Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information of

Self-association and Columnar Liquid Crystalline Phase of Cationic Alkyl-substituted-Bipyridine Benzenedithiolato Gold(III) Complexes

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Contents

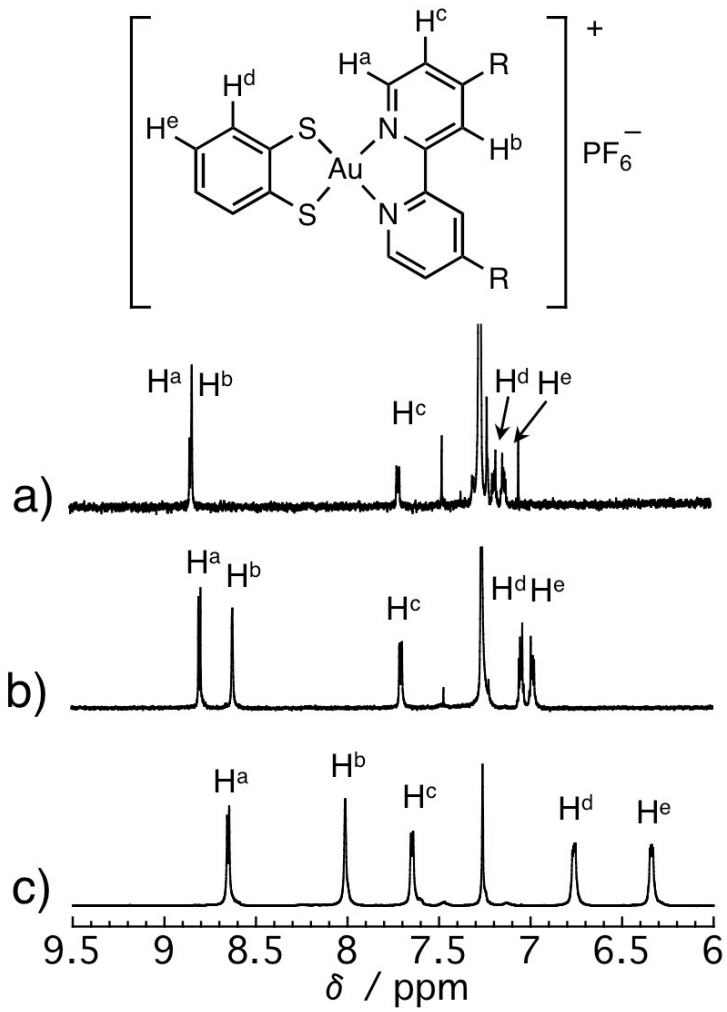

Figure S1. Concentration dependent ^{1}H NMR spectra of **3** in chloroform-*d* at a) 1.16 × 10^{-4}, b) 0.96 × 10^{-3} and c) 0.99 × 10^{-2} M.

