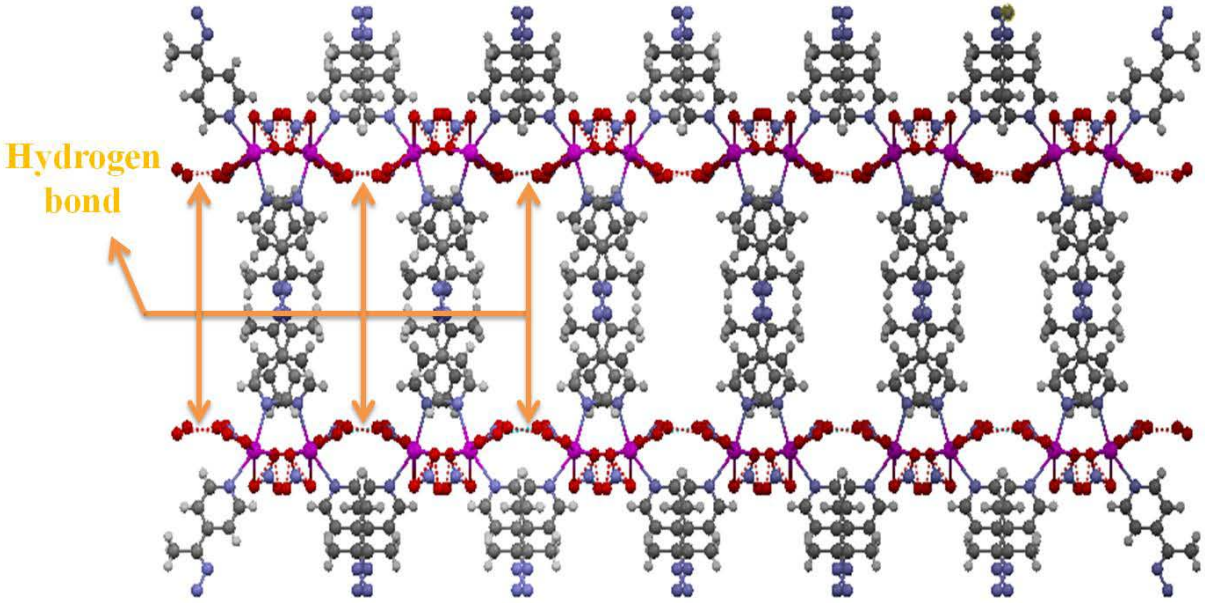


Figure S2. A schematic diagram illustrating the interactions in polymeric chains of compound (**HMTI-1)**, H atoms have been omitted for clarity. (Pb= violet, O = red, C = gray and N= blue)

