inorganics

Supplementary Materials: Synthesis and Physical Properties of Tetrathiafulvalene-8-Quinolinato Zinc(II) and Nickel(II) Complexes

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(1) Emission spectra of the 10^{-6} M $CHCl_3$ solution of complexes **1**, **2**, Znq_2 and Niq_2.

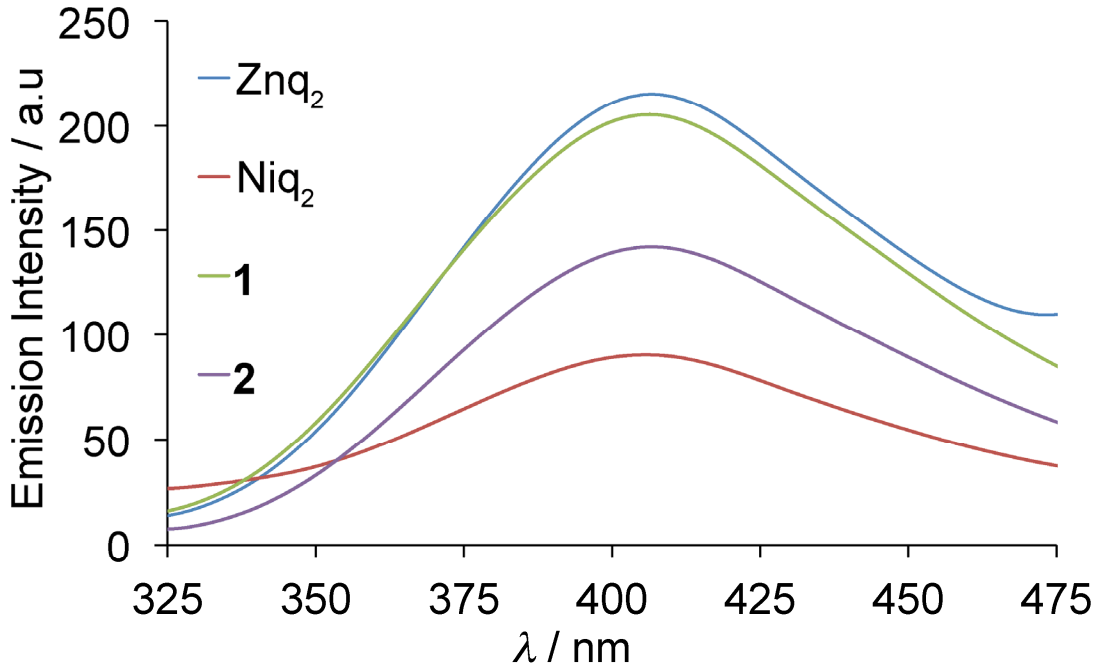


Figure S1. Emission spectra of the 10^{-6} M $CHCl_3$ solution of complexes **1** and **2**, Znq_2 and Niq_2 measured at room temperature under the identical conditions using an excitation light of 268 nm.

(2) Molecular orbital calculation of complexes **1** and **2** on the basis of the DFT and TD-DFT theory at the B3LYP level using the LANL2DZ basis set for the central zinc and nickel atoms and the 6-31G(d, p) basis set for the other atoms.

