Supporting Information for

Encapsulation of Ln^{3+} hydrate species for tunable luminescent materials based on a porous Cd(II)-MOF

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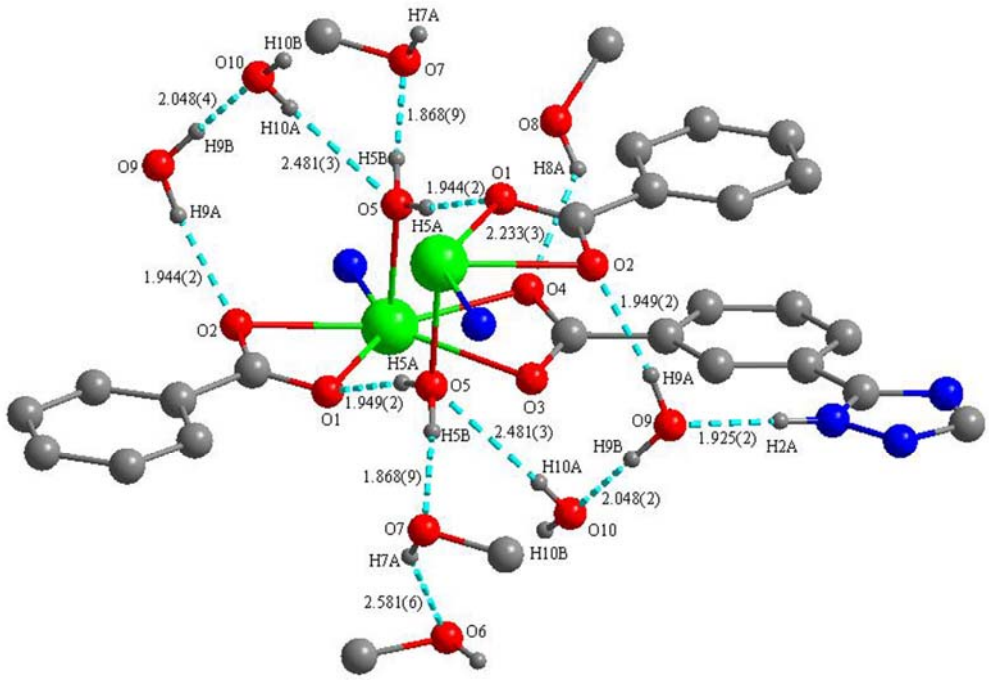

Fig. S1 The H_2O and MeOH guest molecules in **1** are hydrogen bonded to the framework through O-H···O, O-H···N and N-H···O bonds.

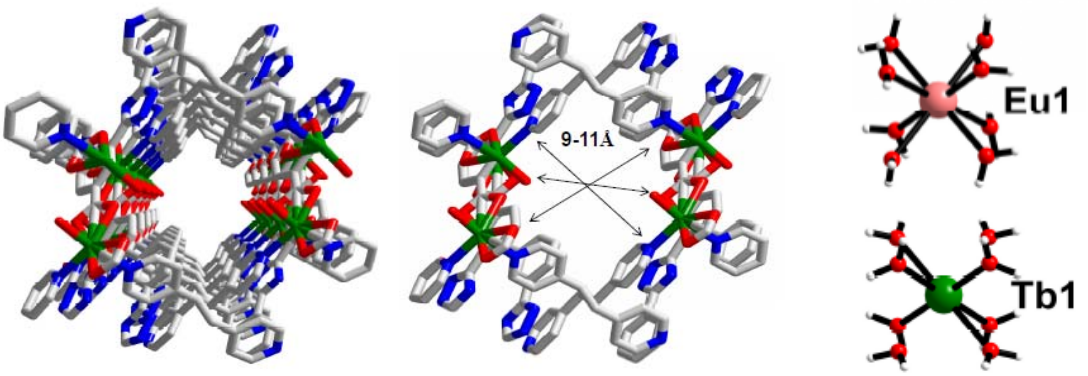

Fig. S2 Perspective and side views of a single channel in **1**. The cavities in **1** are embedded with heteroatoms such as N and O. The opposite O···O and N···N contacts in the channel are ca. 9-11 Å. Thus the cavity in **1** perfectly matches the lanthanide hydrate $Ln(H_2O)_8^{3+}$ and is able to bind it through O-H···E (E = O and N) hydrogen bonding interactions. The crystallographic size of $Ln(H_2O)_8^{3+}$ (Ln = Eu and Tb) is about 2.80 $Å^3$.[1]

