Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supplementary Information for MS:

New lead(II) nano-porous three-dimensional coordination polymer; pore size effect on iodine adsorption affinity

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Table S1 Crystal data and structure refinement of $[Pb(4\text{-bpdb})(\mu\text{-}NO_3)(\mu\text{-}SCN)]_n.1.5\ CH_3OH$ (**TMU-15**).

Identification code	**TMU-15**
Empirical formula	$C_{14.50}\,H_{16}\,N_6\,O_{4.50}\,Pb\,S$
Formula weight	585.58
Temperature(K)	100(2)
Wavelength	0.71073
Crystal system	Monoclinic
Space group	C 2/c
Unit cell dimensions	a = 31.684(4) Å
	b = 10.0017(12) Å
	c = 13.3763(17) Å
	α = 90.00
	β =106.607(3)°
	γ = 90.00
Volume	4062.1(9) Å3
Z	8
Density (calculated)	1.915 Mg/m3
F(000)	2232
Theta range for data collection	2.55 to 29.83°
Index ranges	$-43 \le h \le 43$
	$-13 \le k \le 13$
	$-18 \le l \le 18$
Reflections collected	24504
Independent reflections	5776 [R(int) = 0.0575]
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5776 / 0 / 257
Goodness-of-fit on F^2	1.000
Final *R* indices [$I>2\sigma(I)$]	$R_1 = 0.0345$, $wR_2 = 0.0800$
R Indices (all data)	$R_1 = 0.0524$, $wR_2 = 0.0885$

Table S2 Hydrogen bonding in $[Pb(4\text{-bpdb})(\mu\text{-}NO_3)(\mu\text{-}SCN)]_n.1.5\ CH_3OH$ (**TMU-15**).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(4)-H(4O)...O(5)#5	0.84	2.08	2.77(2)	138

#1 -x+1/2,-y+1/2,-z #2 x-1/2,y+1/2,z #3 -x+1/2,y-1/2,-z+1/2 #4 x+1/2,y-1/2,z #5 -x+1,y,-z+1/2