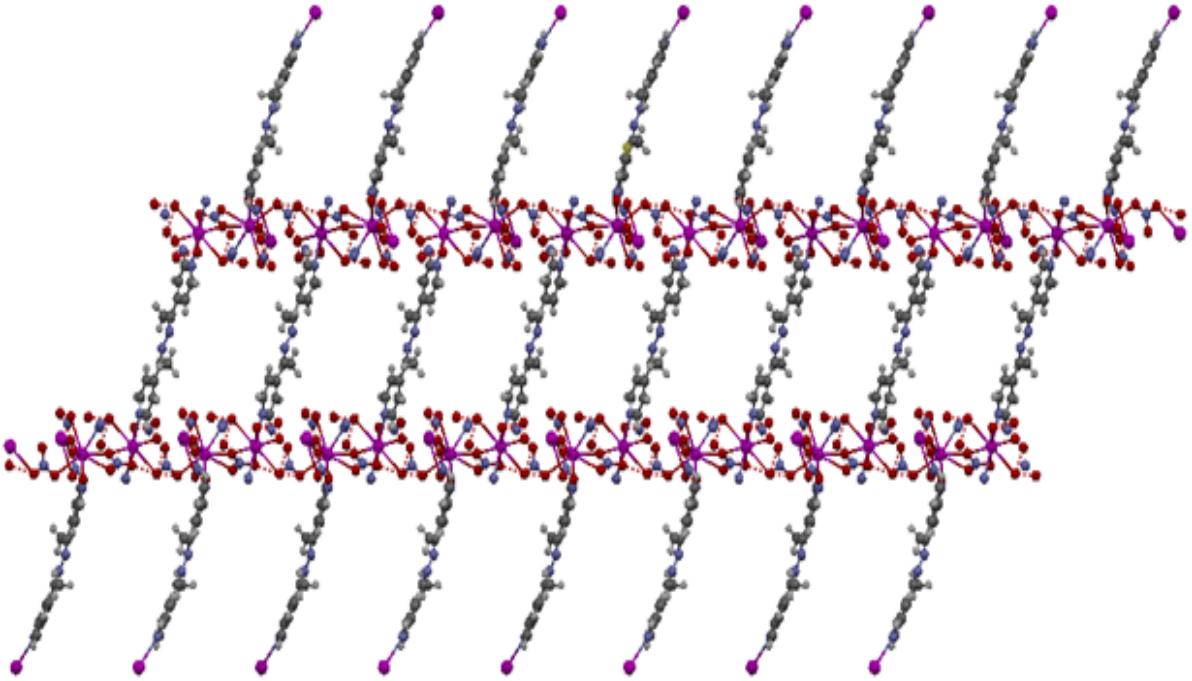


Figure S3. A schematic diagram illustrating the interactions in polymeric chains of compound (**HMTI-2)**, H atoms have been omitted for clarity. (Pb= violet, O = red, C = gray and N= blue)