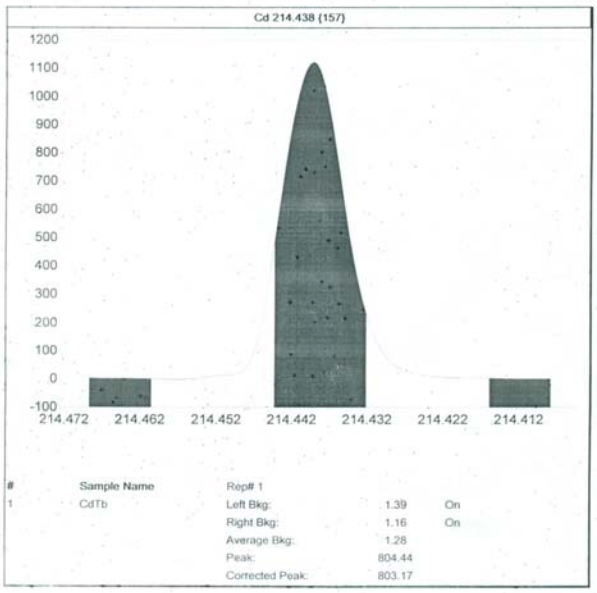

Fig. S3 The Cd^{2+} amount found in **1** is 18.00 % based on ICP measurement.

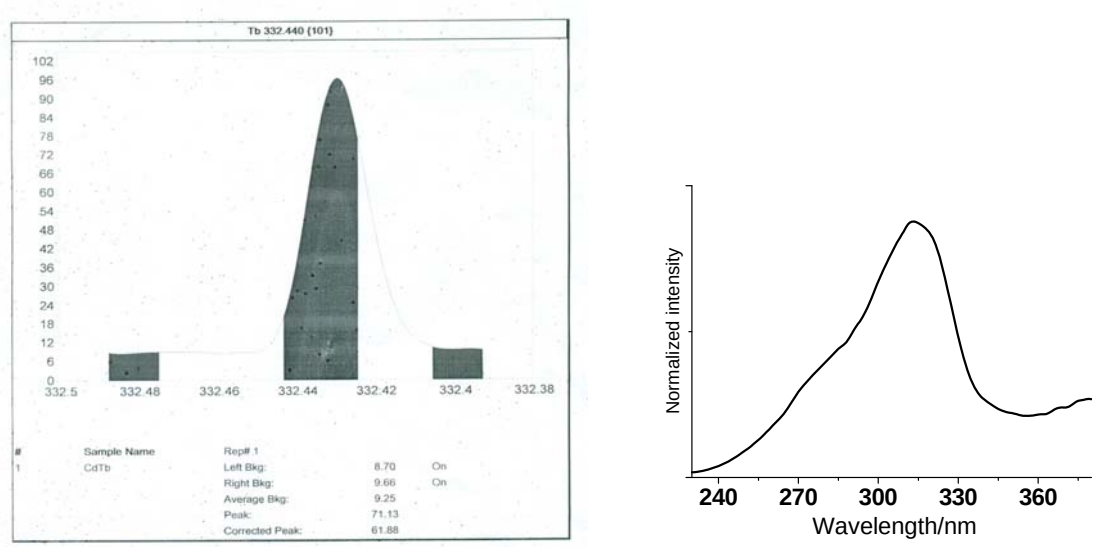

Fig. S4 Left: The encapsulated amount of Tb^{3+} in **1b** is up to 15.37 % based on ICP measurement. Right: Excitation spectrum of **1b**.

