

Structural diversity of the encapsulated water clusters in the 3D supramolecular assemblies: a cyclic quasi-planar hexamer of water constructed through strong hydrogen bonding interactions

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Supplementary Information

Table S1 Selected bond distances (Å) for **1**, **2** and **3**.

	1	2	3
Mn1-N1	2.2349(14)	2.244(3)	2.255(2)
Mn1-N2	2.3346(13)	2.354(3)	2.383(2)
Mn1-N3	2.3097(13)	2.265(3)	2.369(2)
Mn1-N4	2.3106(14)	2.303(3)	2.332(2)
Mn1-O1	2.1242(12)	2.133(2)	2.249(3)
Mn1-O2	2.1415(13)	2.088(2) [#]	2.1122(18)
Mn1-O4	-----	-----	2.529(3)
C20-C21	1.197(2)	-----	-----

[#]-x+1/2, -y+3/2, -z

Table S2 Selected bond angles (degrees) for **1**, **2** and **3**.

	1	2	3
O2-Mn1-O1	104.52(5)	99.28(8) [#]	103.25(8)
O1-Mn1-N1	162.20(5)	163.69(9)	163.31(8)
O1-Mn1-N4	89.02(5)	87.12(9)	135.06(9)
O2-Mn1-N3	129.12(5)	118.79(10) [#]	87.68(7)
N1-Mn1-N3	82.88(5)	85.46(9)	90.01(8)
O2-Mn1-N2	154.07(5)	164.98(9) [#]	87.81(8)
N1-Mn1-N2	76.57(5)	76.09(9)	75.83(8)
N3-Mn1-N2	73.93(5)	73.84(9)	71.06(7)
O2-Mn1-N1	93.27(5)	95.99(9) [#]	163.31(8)
O2-Mn1-N4	84.01(5)	93.98(10) [#]	87.23(7)
O1-Mn1-N3	85.22(5)	92.13(9)	81.04(9)
N4-Mn1-N3	146.75(5)	146.82(9)	143.64(8)
O1-Mn1-N2	87.44(5)	87.71(9)	149.58(9)
N4-Mn1-N2	73.11(5)	72.99(9)	72.79(7)
N1-Mn1-O4	-----	87.12(9)	87.97(8)
O1-Mn1-O4	-----	-----	54.15(9)
N4-Mn1-O4	-----	-----	80.91(8)
N2-Mn1-O4	-----	-----	150.05(9)
N1-Mn1-N4	93.69(5)	86.16(9)	84.86(8)
O2-Mn1-O4	-----	-----	105.27(8)
N3-Mn1-O4	-----	-----	134.95(8)
C21 [#] -C20-C19	175.60(18)	-----	-----
C20 [#] -C21-C22	172.15(17)	-----	-----
[#] -x+1/2, y+3/2, -z		[#] -x+1/2, -y+1/2, -z+1	

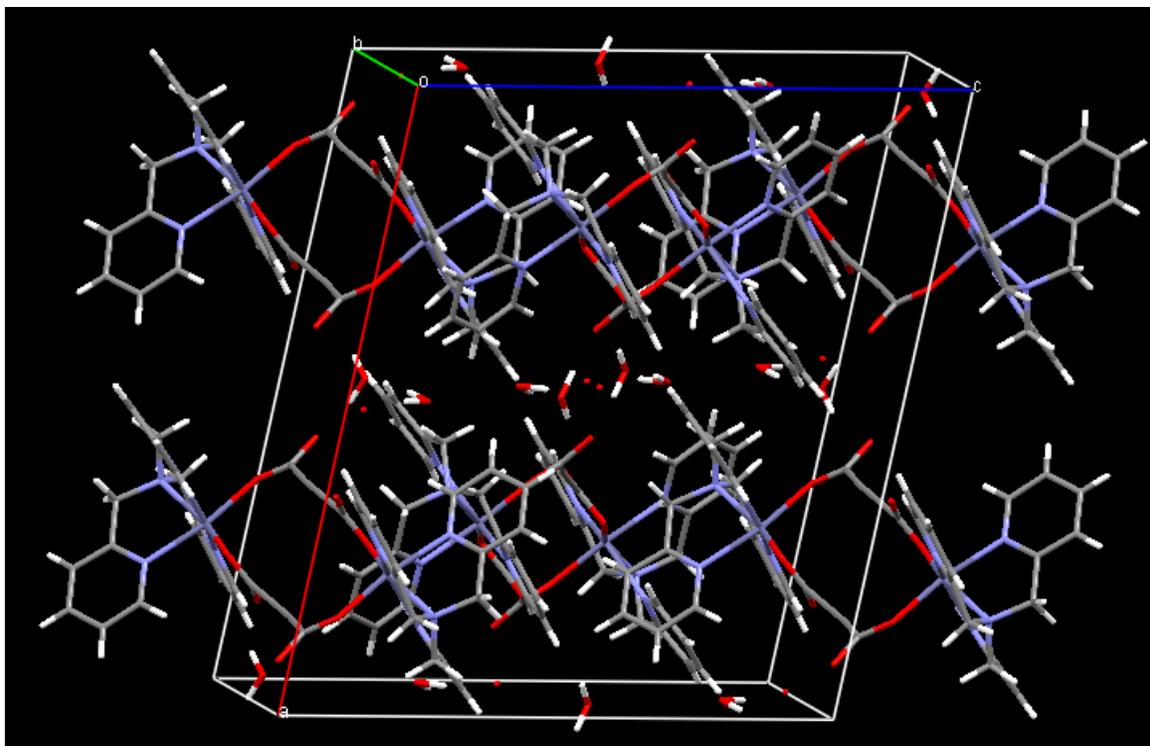


Fig. S1 Unit cell packing diagram of **1**.