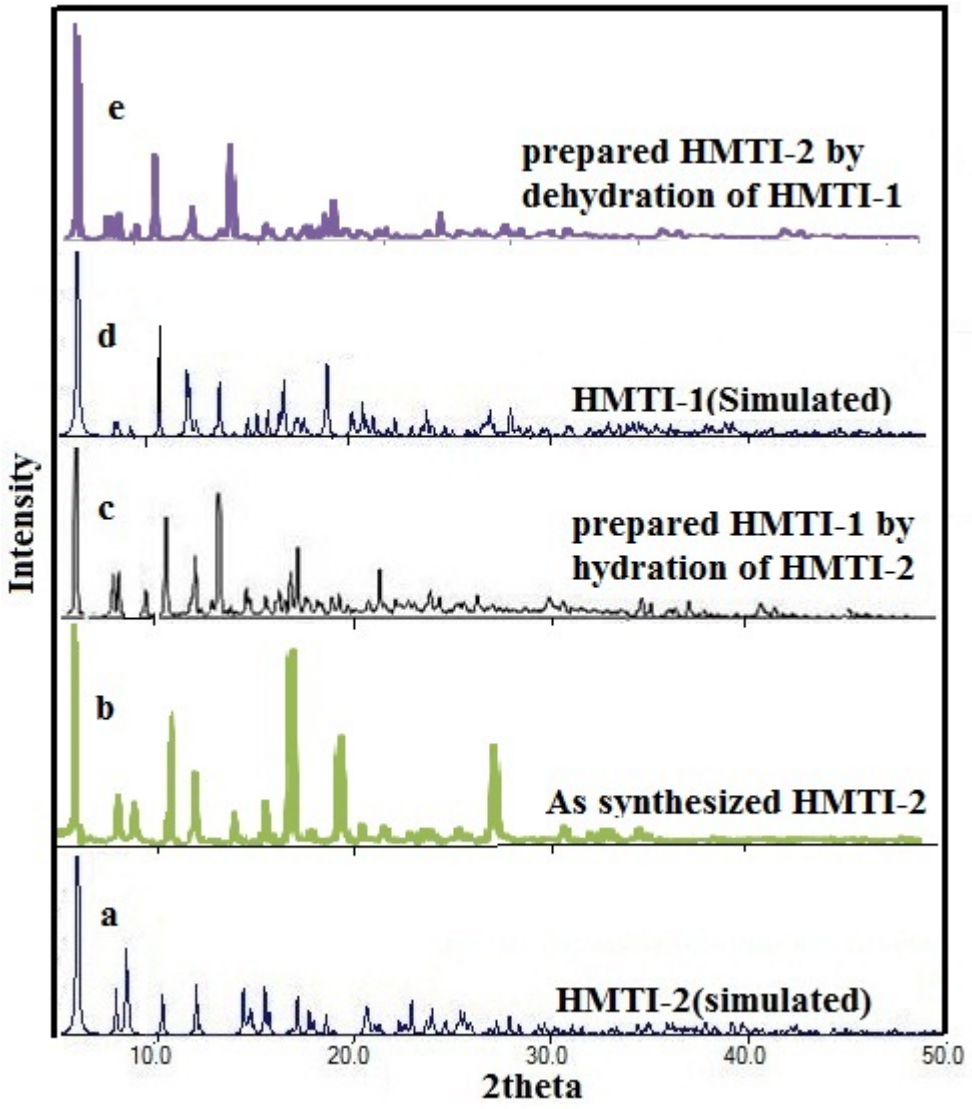


Figure S4. The XRD patterns of (**a**) simulated from single crystal X-ray data of compound **HMTI-2**; (**b**) bulk materials as synthesized **HMTI-2**; (**c**) bulk materials obtained by hydration of compound **HMTI-2**; (**d**) simulated from single crystal X-ray data of compound **HMTI-1** and (**e**) bulk materials obtained by dehydration of compound **HMTI-1.**

