Investigation on Structures, Luminescent and Magnetic Properties of Ln^{III}–M (M = Fe^{II}_{hs}, Co^{II}) Coordination Polymers

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Explanation to the alert level A in CheckCIF

CIF files associated with the manuscript were checked by the program of ICUR, and the results exhibited that CIF files appeared some similar alerts level A.

The alerts level A about the shorter inter O...O distances is related to the disordered lattice water molecules, and the isolate O atoms are lattice water molecules. **17** possess large 1D channel, therefore, an alert level A is related to this.

To explain other alerts level A, taken **1** as an example, the shorter inter X…Y contact was found in the **1**- CheckCIF. Actually, after these A-alerts were checked carefully, we will find that so called shorter inter X…Y contact should be wrongly determined by program. In **1**, only half a molecule of ligand (L^1) is crystallographically independent, as shown in following Figure S1 (left), and a complete L^1 molecule is displayed by proper symmetry operation, shown in Figure S1 (right). As a result, the distances among different atoms intra a molecule of L^1, displaying in Figure 1(right), especially among six atoms from pyridine ring, were wrongly defined as A-alerts. The shorter inter H…H contact (such as **16**) is also related to a complete coordinated water molecule by symmetry operation.

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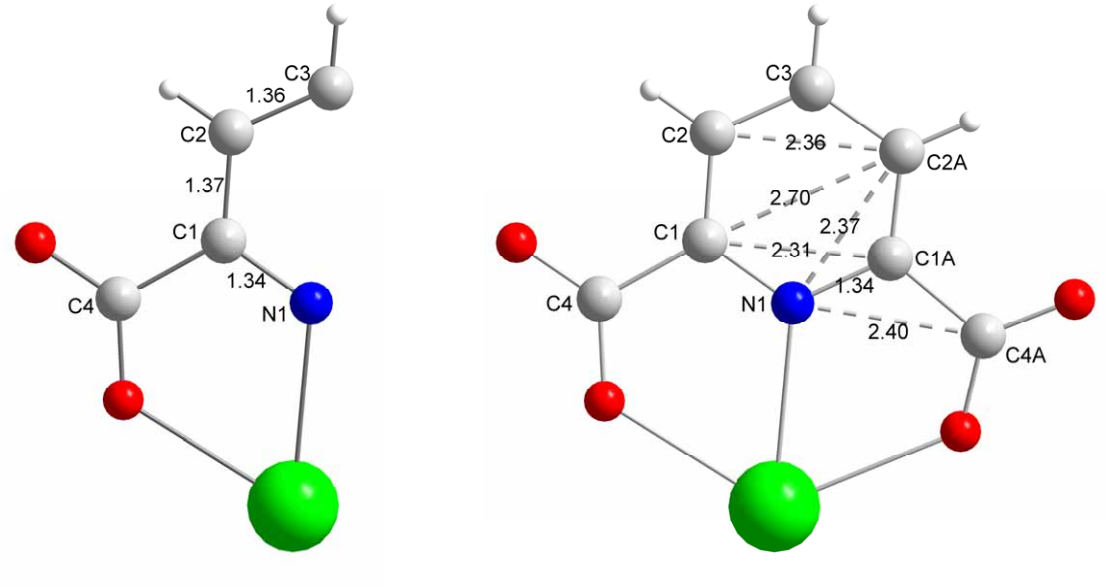


Figure S1. Half a L^1 molecule (left) and a complete L^1 molecule by symmetry operation (–y+1, –x+1, –z+1/2) (right).