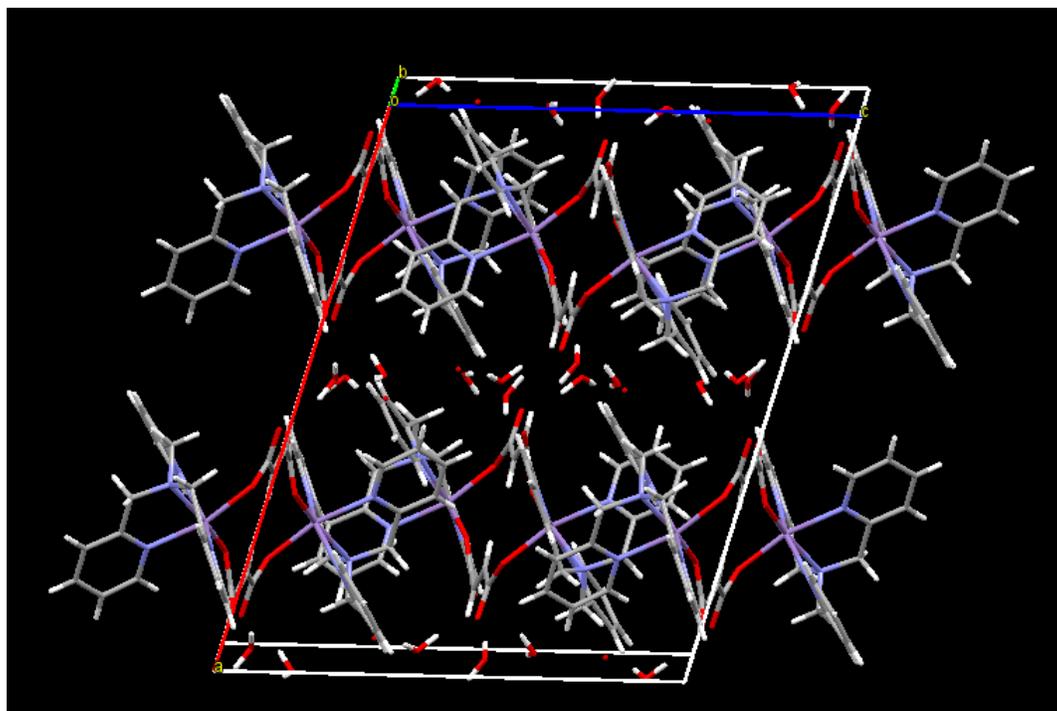


Fig. S2 Unit cell packing diagram of **2**.

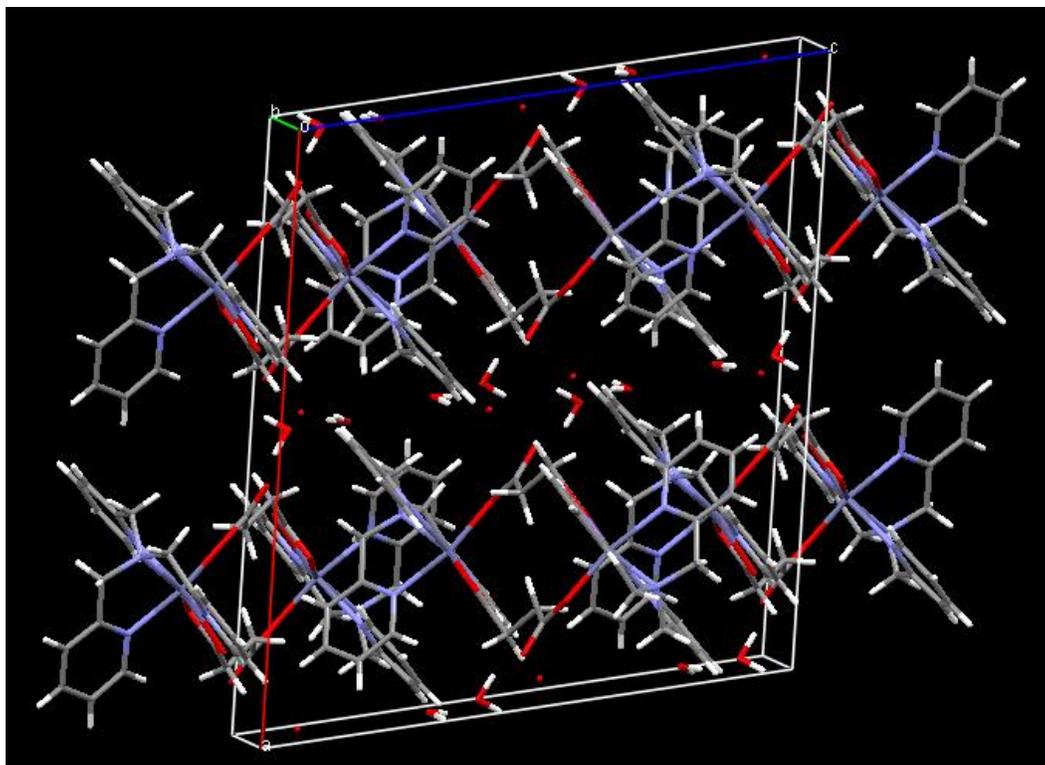


Fig. S3 Unit cell packing diagram of **3**.

