Supporting Information

Structural Characterization of an Enantiopure Hydroxo-bridged Binuclear Iron(III) Complex with Empty One-dimensional Helical Channels

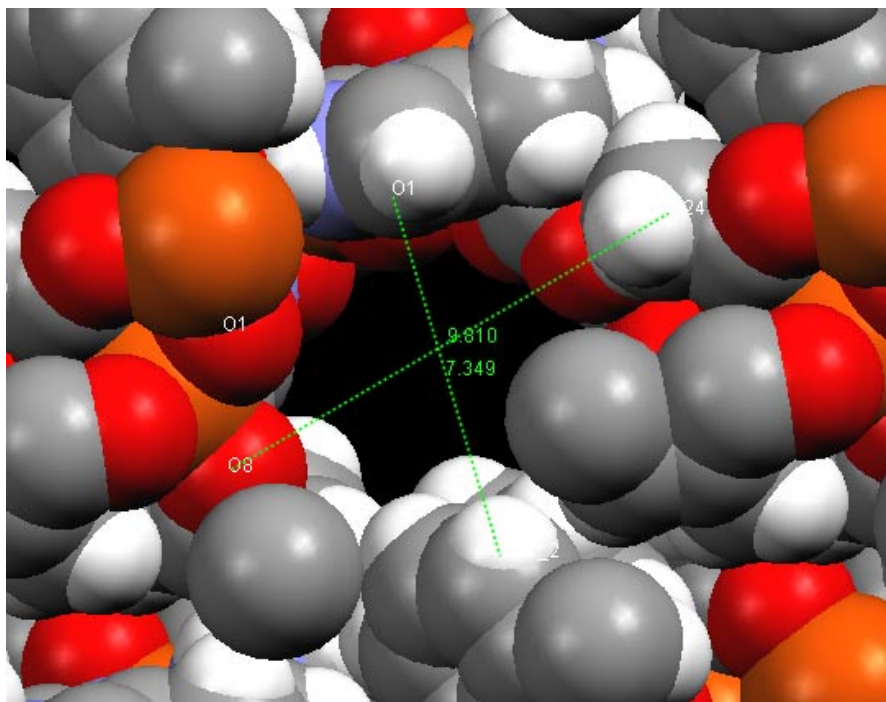Md. Akhtarul Alam†, Munirathinum Nethaji‡*, and Manabendra Ray†*

Figure S1. The cavity diameter in **1** was calculated by atom-atom distances between O8-C24 and O1-C11.
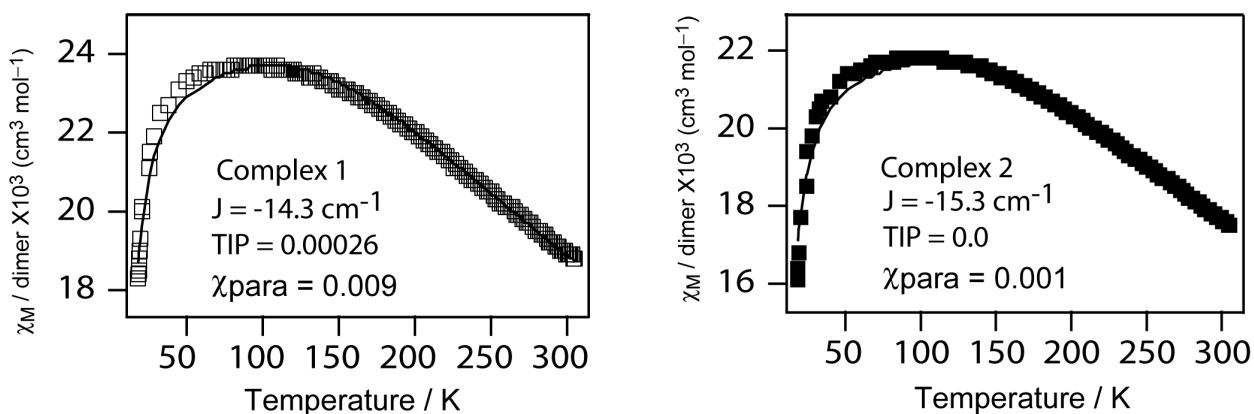