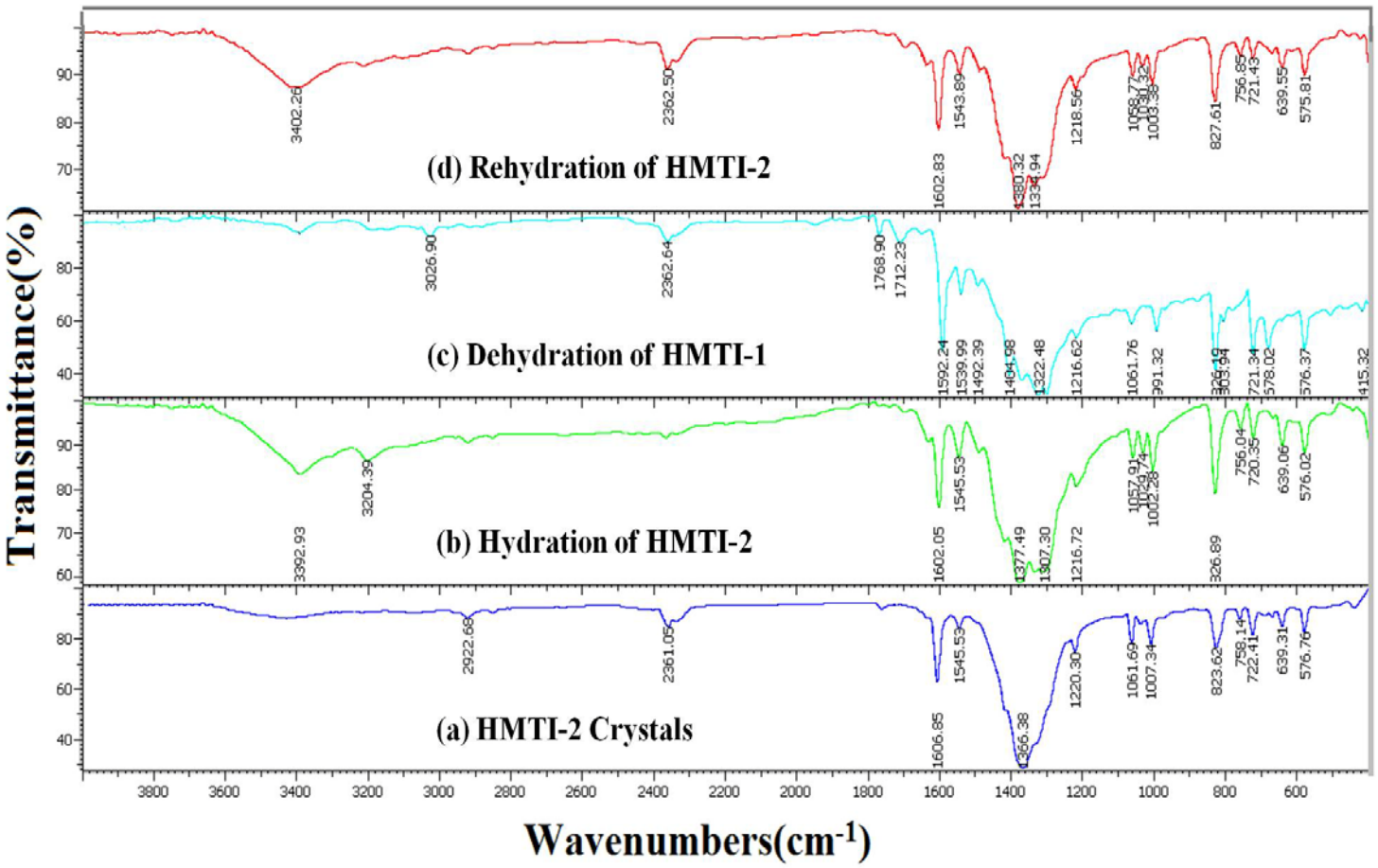


Figure S5. IR spectra of **a**) compound **HMTI-2, b**) bulk materials obtained by hydration of compound **HMTI-2** by dispersion of the compound **HMTI-2** **c**) the species obtained by heating of compound **HMTI-1** prepared by hydration of compound **HMTI-2** and **d**) compound **HMTI-1** prepared by rehydration of compound **HMTI-2** prepared by dehydration of compound **HMTI-1**.

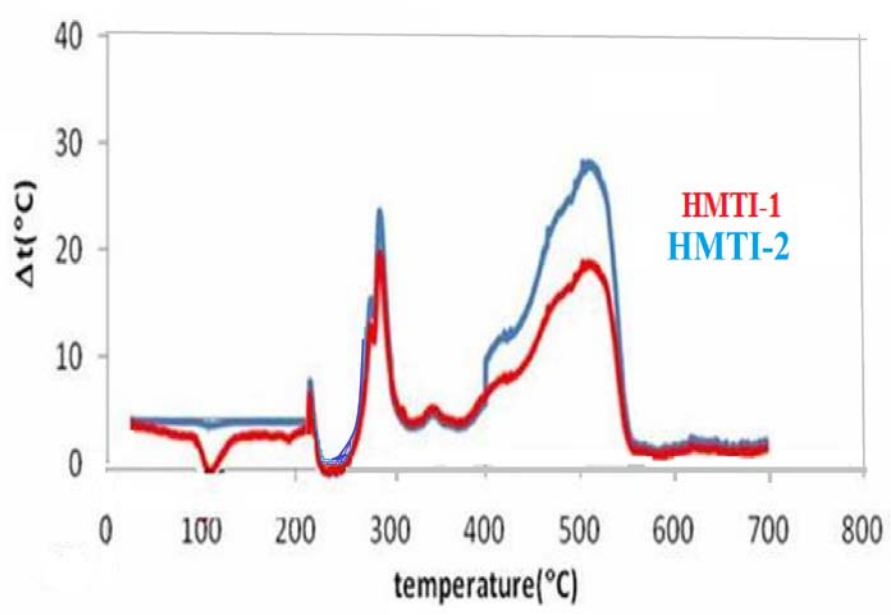


Figure S6. DTA diagrams of compounds **HMTI-1** and **HMTI-2**.