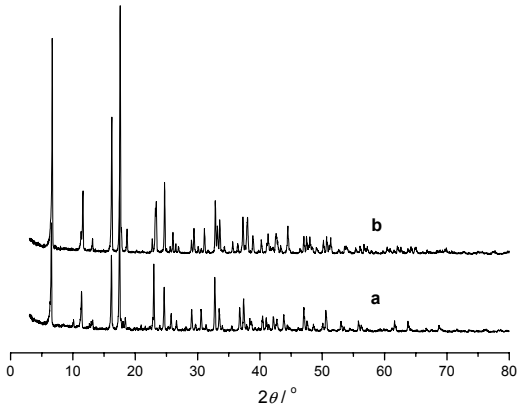
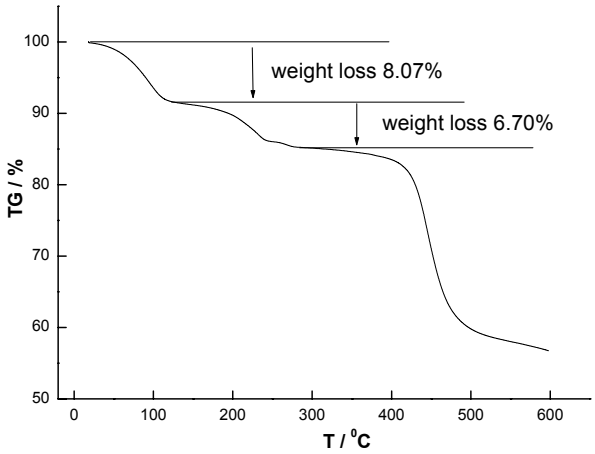


Figure S2. PXRD patterns of compounds **2** (**a**) and **7** (**b**).



Figuer S3. TGA curve for **7**.

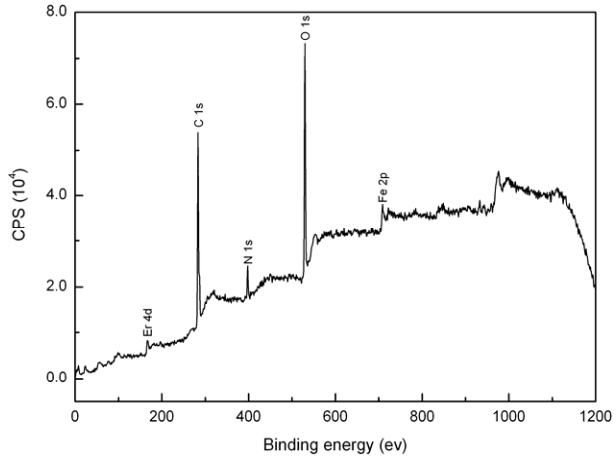


Figure S4. XPS for **9** at room temperature.