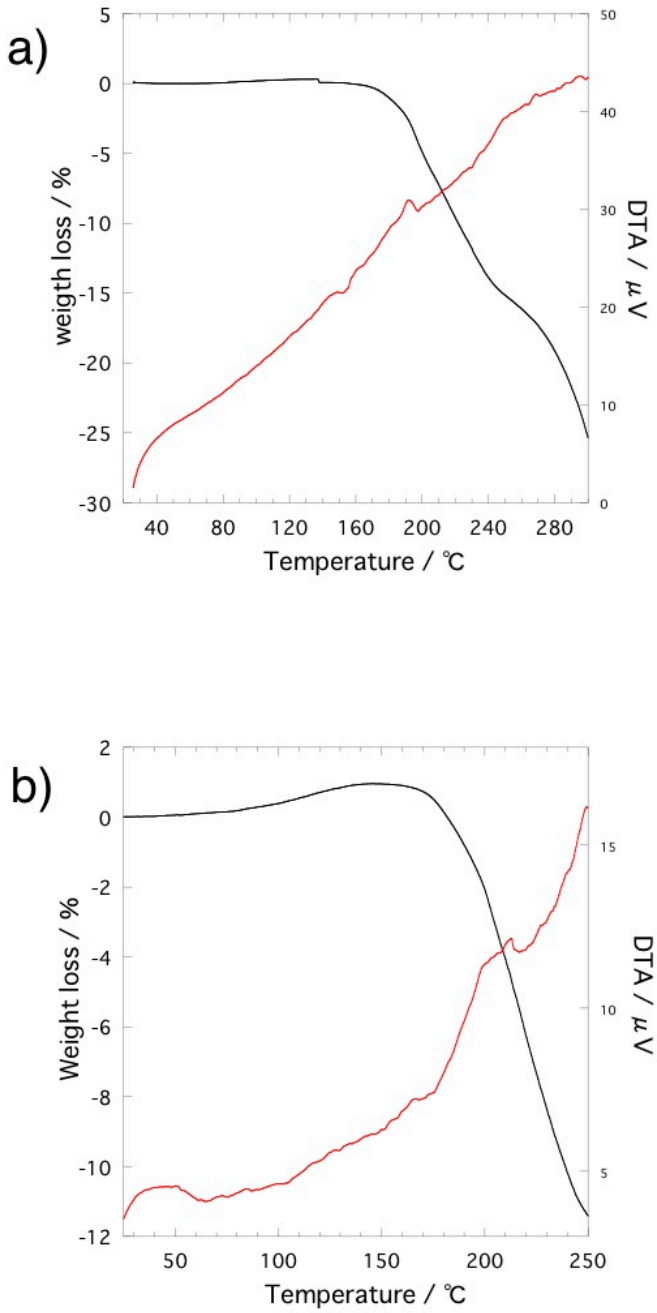

Figure S2. Thermogravimetry-differential thermal analyses of a) **3** and b) **4** at scan rate of 5 K/min (TG (–) and DTA (–)).

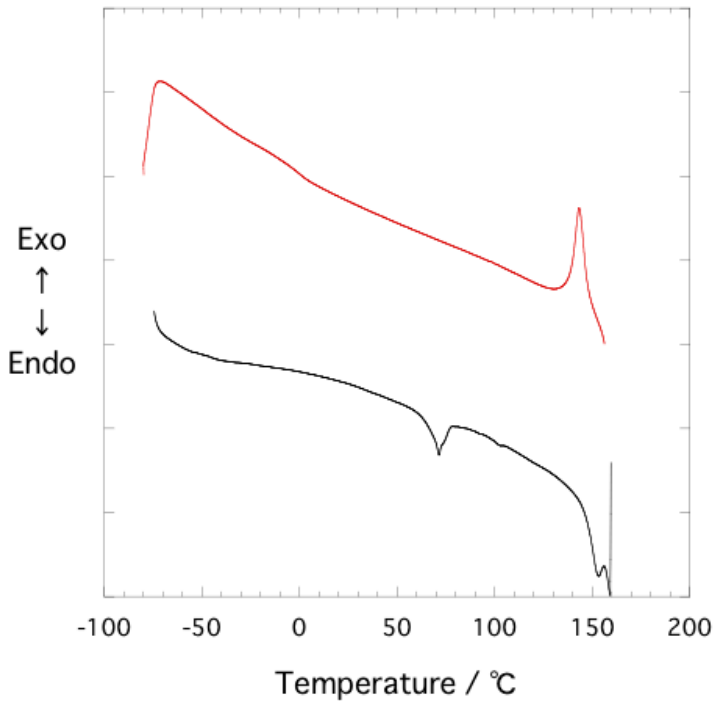

Figure S3. DSC curves of **3** at a scan rate of 5 K/min (first heating scan (–) and second cooling scan (–)).