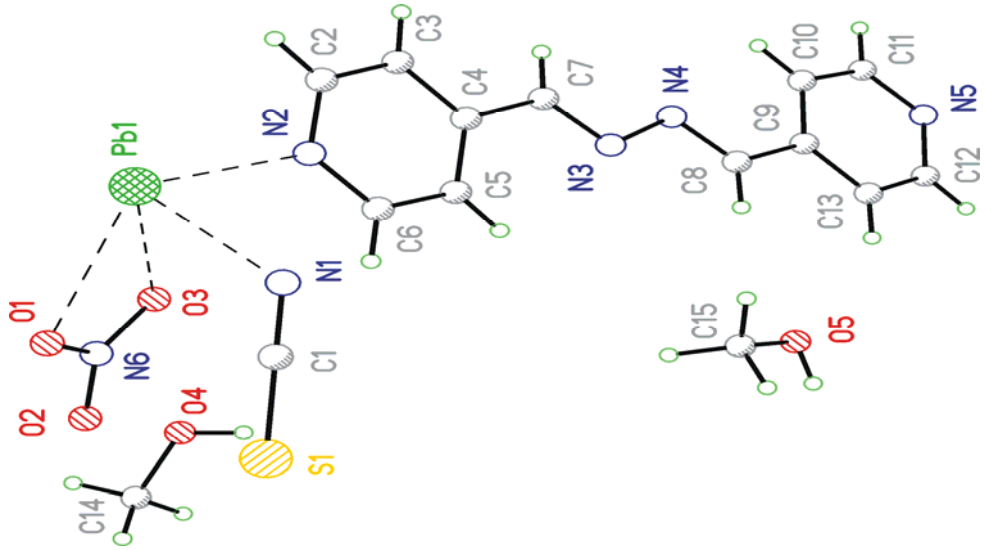


Fig. S1. Molecular view of independent part of unit cell

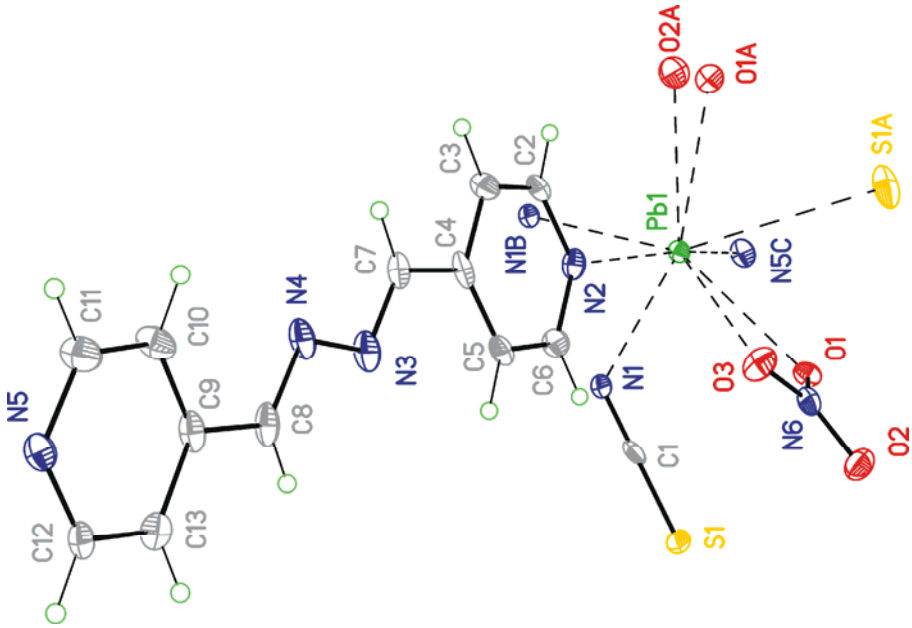
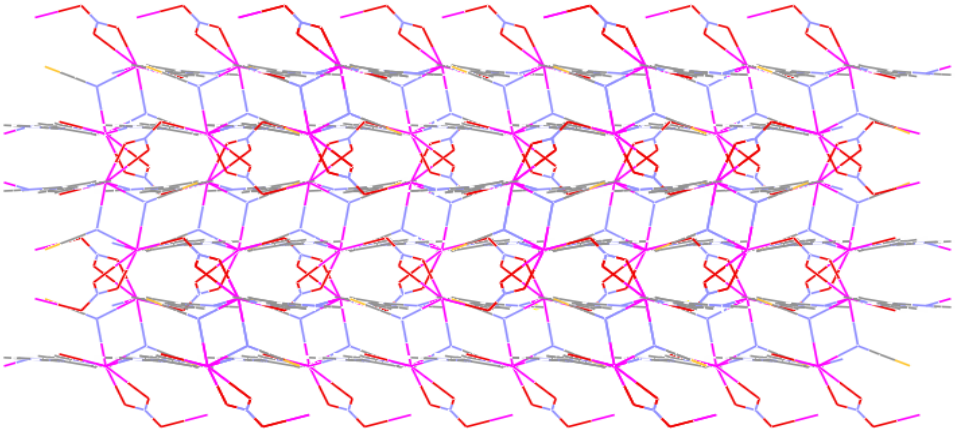
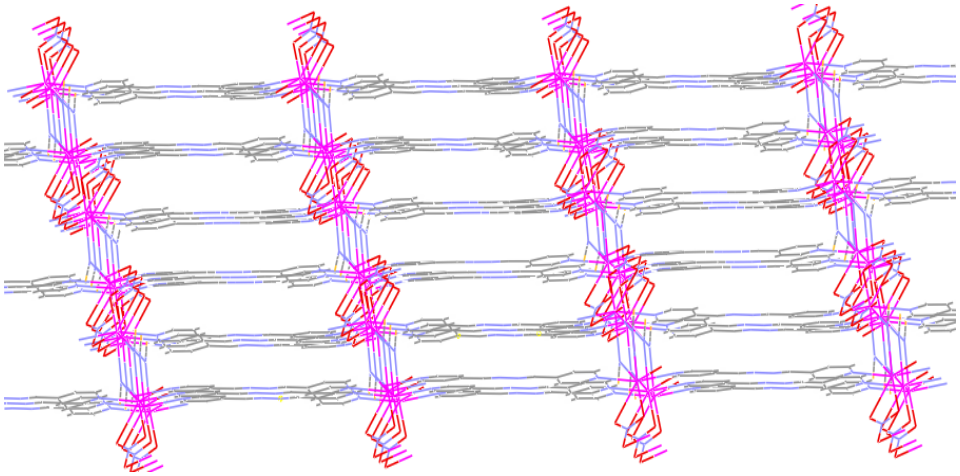