Figure S2. The magnetic susceptibility plots with parameters used in the fit. The fitting equation was taken from *J. Chem. Soc., Dalton Trans.*, **2001**, 2616 where g was kept fixed at 2.00 and Θ was taken as zero.
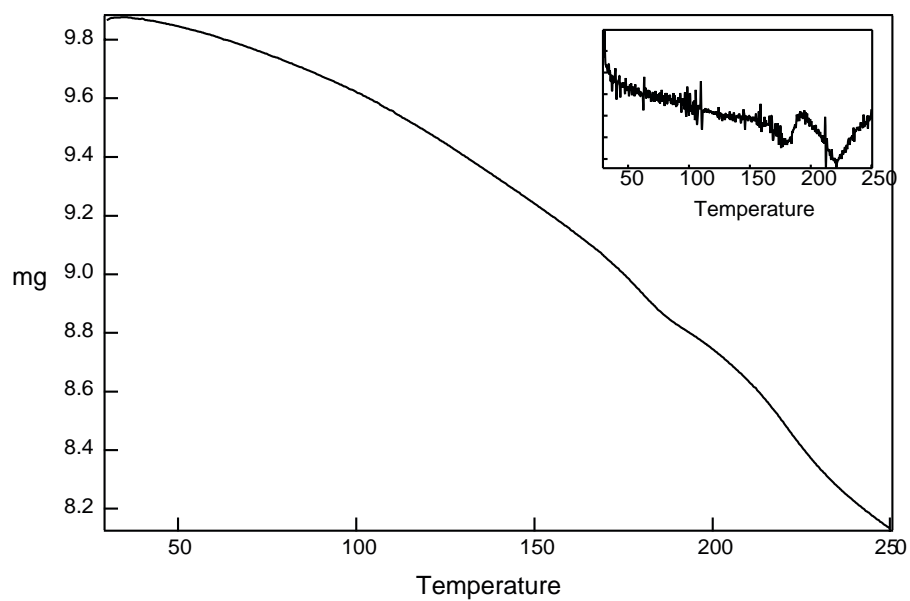
Figure S3. TGA plot of iodine doped **2** with derivative (DTA) plot of TGA as inset.

Rehydration of the dried crystals

Complex 2+ Water

35 -100 °C wt. loss 5.2 %
100 - 130 °C wt. loss 1.6%

Dried Complex 1a + Water

35 -90 °C wt. loss 4.3 %
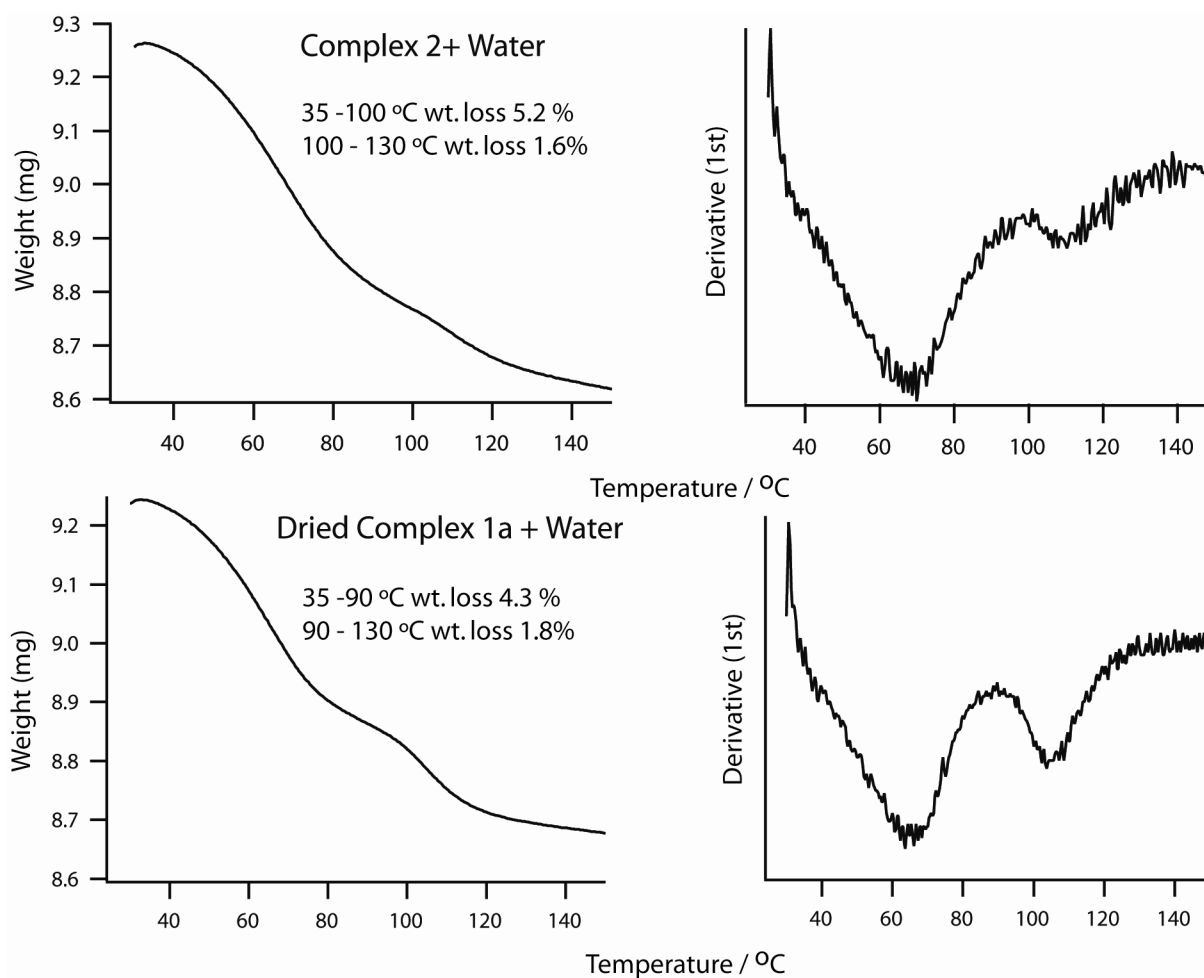90 - 130 °C wt. loss 1.8%