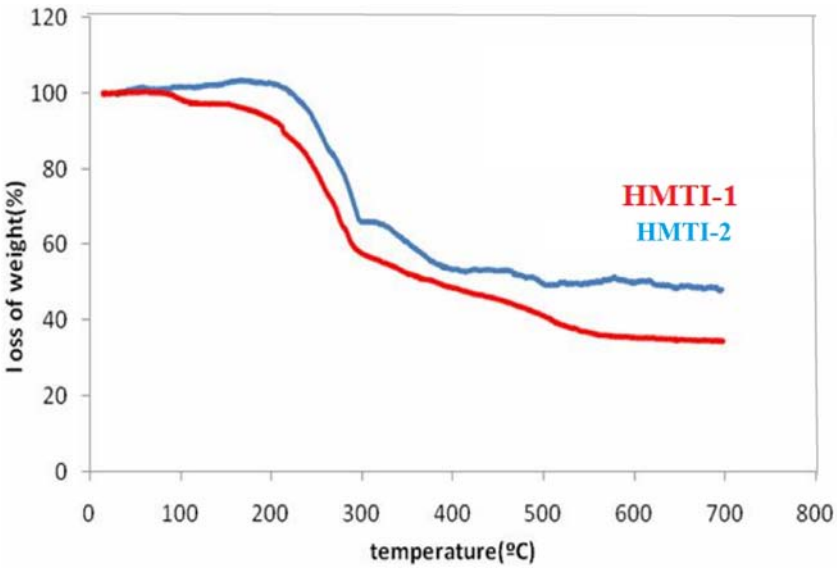


Figure S7. TGA diagrams of compounds **HMTI-1** and **HMTI-2**.