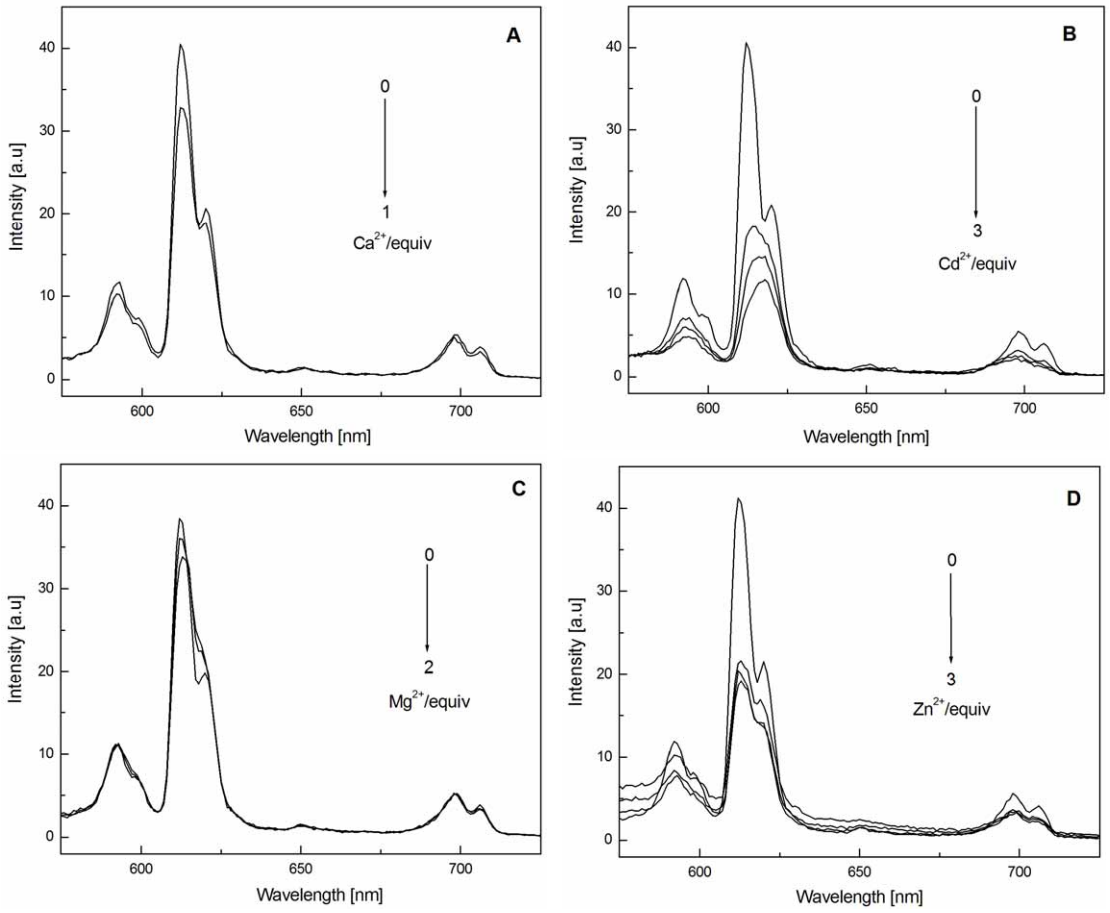


Figure S5. Emission spectra of **13** in DMF (10^{-4} M) at room temperature (excited at 280nm) in the presence of ~0-1 equivalents Ca^{2+} (**A**), 0-2 equivalents Mg^{2+} (**C**), 0-3 equivalents Cd^{2+} (**B**), Zn^{2+} (**D**) with respect to **13**.