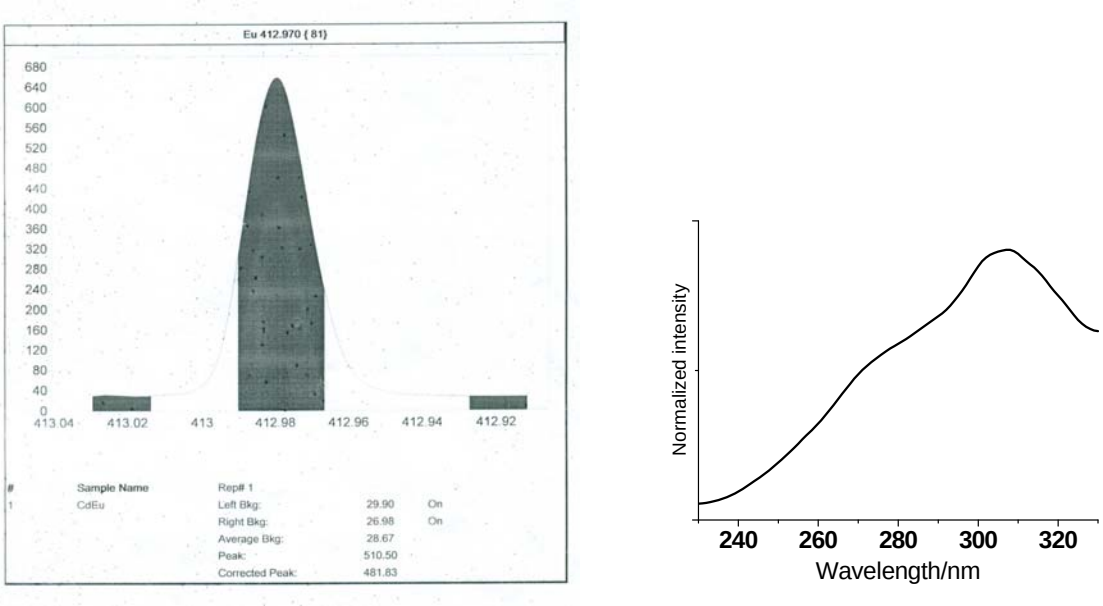

Fig. S5 Left: The encapsulated amount of Eu^{3+} in **1c** is up to 9.39 % based on ICP measurement. Right: Excitation spectrum of **1c**.

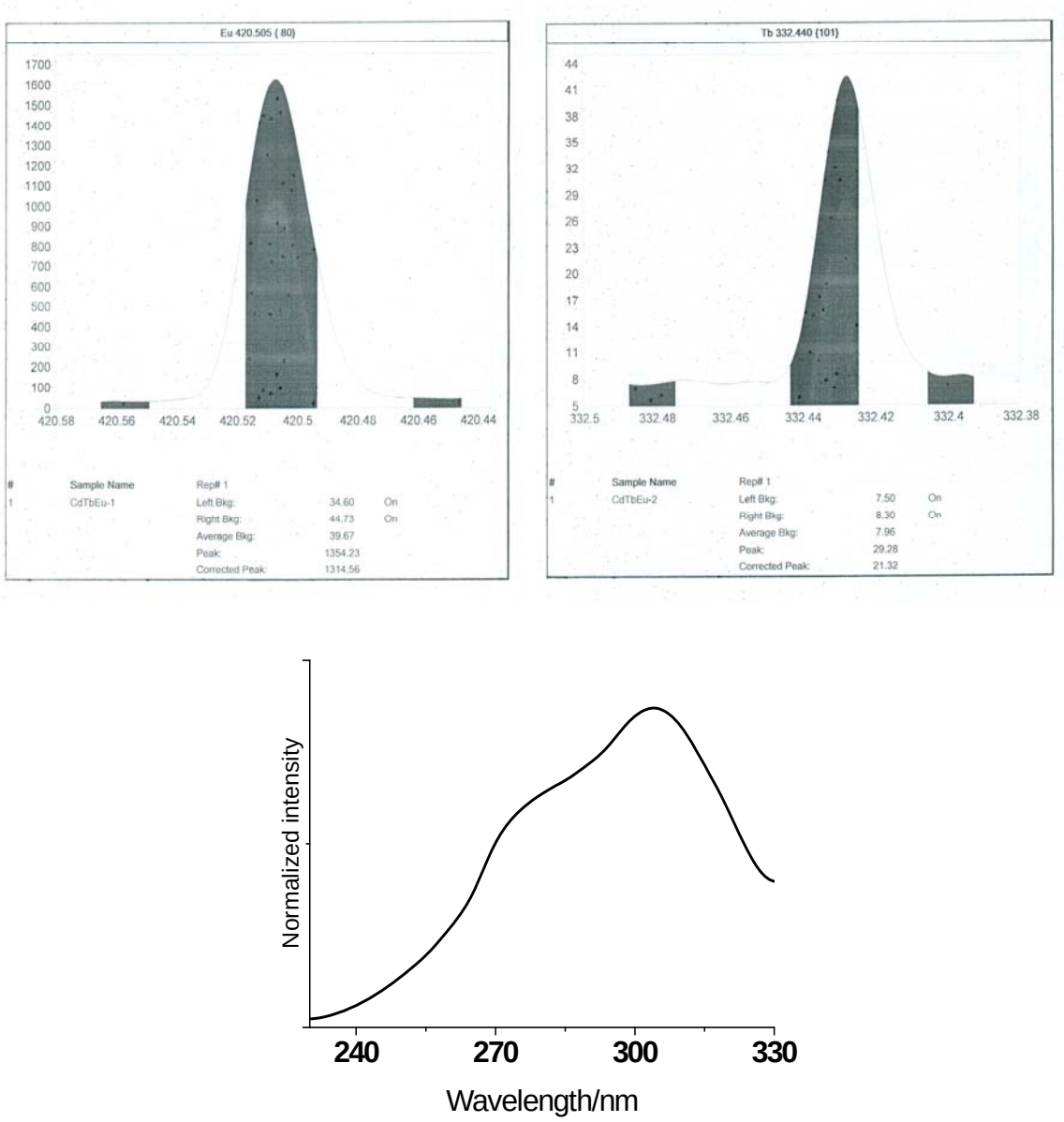

Fig. S6 Up: The encapsulated amounts of Eu^{3+} and Tb^{3+} in **1d** are 3.20 and 1.80 %, respectively, based on ICP mensurement. Bottom: Excitation spectrum of **1d**.