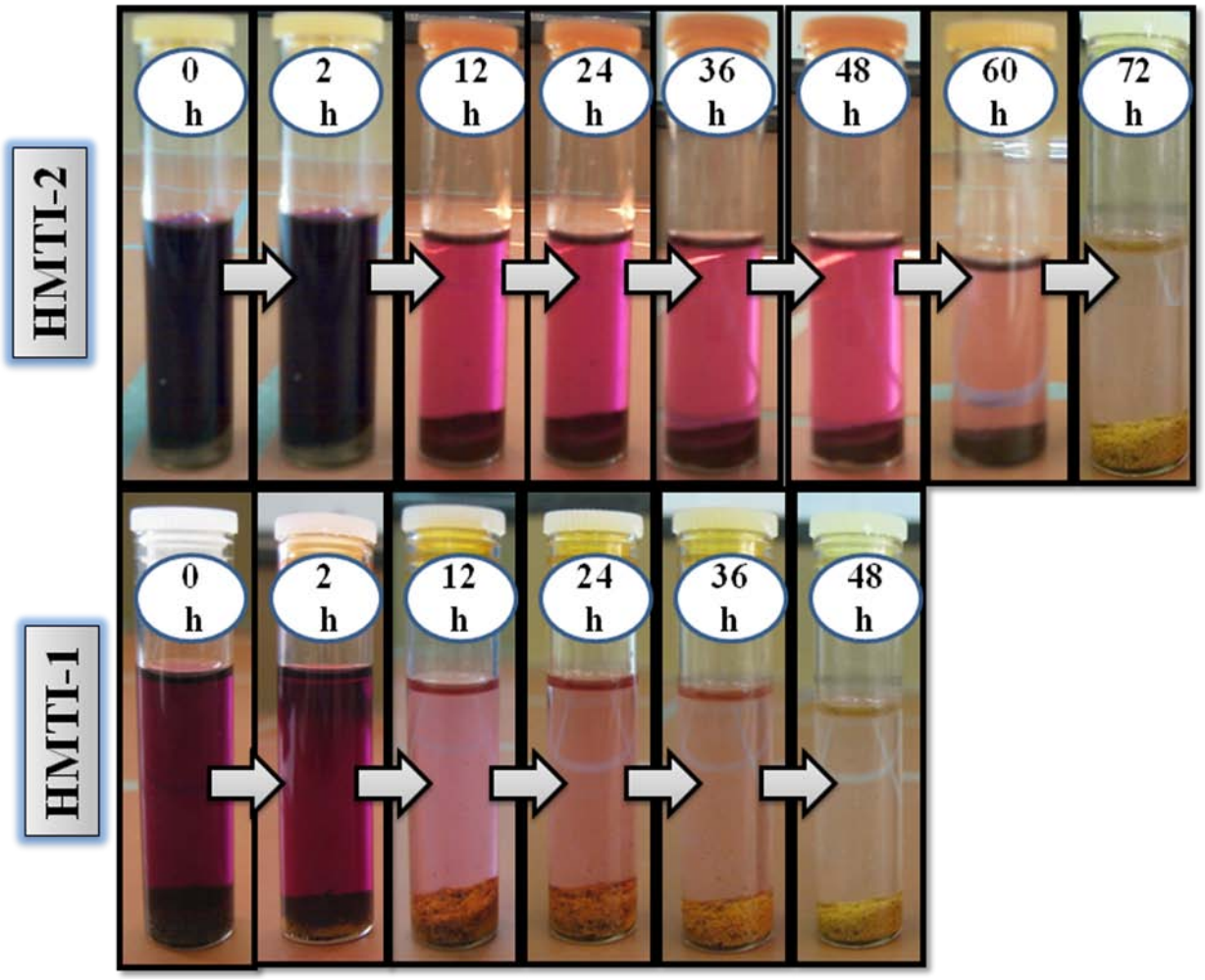


Figure S8. Comparison of I_2 enrichment progress between **HMTI-2** and **HMTI-1** when 100 mg of crystals were soaked in 3 mL of a cyclohexane solution of I_2 (0.1 M/L).

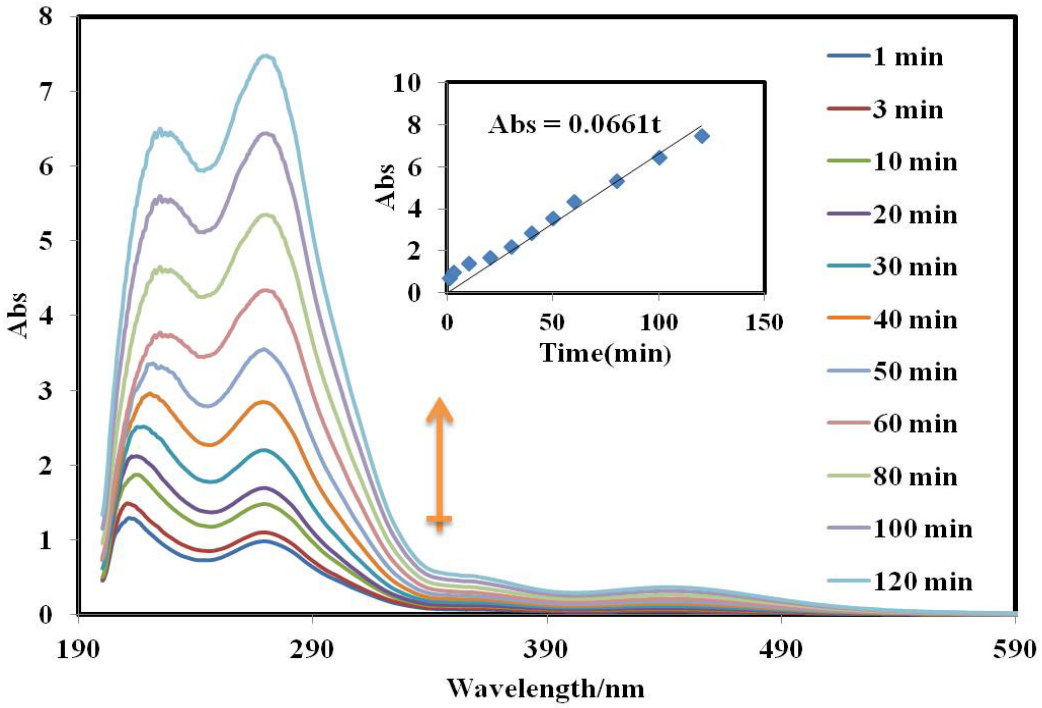


Figure S9. Temporal evolution of UV/vis absorption spectra for the delivery of I_2 from **HMTI-2** in the first 2 h.