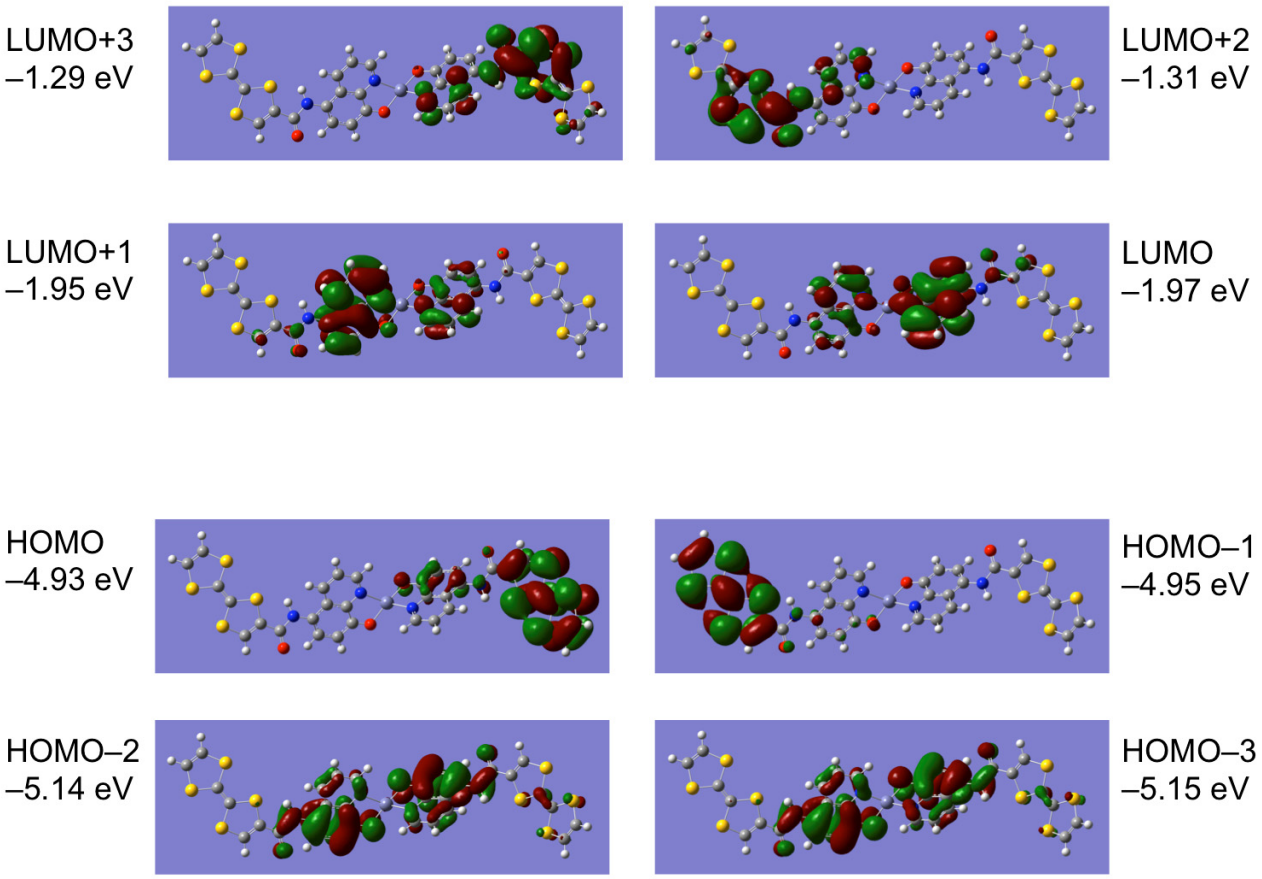


Figure S2. Molecular orbitals and energy levels of Zn complex **1**.