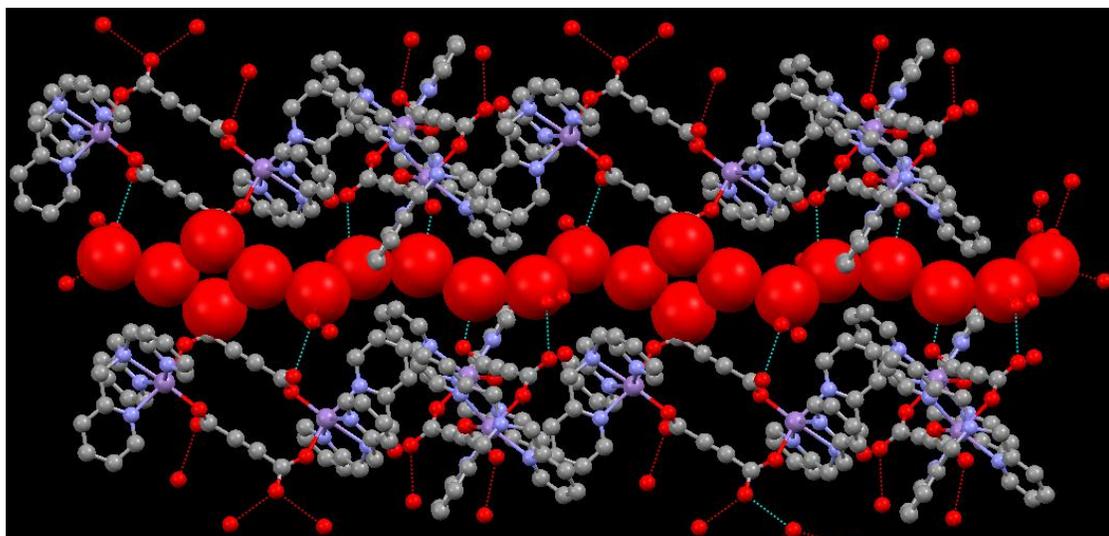


Fig. S4 A perspective view of the chain of encapsulated water molecules (space-fill) in **1**.

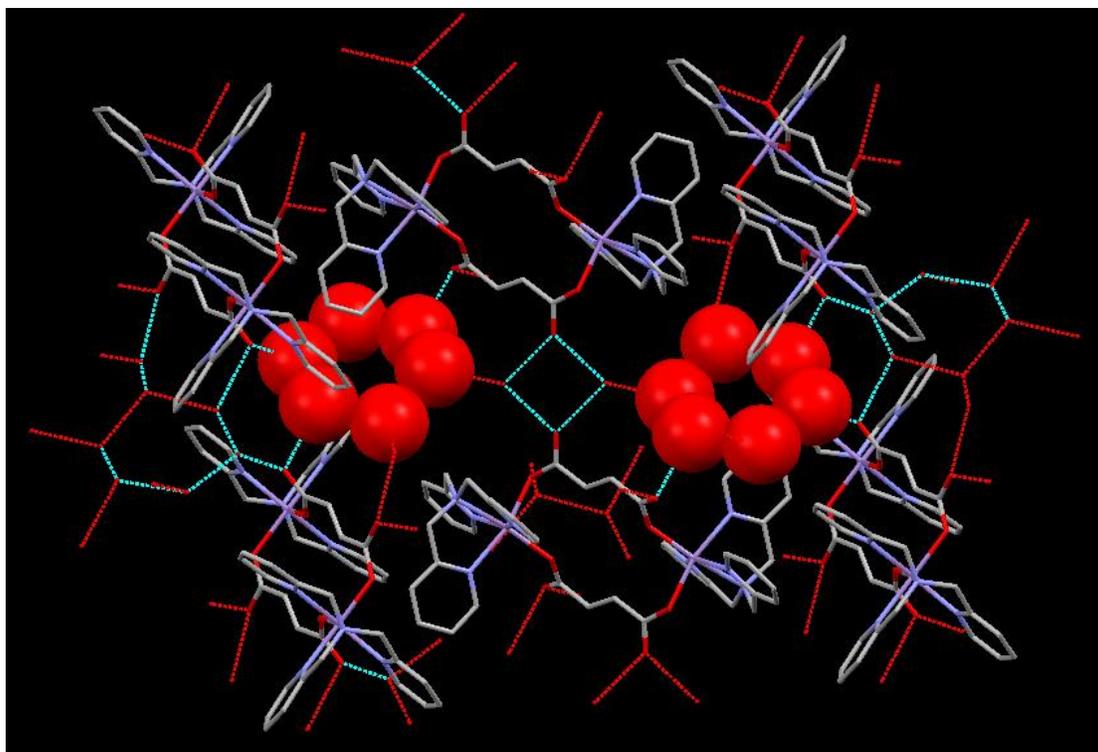


Fig. S5 A perspective view of the network of encapsulated water molecules (space-fill) in **2**.