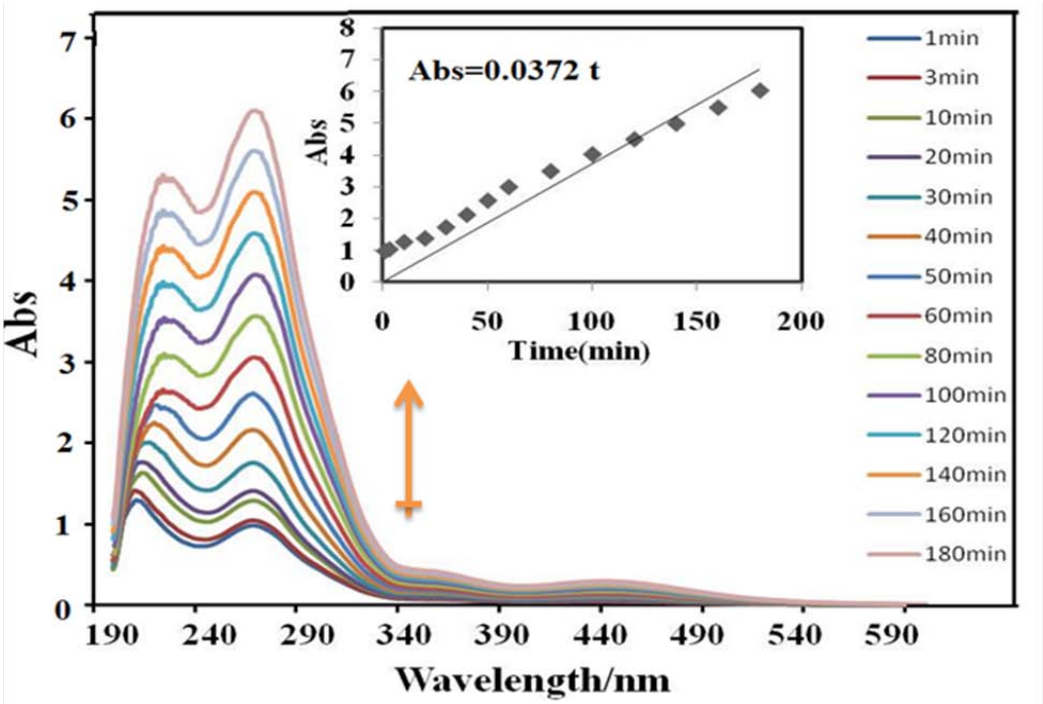


Figure S10. Temporal evolution of UV/vis absorption spectra for the delivery of I_2 from **HMTI-1** in the first 3 h.