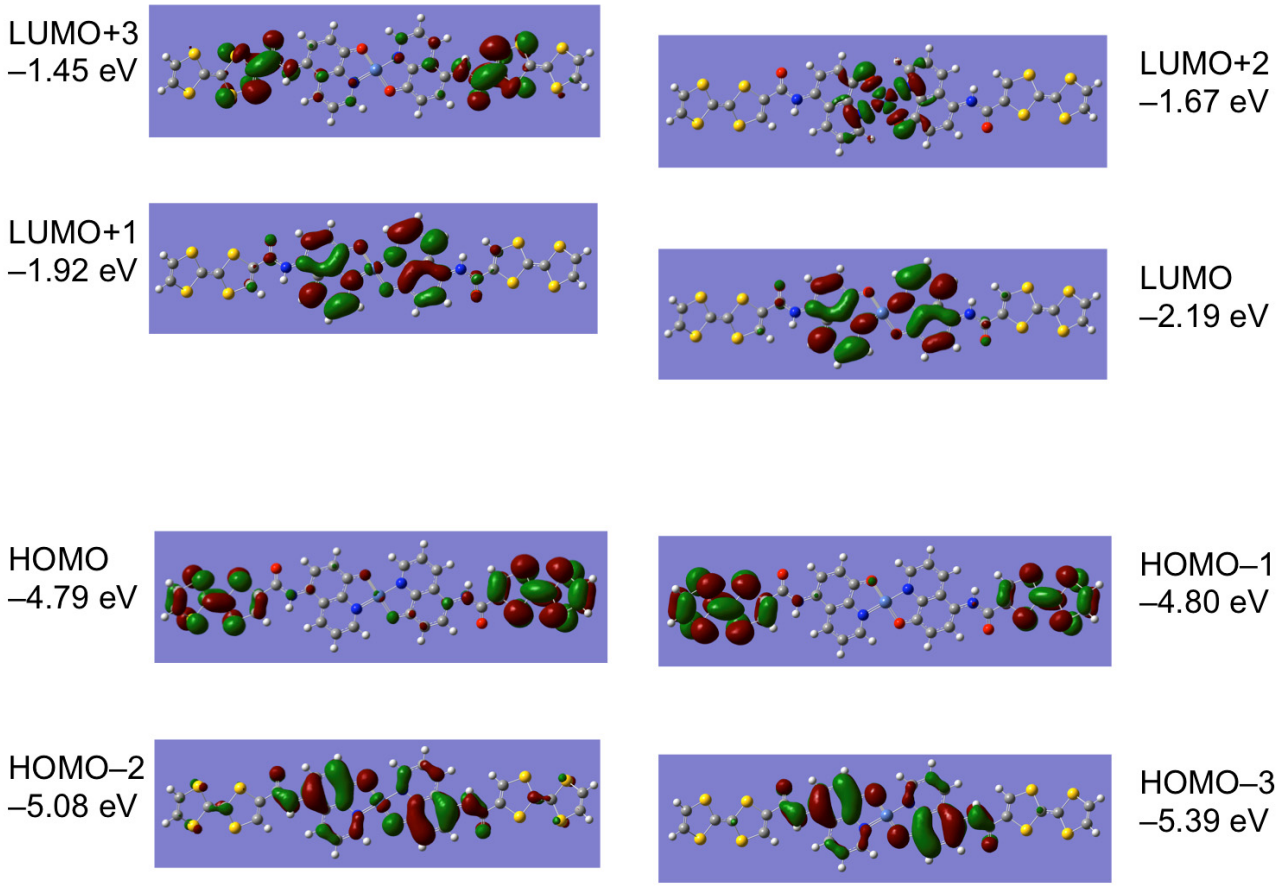
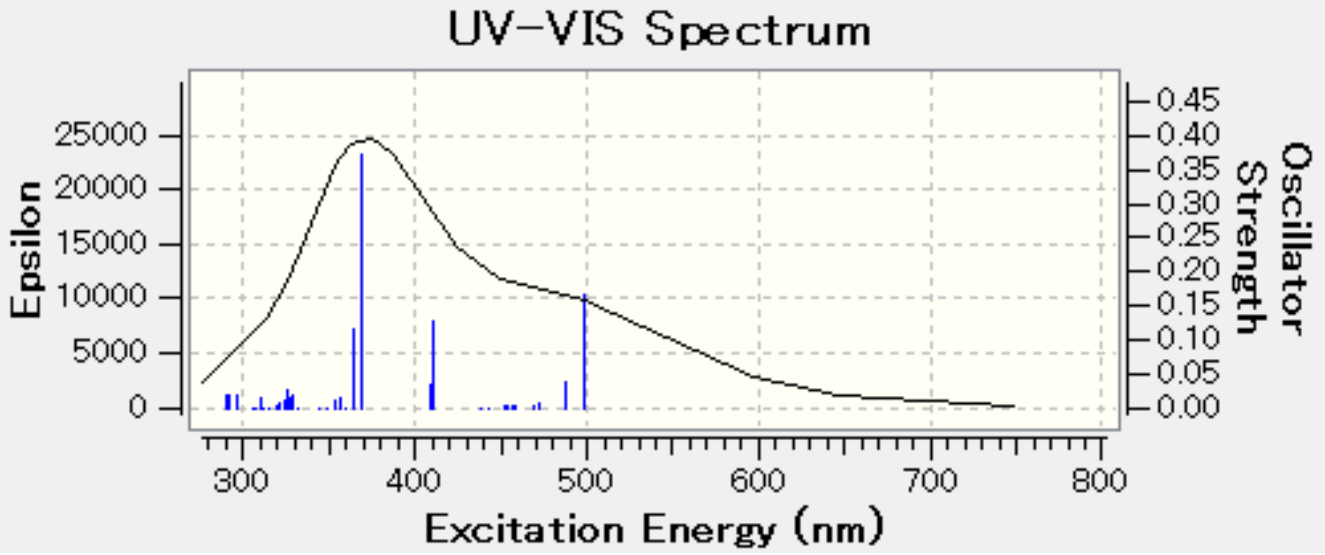


Figure S3. Molecular orbitals and energy levels of Ni complex **2**.

(a) Zn complex **1**.



(b) Ni complex **2**.