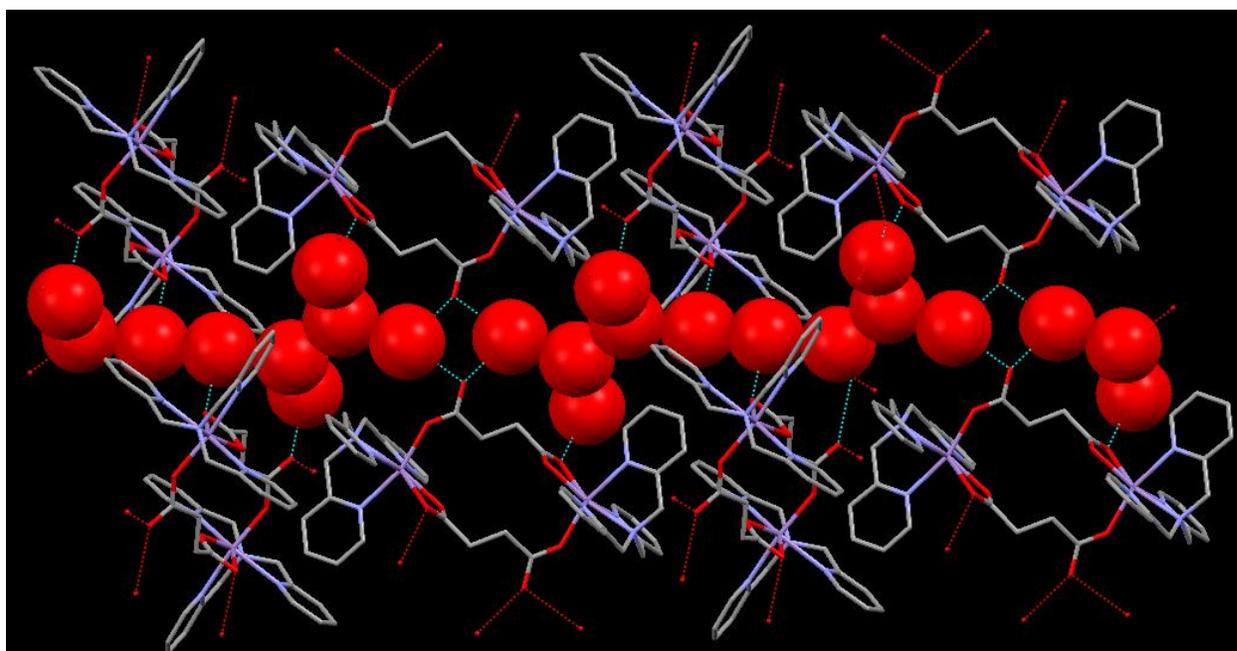


Fig. S6 A perspective view of the network of encapsulated water molecules (space-fill) in **3**.

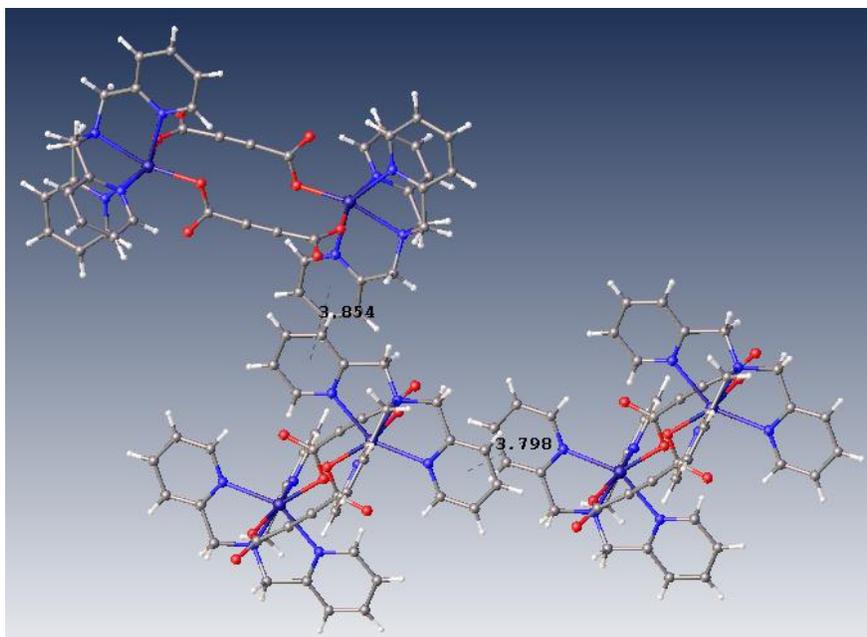


Fig. S7 A perspective view of **1** showing π - π interactions between two pyridine rings in two different planes.