Fig. S2. Lead coordination environment given in thermal ellipsoids with 50% probability level. Symmetry transformations used to generate equivalent atoms: #A-x+1/2,y-1/2,-z+1/2 1Bx+1/2,-y+1/2,-z #C-1/2,y+1/2,z

view along crystallographic axic a



view along crystallographic axic b



view along crystallographic axic c

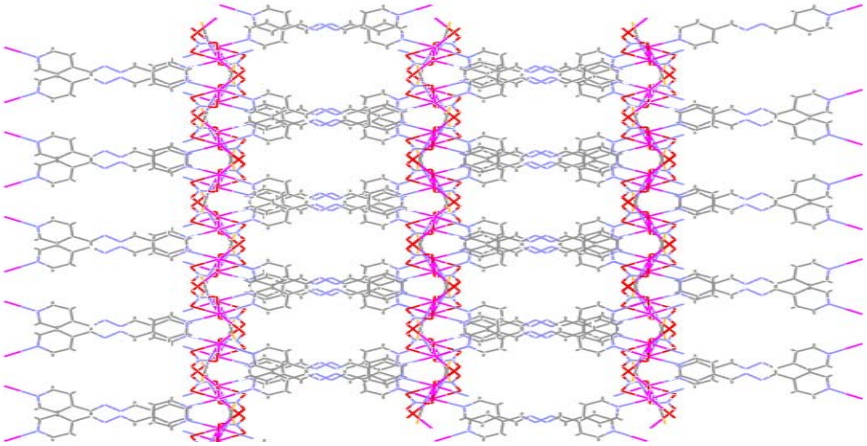


Fig. S3. A fragment of nano-porous 3D coordination polymer in [Pb(4-bpdb)(μ-NO_3)(μ-SCN)]$_n$.1.5 CH_3OH (**TMU-15**) (view along crystallographic axic a, b and *c*). The lead atoms are connected into infinite chains through the ($C_{10}H_{10}N_4$) ligands and the chains are further linked into MOF by NO_3^- and SCN^- anions.

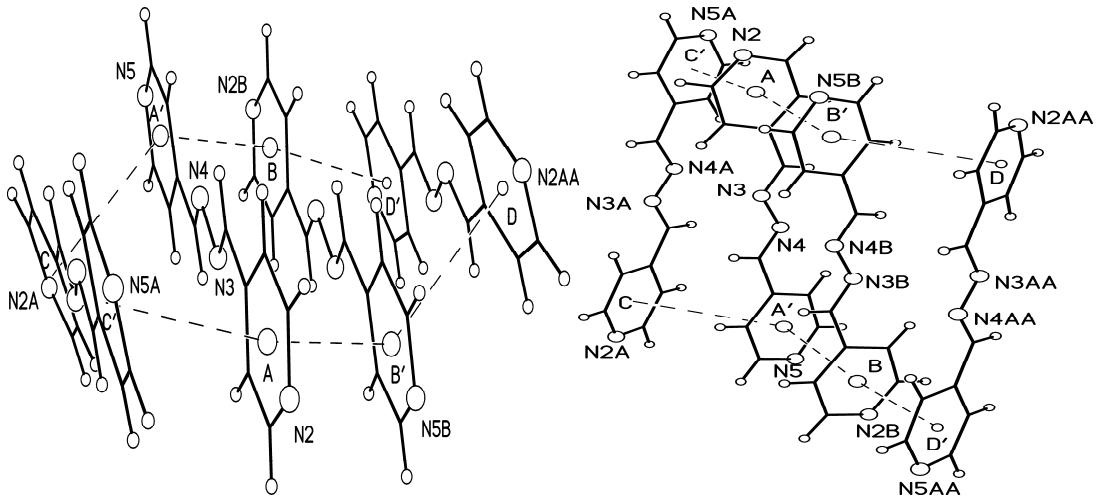


Fig. S4. Fragment of π-stacking ($C_{10}H_{10}N_4$) ligands (the stacks are parralel with the crystallographic axis *a*). The angle between the meanplanes of pyridine moieties and the distance between their centres for the pairs of cycles denoted A and B', B and D', A' and C are equal to, respectively, 8.3º and 3.58Å; that for the A' and B, B' and D, A and C' cycles - to 7.0º and 3.78Å.