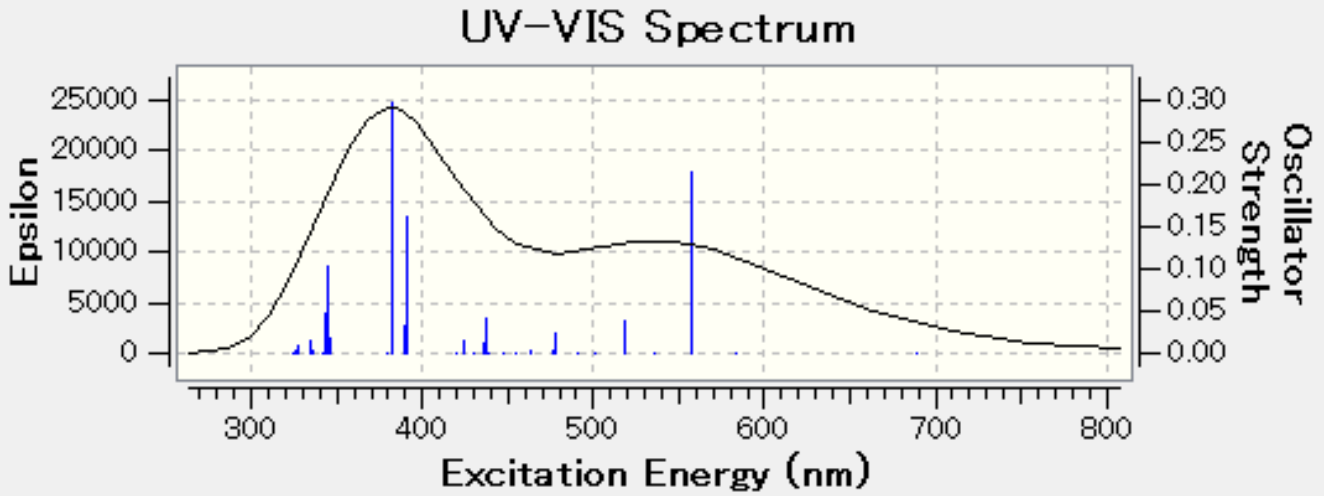
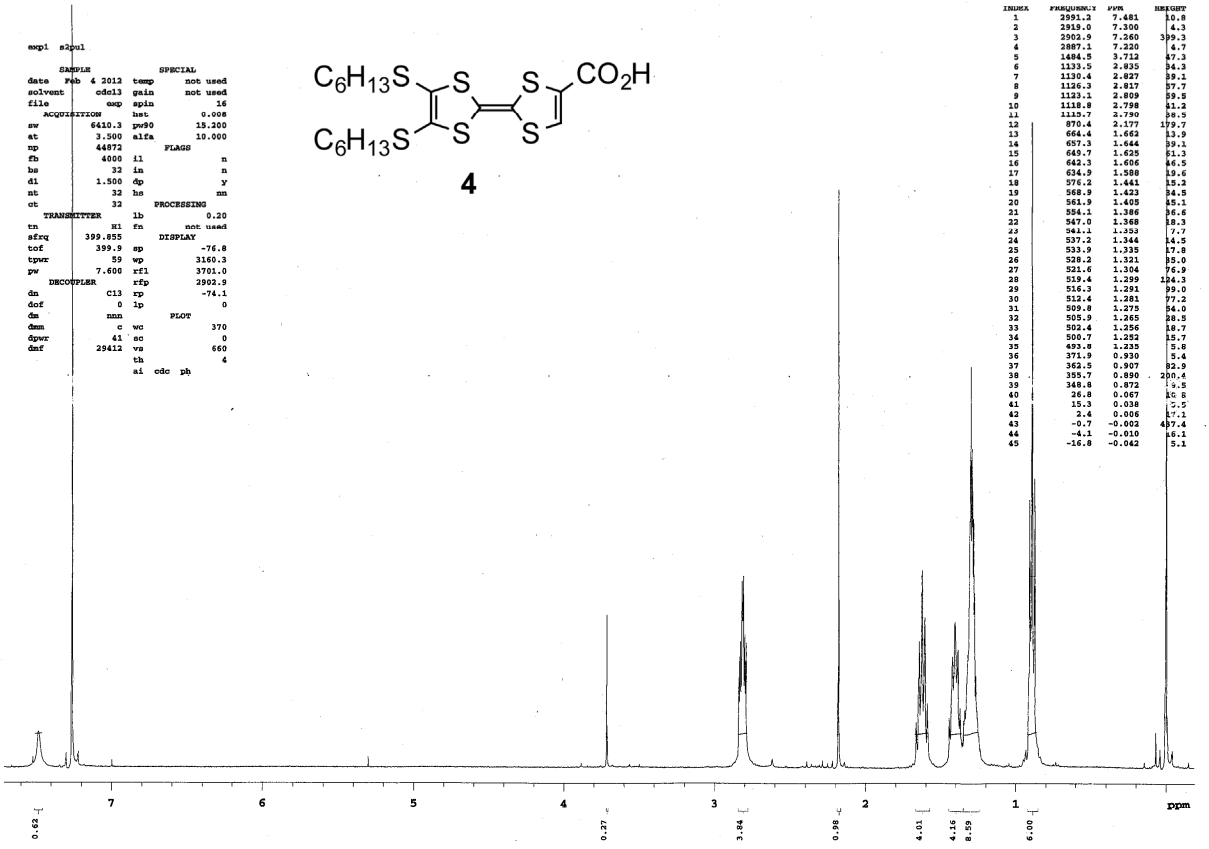