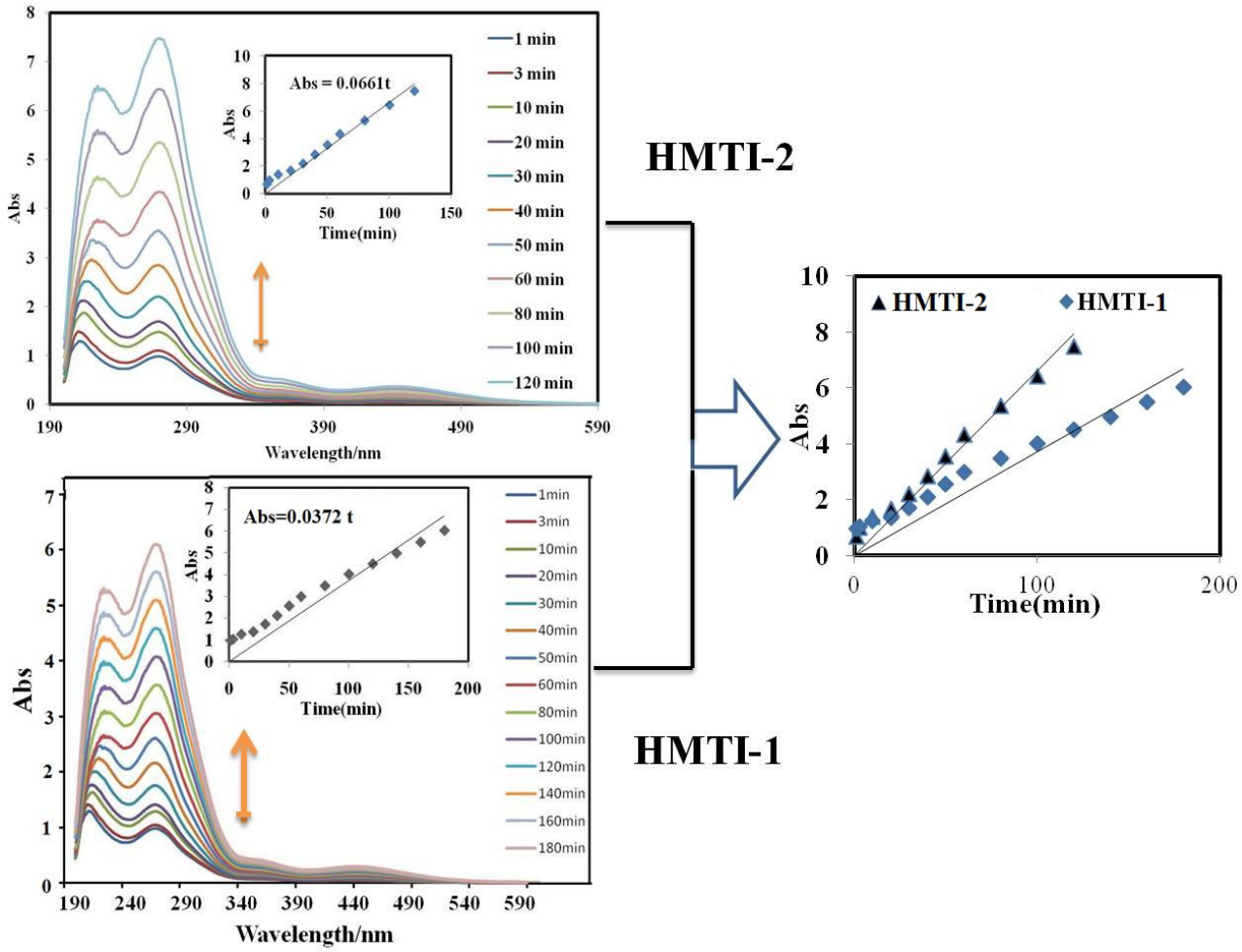


Figure S11. Comparison of desorbed rate of **HMTI-1** and **HMTI-2**.

Table S1 Crystal data and structure refinement of [Pb(4-bpdh)(NO_3)$_2$] (**HMTI-2**).

Identification code	**HMTI-2**
Empirical formula	$C_{15}H_{16}N_{6.6}O_6Pb$
Formula weight	596.88
Temperature(K)	120(2)
Wavelength	0.71073
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a =30.9991(10)Å
	b =10.1021(4)Å
	c =20.4318(8)Å
	β =110.727(3)^o
Volume	5984.2(4)Å^3
Z	4
Density (calculated)	1.987 g/m^3
F(000)	3416
Theta range for data collection	2.10 to 29.16 ^{o}
Index ranges	-42 ≤ *h* ≤ 32
	-13 ≤ *k* ≤ 11
	-27 ≤ *l* ≤27
Reflections collected	8045
Independent reflections	5075
Absorption correction	Integration
Refinement method	F^2 > 2sigma(F^2)
Data / restraints / parameters	8045 / 0 / 394
Goodness-of-fit on F^2	1.114
Final *R* indices [$I>2\sigma(I)$]	R_1= 0.1076 and wR_2= 0.2029
R Indices (all data)	R_1= 0.1702 and wR_2= 0.2286