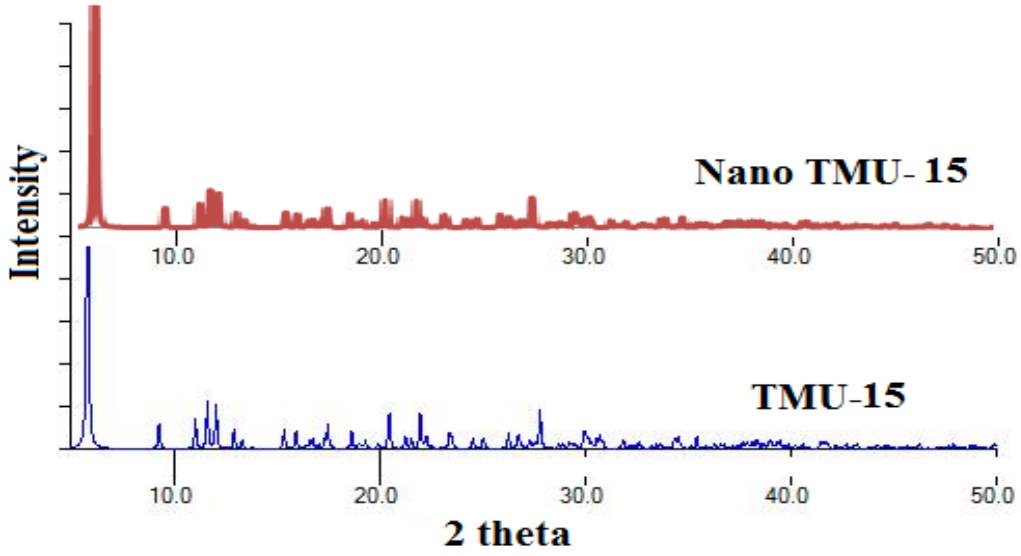


Fig. S5. XRD patterns of simulated based on single crystal data of compounds **TMU-15** and nano-**TMU-15** prepared by sonochemical process.

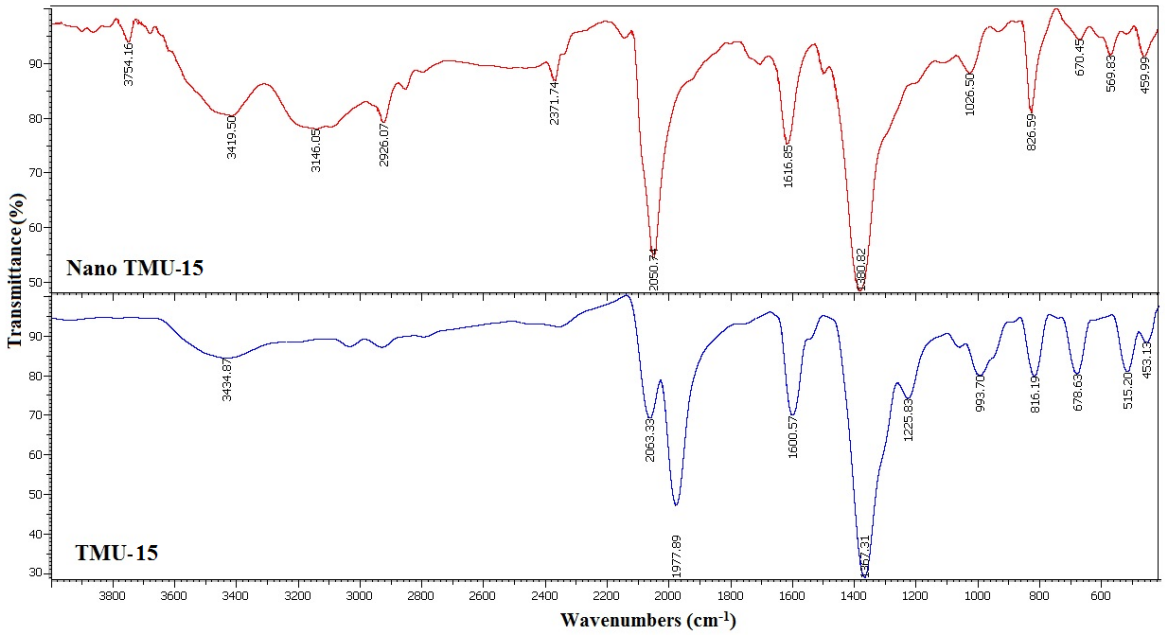


Fig. S6. The IR spectra of bulk materials as synthesized of compounds **TMU-15** and nano-sized compounds **TMU-15** prepared by sonochemical method.