Temperature / °C

Figure S4. TGA (left) and DTA (right) plot of **2** and **1a** (dried at 90°C 2h) after exposure to water vapor for three days. Longer exposure to water does not have any effect on weight loss.

Figure S5 showing the 3H$_2$O waters (disordered in **1**) and 1H$_2$O in the channels of **1** and **1a** respectively. Table S1 have the bond parameters and occupancy used while solving the structure of **1**.
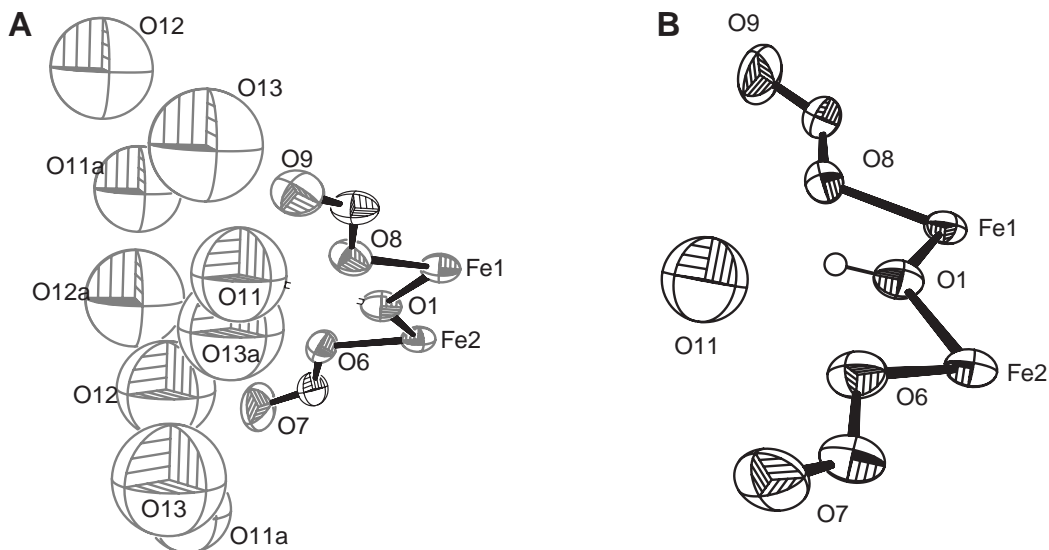

Figure S5. Water molecules in the channel of **1** (A) and **1a** (B).

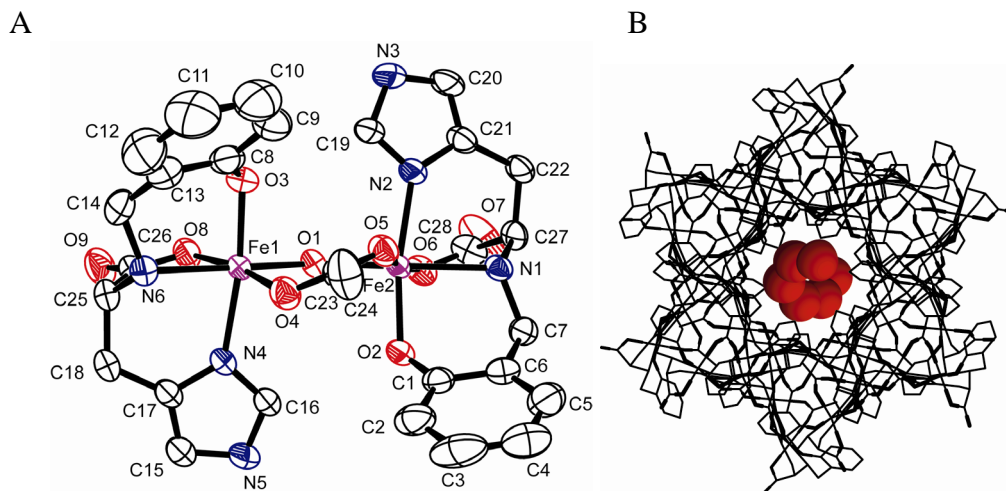|		*Table- S1*	
Atom	Occupancy		Distances (Å)
In **1**			
O11	0.6	O11-O11a	2.6002(0.0302)
O11a	0.4	O11-O12a	2.9682(0.0275)
O12	0.5	O11-O13	2.4368(0.0311)
O12a	0.5	O11a-O13a	3.1709(0.0366)
O13	0.6	O12a-O13a	2.7710(0.0400)
O13a	0.4	O1-O13a	2.7850(0.0479)
		O13-O13a	3.3874(0.0419)
		O11-O12	3.1002(0.0301)
In **1a**			
O11	1.0	O1-O11	2.790