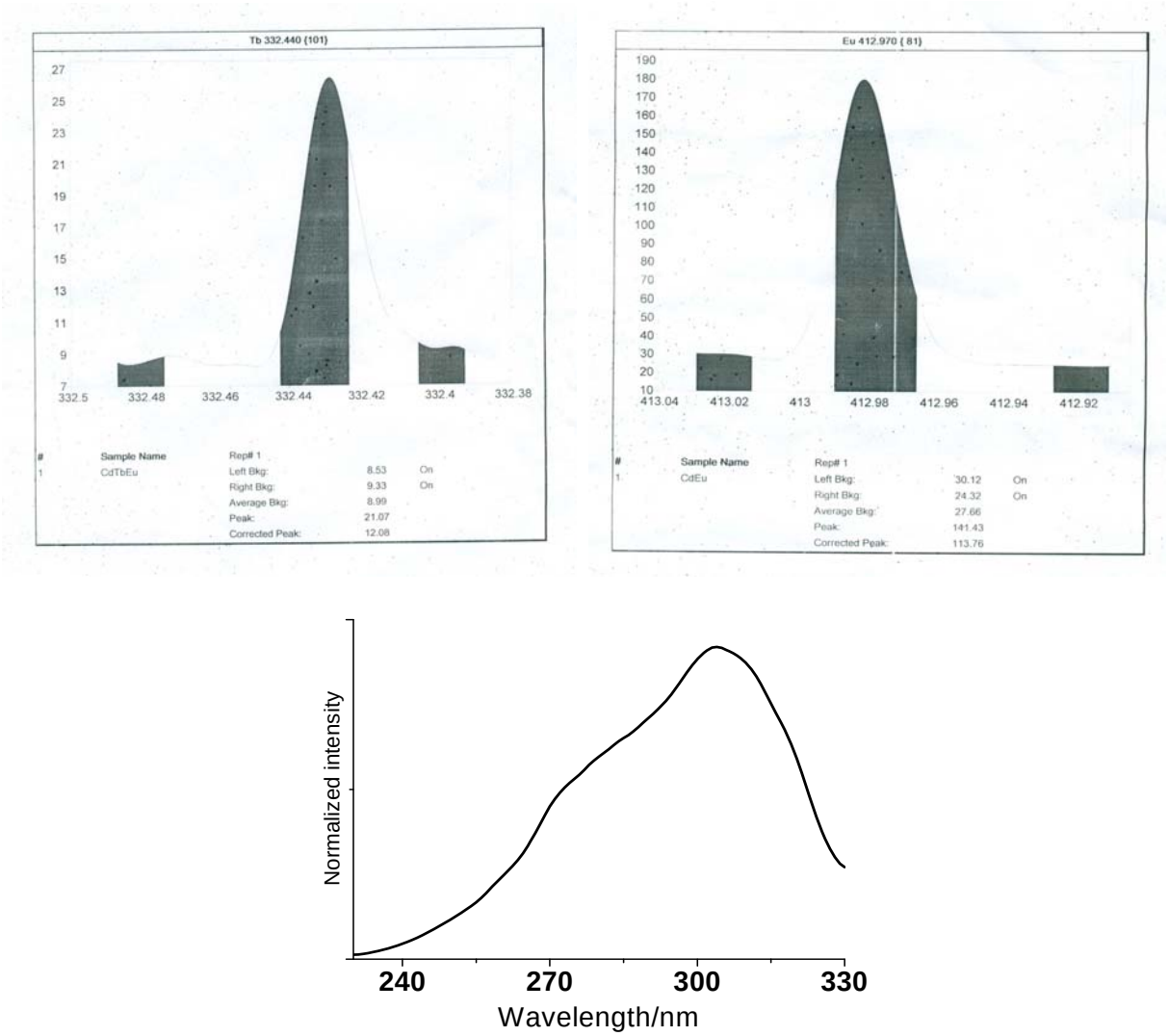

Fig. S7 Up: The encapsulated amounts of Tb^{3+} and Eu^{3+} in **1e** are 1.52 and 8.92 %, respectively, based on ICP measurement. Bottom: Excitation spectrum of **1e**.