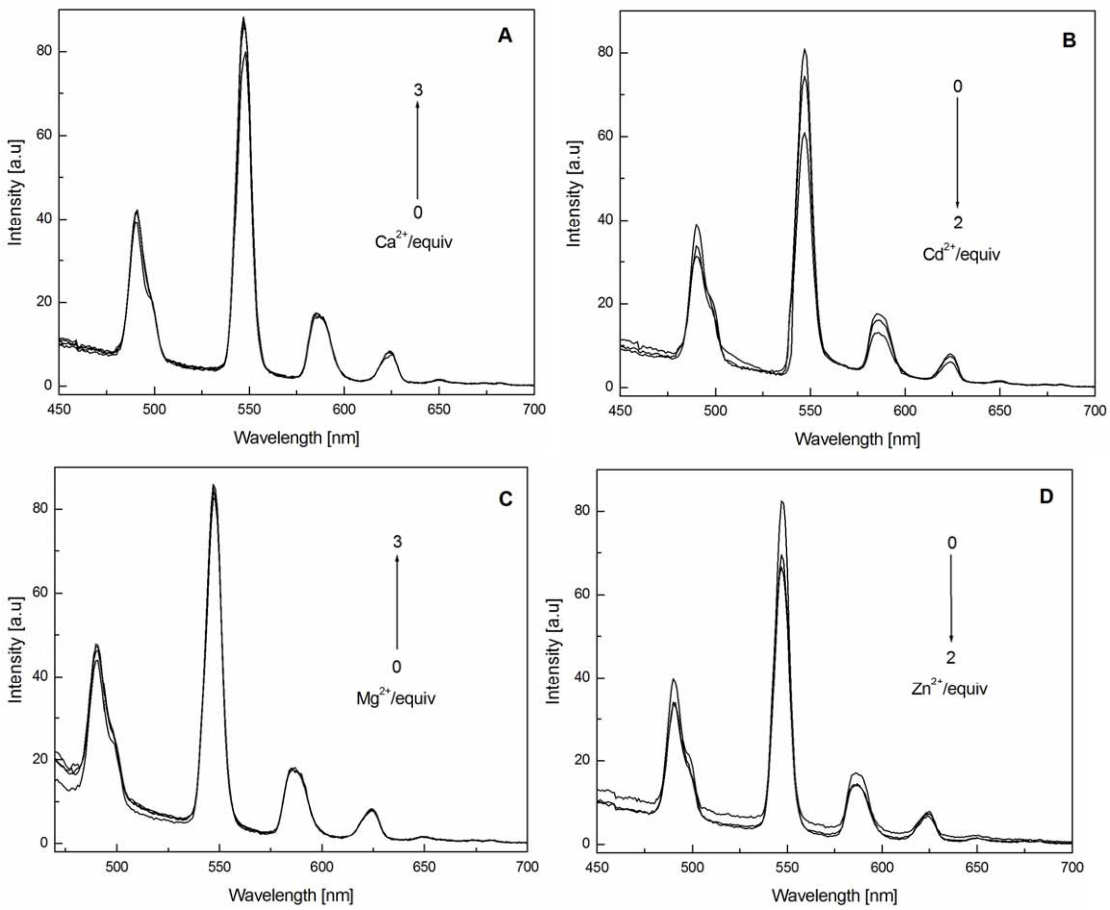


Figure S6. Emission spectra of **15** in DMF (10^{-4} M) at room temperature (excited at 280 nm) in the presence of ~0-3 equivalents Ca^{2+} (**A**), Mg^{2+} (**C**) and 0-2 equivalents Cd^{2+} (**B**), Zn^{2+}(**D**) with respect to **15**.

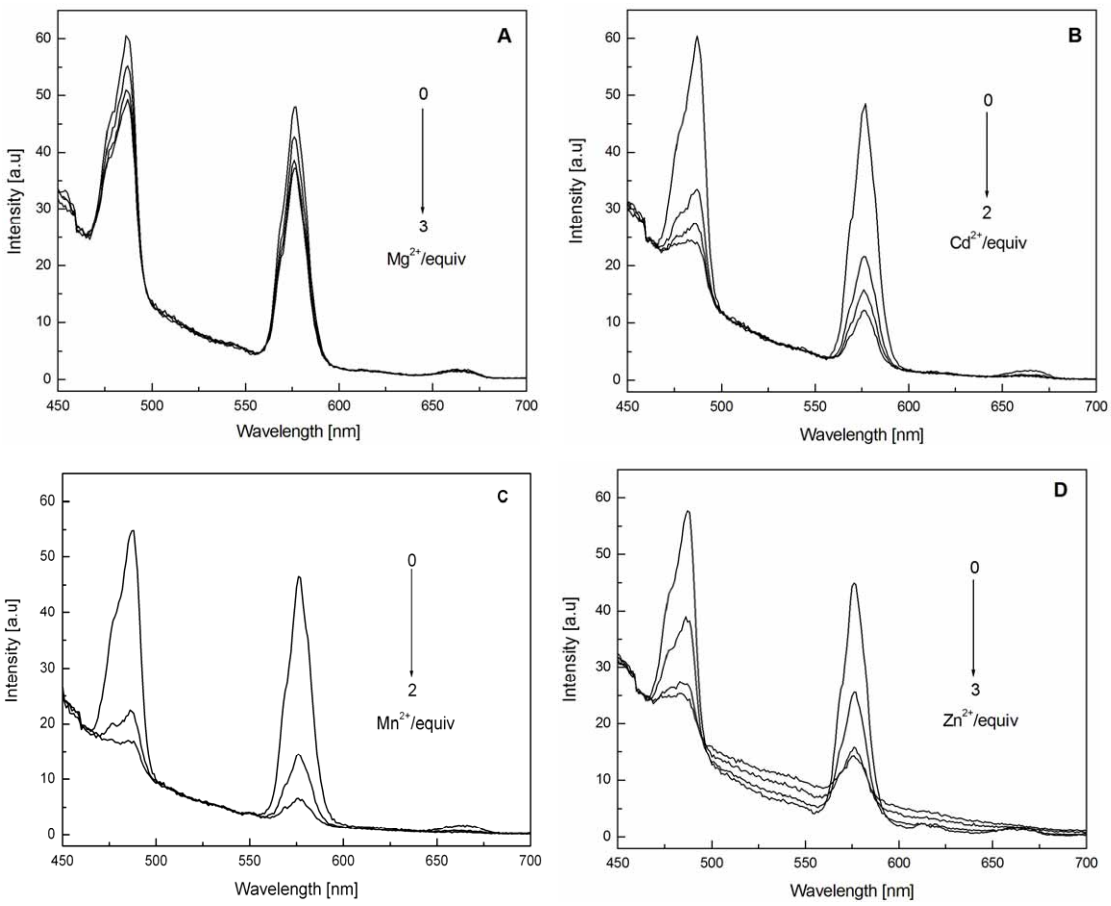


Figure S7. Emission spectra of **16** in DMF (10^{-4} M) at room temperature (excited at 280 nm) in the presence of ~0-3 equivalents Mg^{2+} (**A**), Zn^{2+} (**D**) and 0-2 equivalents Cd^{2+} (**B**), Mn^{2+} (**C**) with respect to **16**.