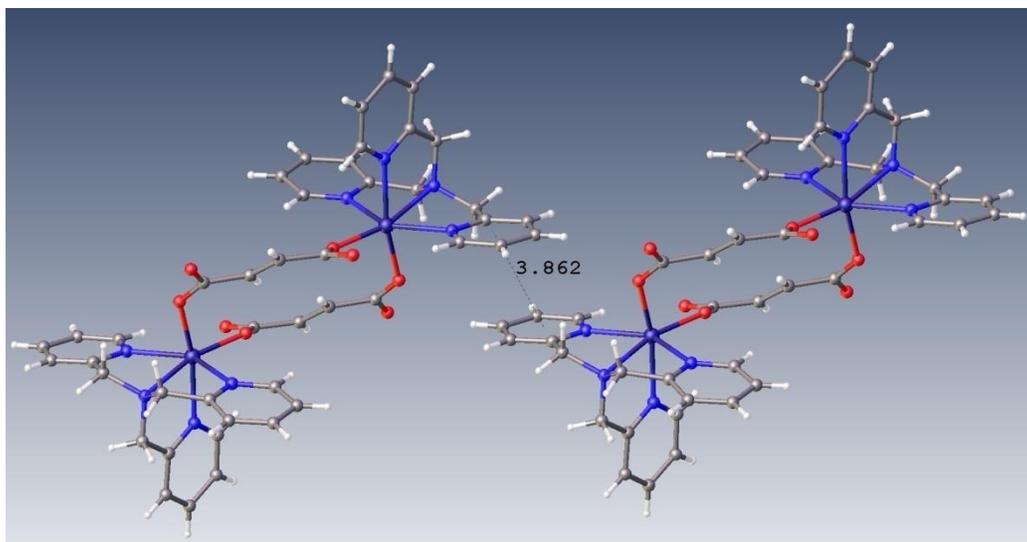


Fig. S8 A perspective view showing π - π interactions between two pyridine rings of two dimanganese subunits in **2**.

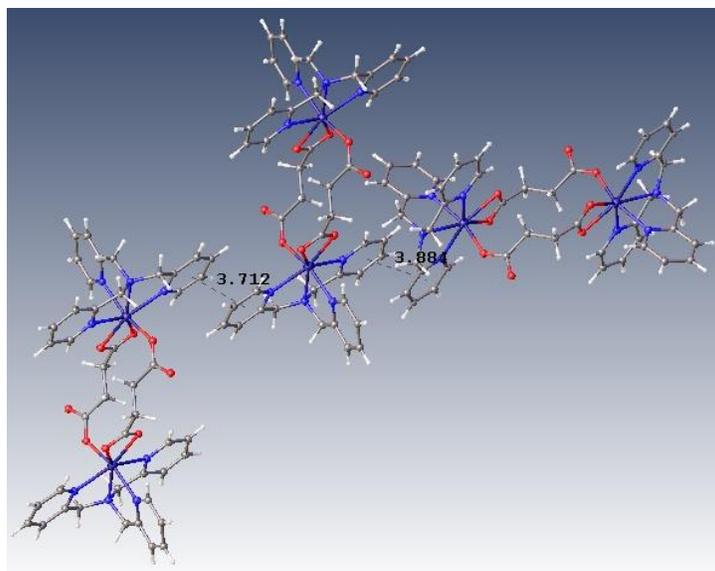


Fig. S9 A perspective view of **3** showing π - π interactions between two pyridine rings in two different planes.

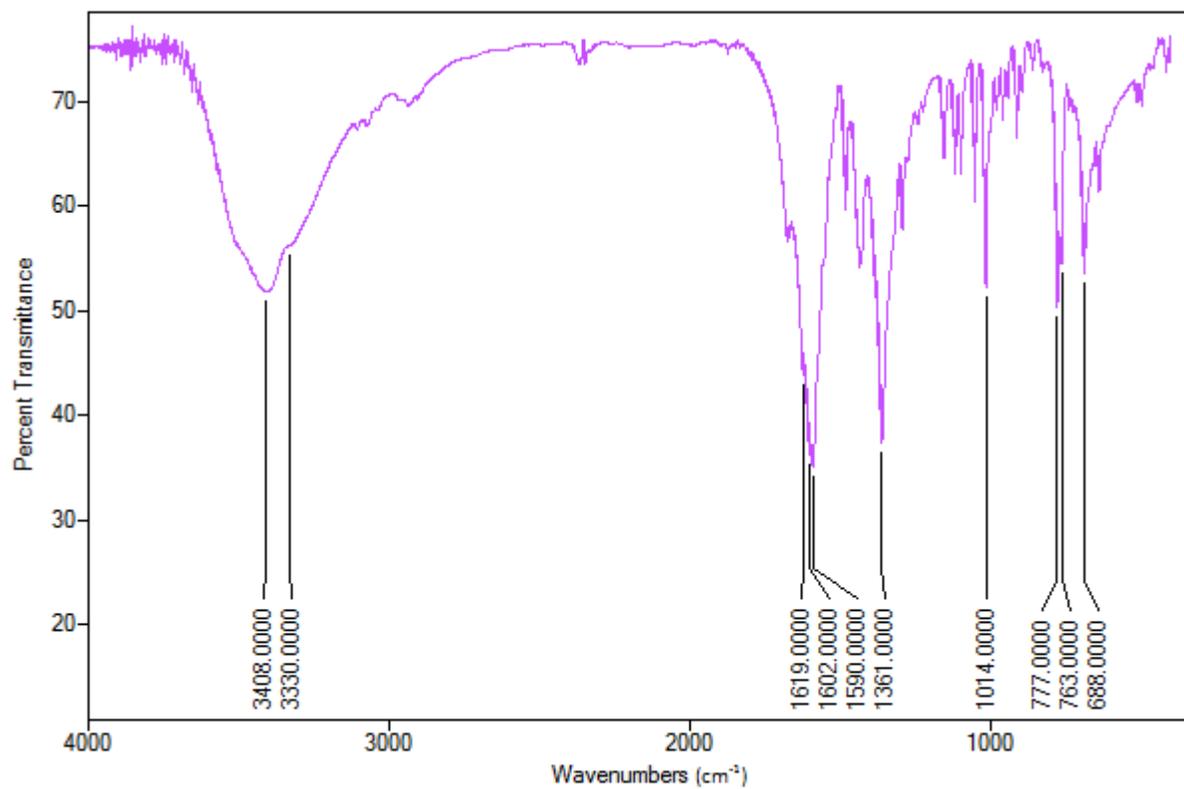


Fig. S10 FTIR spectrum of **1**.