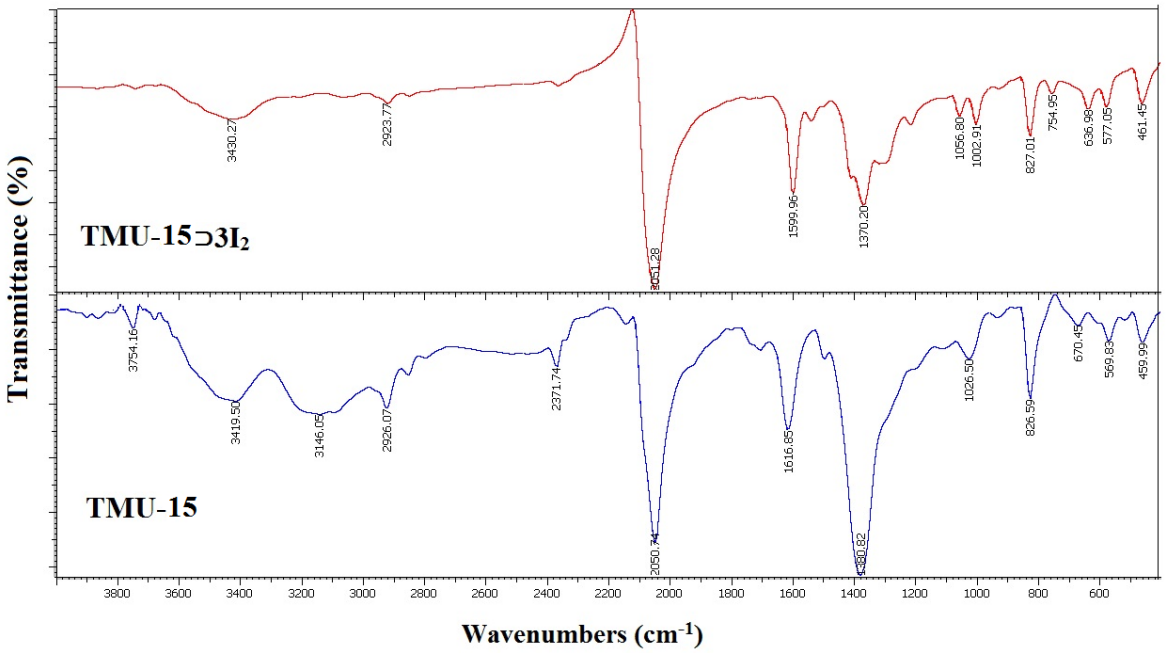


Fig. S7. The IR spectra of bulk materials as synthesized of compounds **TMU-15** and **TMU-15⊃3I$_2$.**

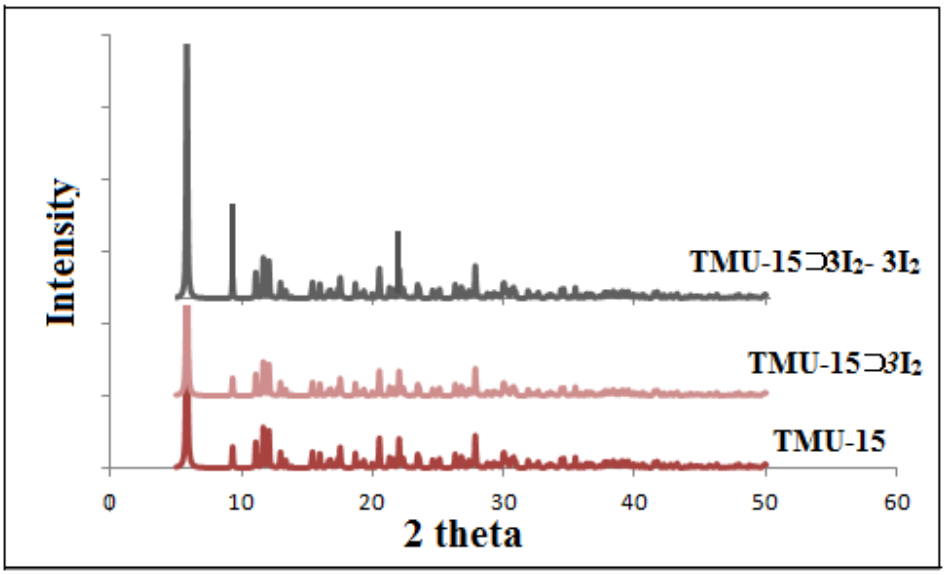


Figure S8. PXRD patterns of as-synthesized **TMU-15**, **TMU-15⊃3I$_2$** and **TMU-15⊃3I$_2$-3I$_2$.**

Elemental analysis data for compound **TMU-15** after the first cycle of iodine adsorption and desorption:

Compound TMU-15: C, 29.65; H, 2.70; N, 14.35%.

Compound TMU-15 after iodine adsorption (TMU-15⊃*3*I_2):

C, 12.91; H, 1.17; N, 6.24%.

Compound TMU-15 after iodine desorption (TMU-15⊃*3*I_2-*3*I_2):

C, 29.63; H, 2.68; N, 14.33%.