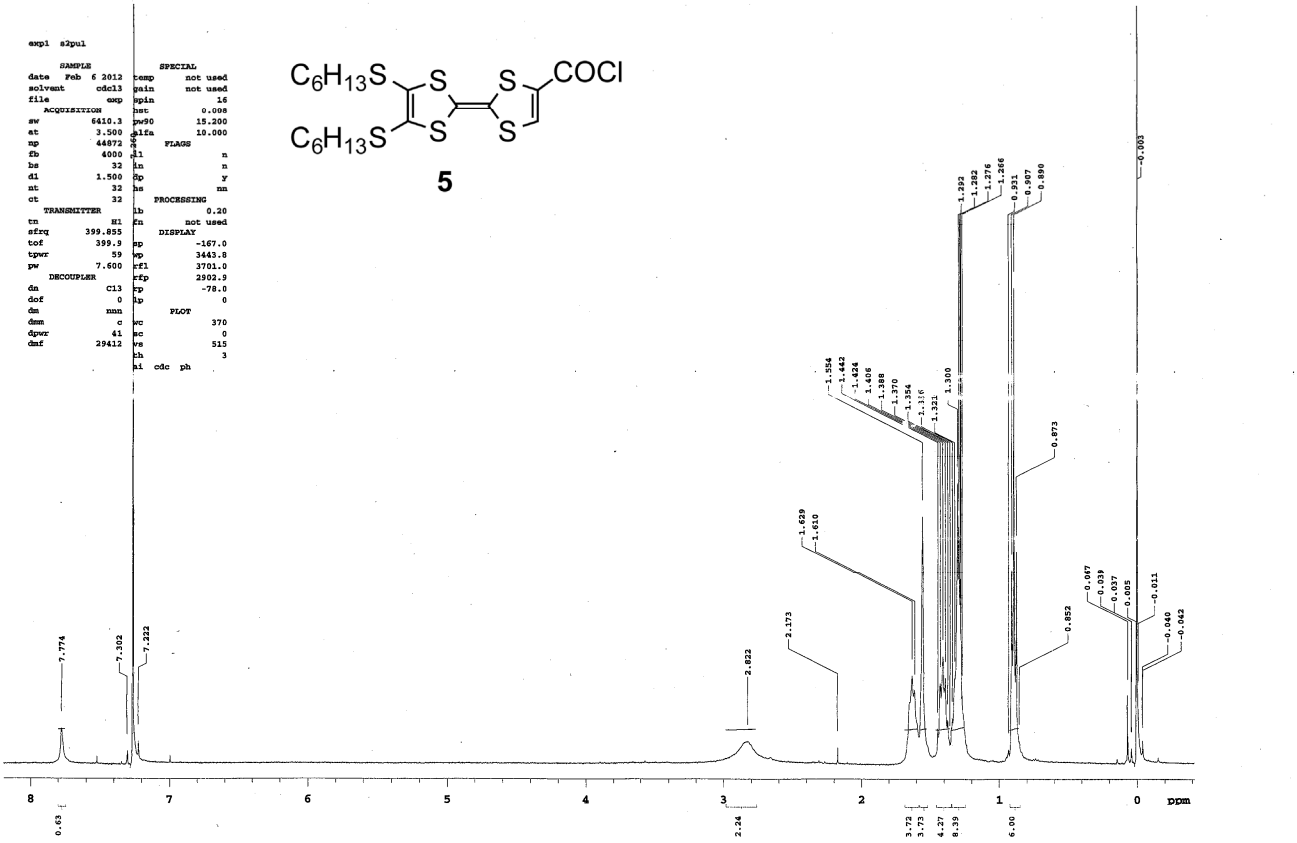