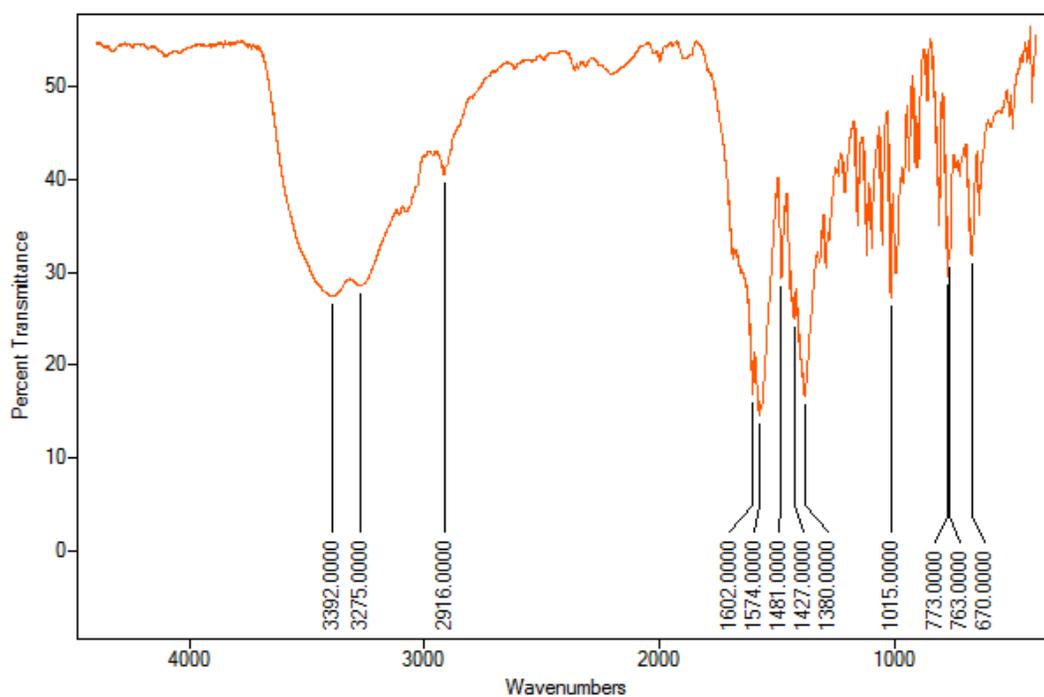


Fig. S11 FTIR spectrum of **2**.

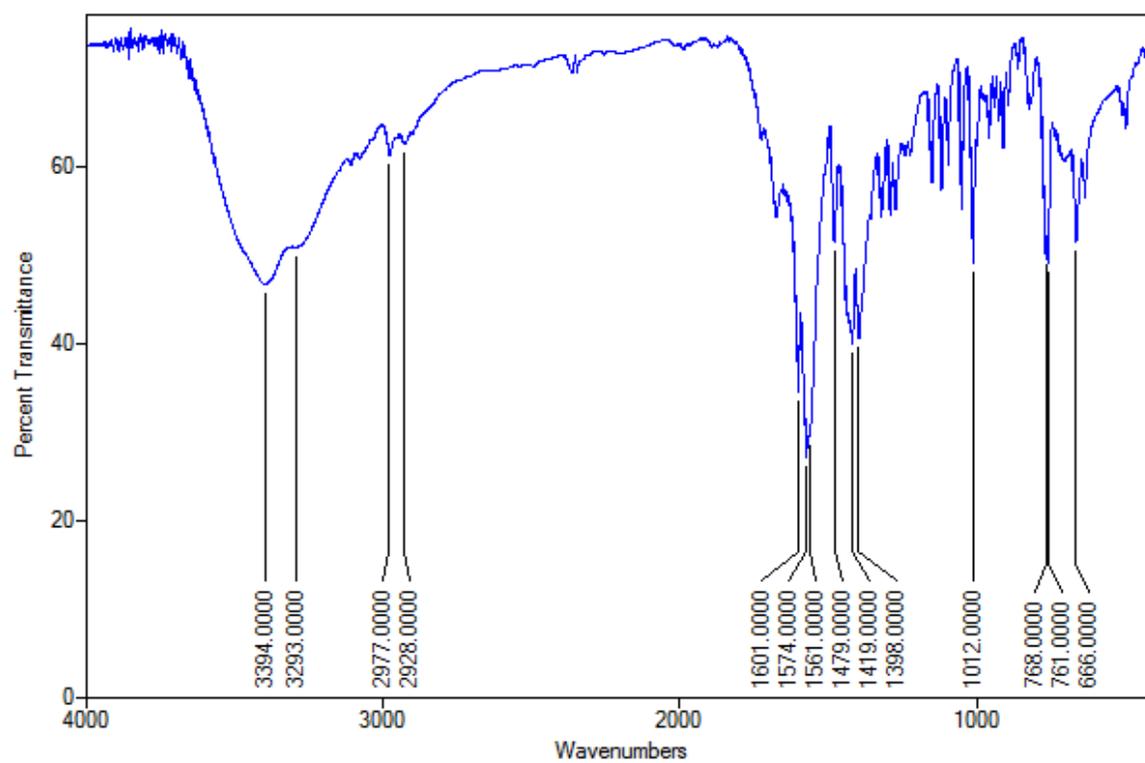


Fig. S12 FTIR spectrum of **3**.