Figure S6. (a) ORTEP diagram of the complex **1a** (b) left handed helix formed by **1a.**
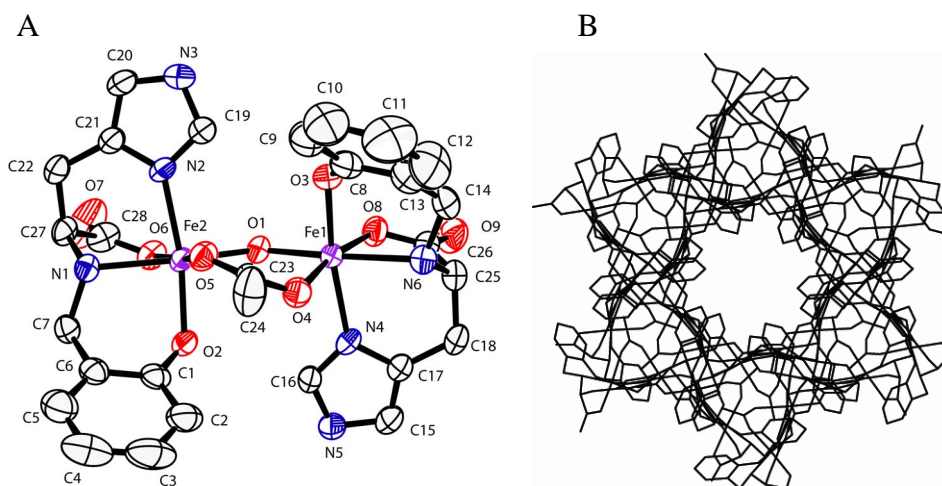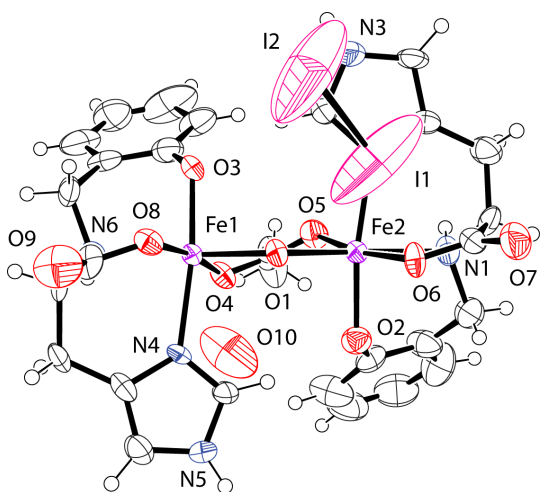

Figure S7. (a) ORTEP diagram of the complex **2** (b) Empty channel of **2.**
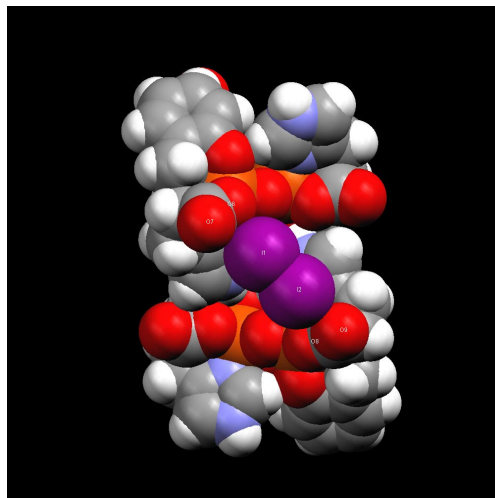
A

B

Figure S8. (a) ORTEP diagram of the complex **3** (b) Iodine molecules between two dimers in **3.**