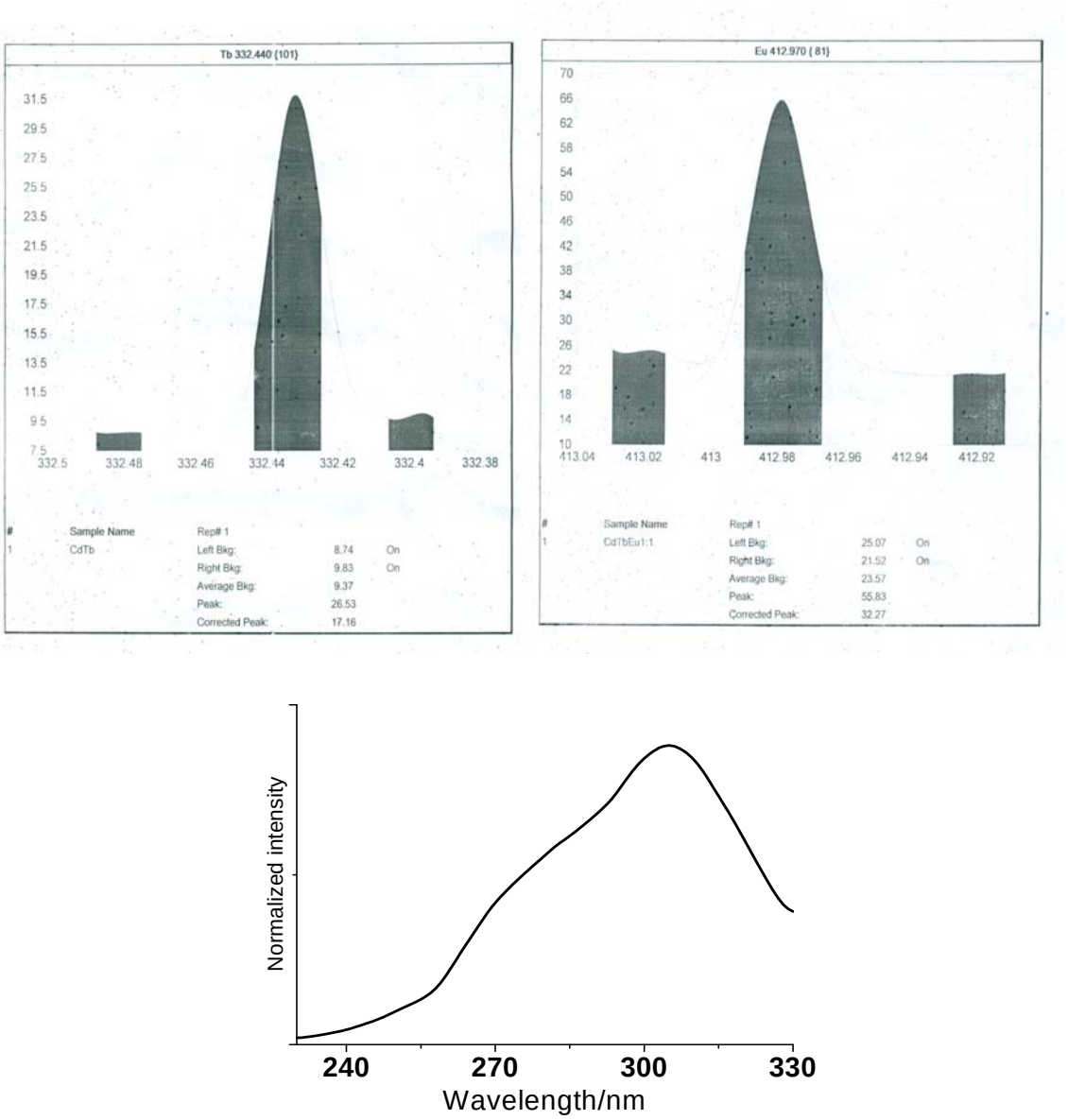

Fig. S8 Up: The encapsulated amounts of Tb^{3+} and Eu^{3+} in **1f** are 0.47 and 0.63 %, respectively, based on ICP measurement. Bottom: Excitation spectrum of **1f**.

References

1. (a) P. Wang, J.-P. Ma, Y.-B. Dong, R.-Q. Huang, *J. Am. Chem. Soc.,* 2007, **129**, 10620. (b) P. Wang, J.-P. Ma, Y.-B. Dong, *Chem. Eur. J.,* 2009, **15**, 10432.