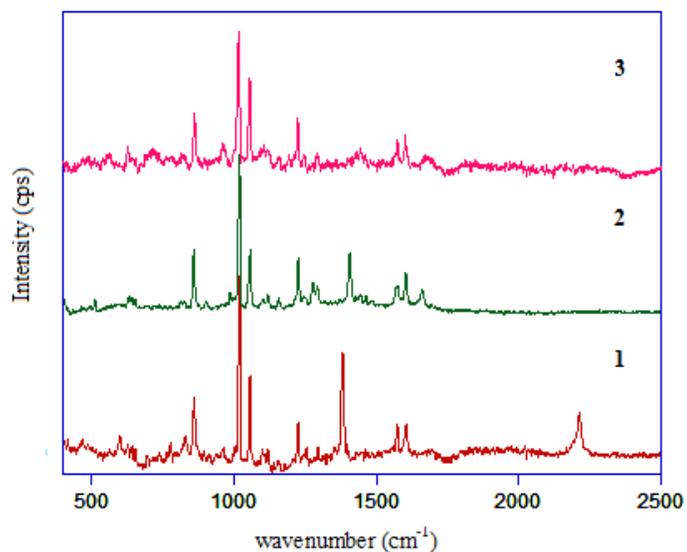


Fig. S13 Raman spectra of 1, 2 and 3.

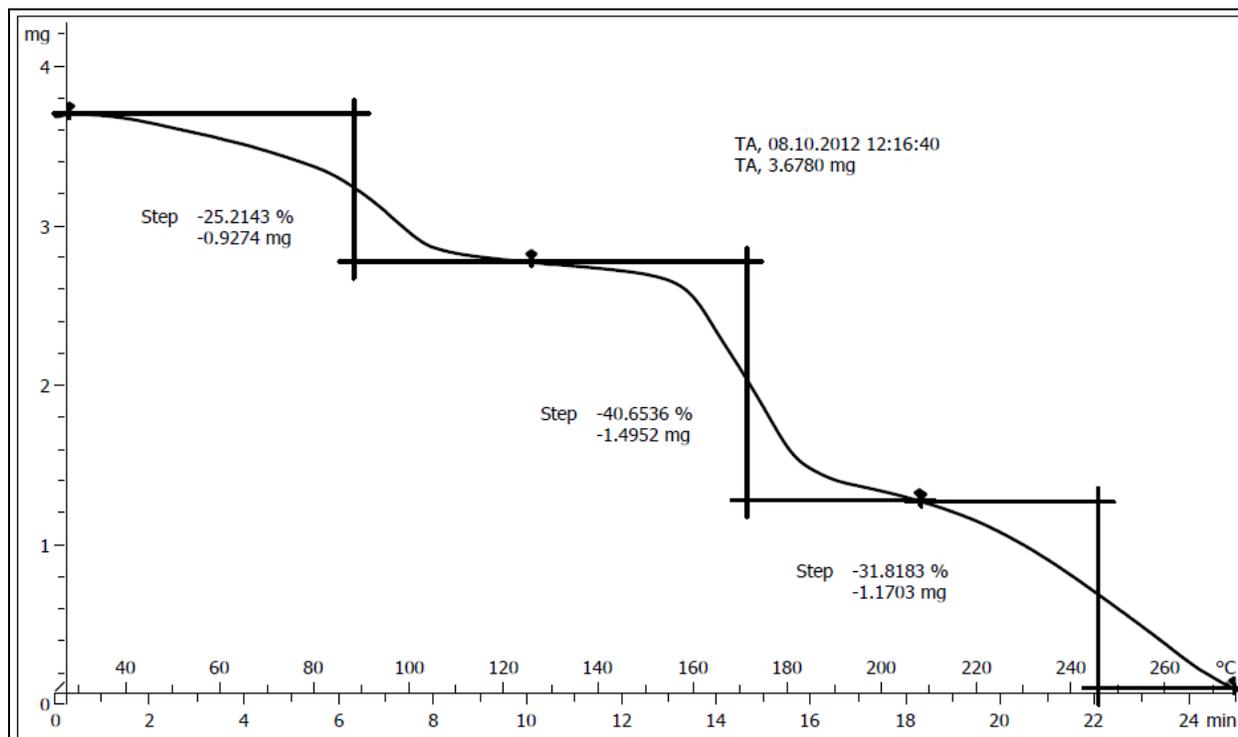


Fig. S14 TGA scan of 1.