Figure S4. UV-Vis simulated spectra of **1** and **2** calculated on the basis of a TD-DFT method.

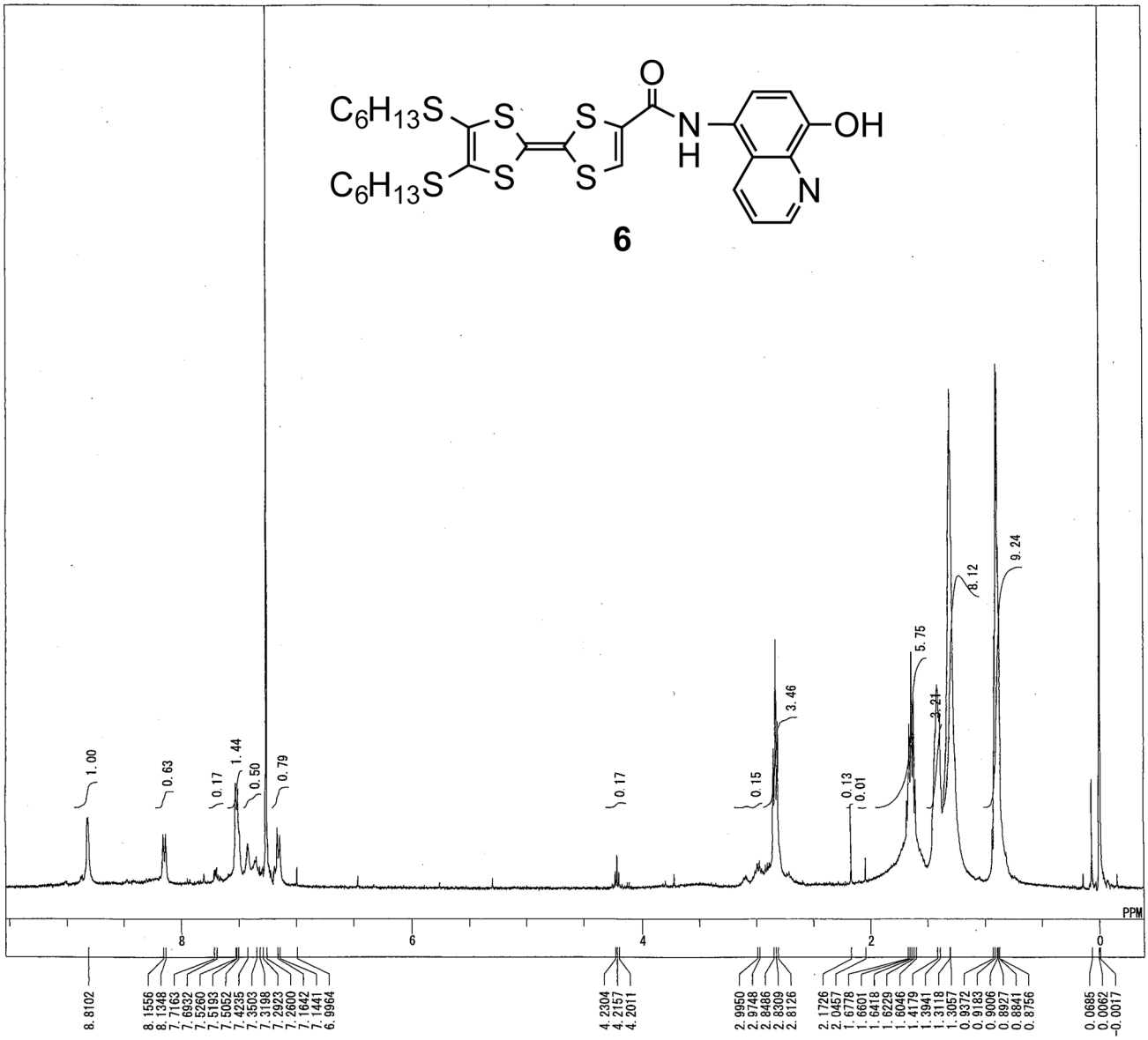
(3) NMR charts of compounds **4**, **5**, **6** and Zn complex **1**.
NMR chart of **4** (400 MHz, $CDCl_3$)



NMR chart of **5** (400 MHz, $CDCl_3$)



NMR chart of **6** (400 MHz, $CDCl_3$)



NMR chart of Zn complex **1** (400 MHz, DMSO-d$_6$)