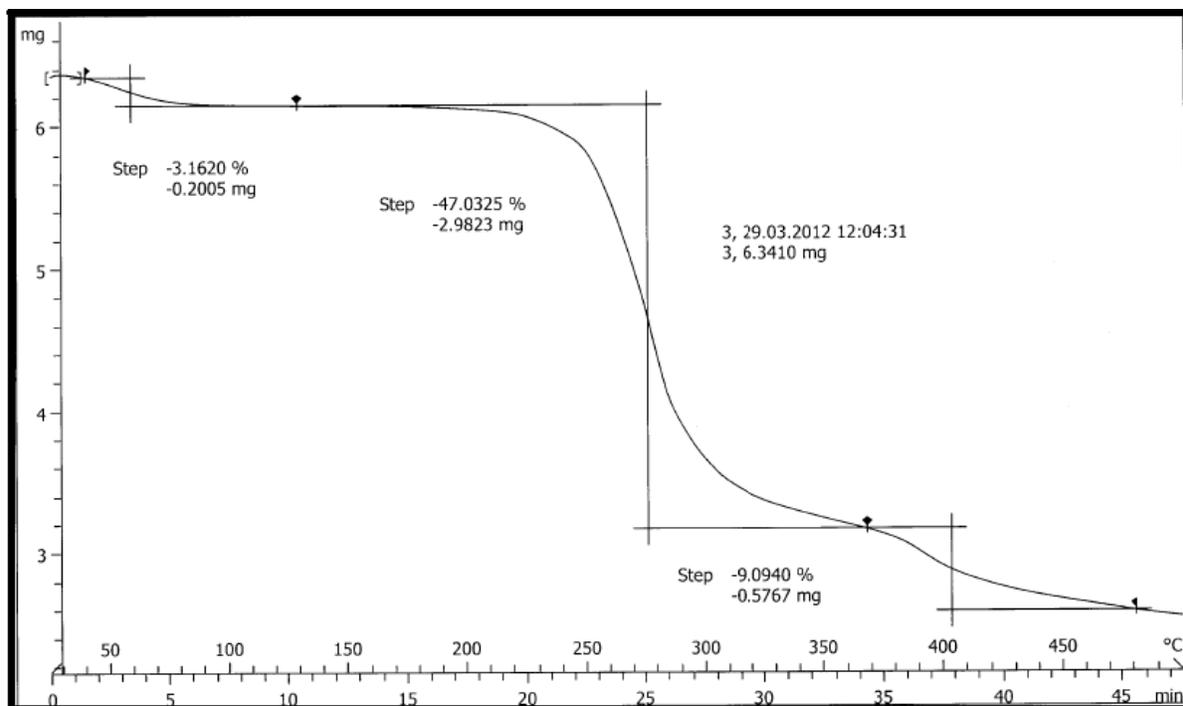


Fig. S15 TGA scan of 2.

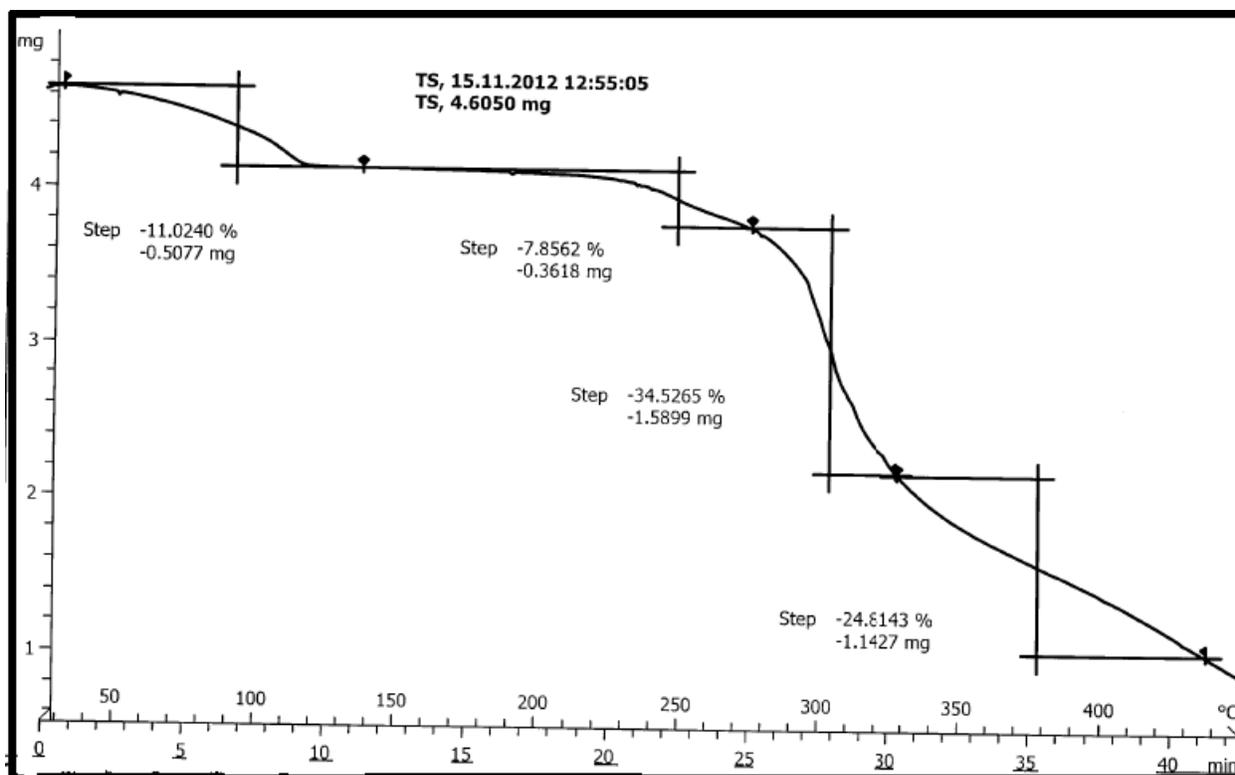


Fig. S16 TGA scan of 3.