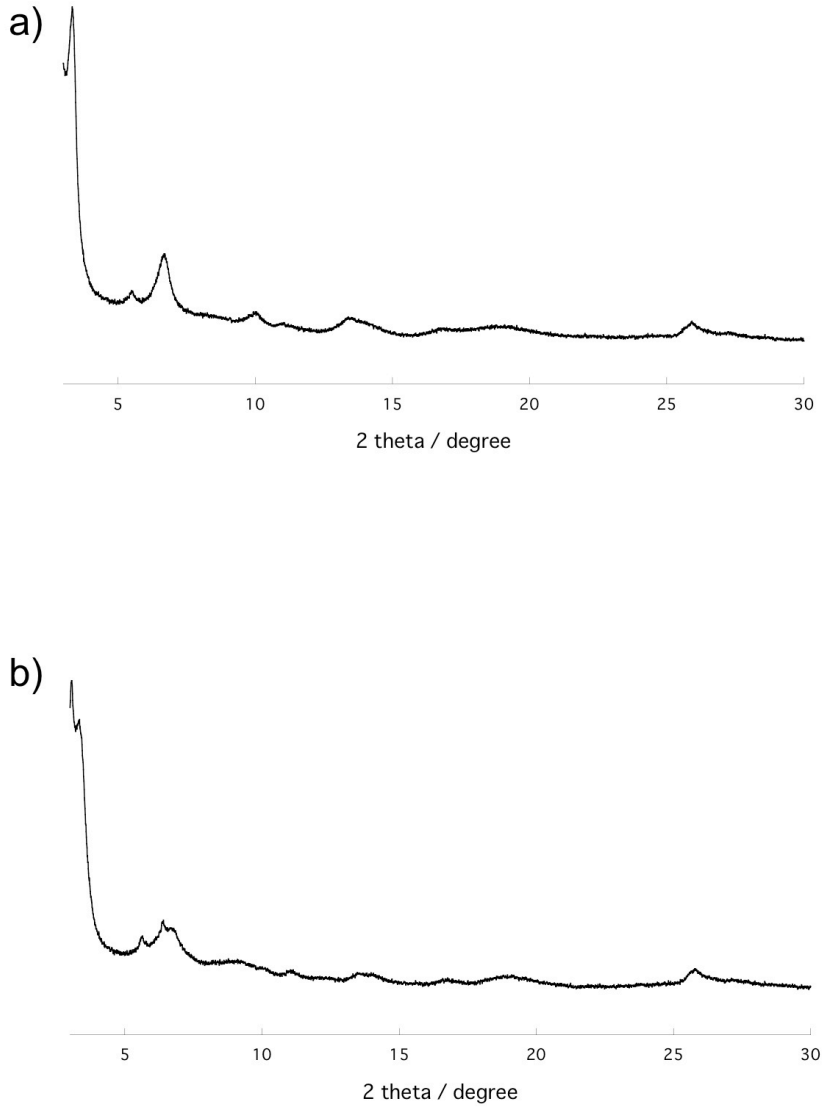

Figure S4. Variable temperature X-ray diffraction patterns of **3** at a) 40 and b) 120 ˚C. Each reflection becomes broad because the complex easily loses its crystallinity. However, the XRD patterns at two temperatures clearly different each other, indicating a crystal-to-crystal phase transition.

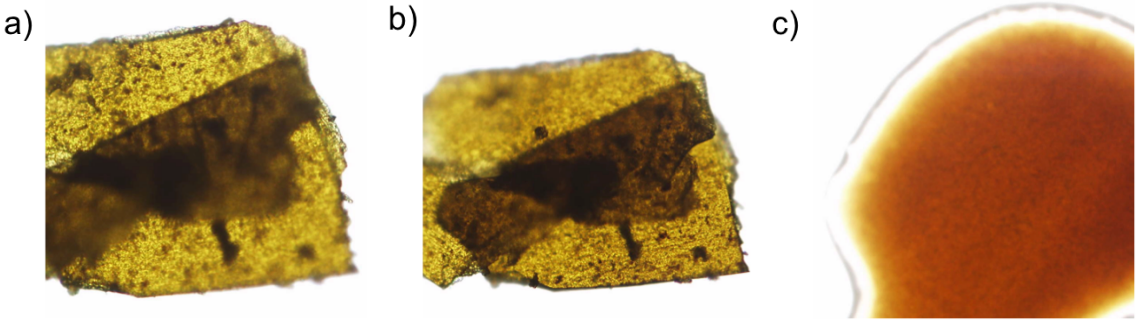

Figure S5. POM images of **3** at a) 25 (Cr1), b) 120 (Cr2) and c) 160 ˚C (Iso).

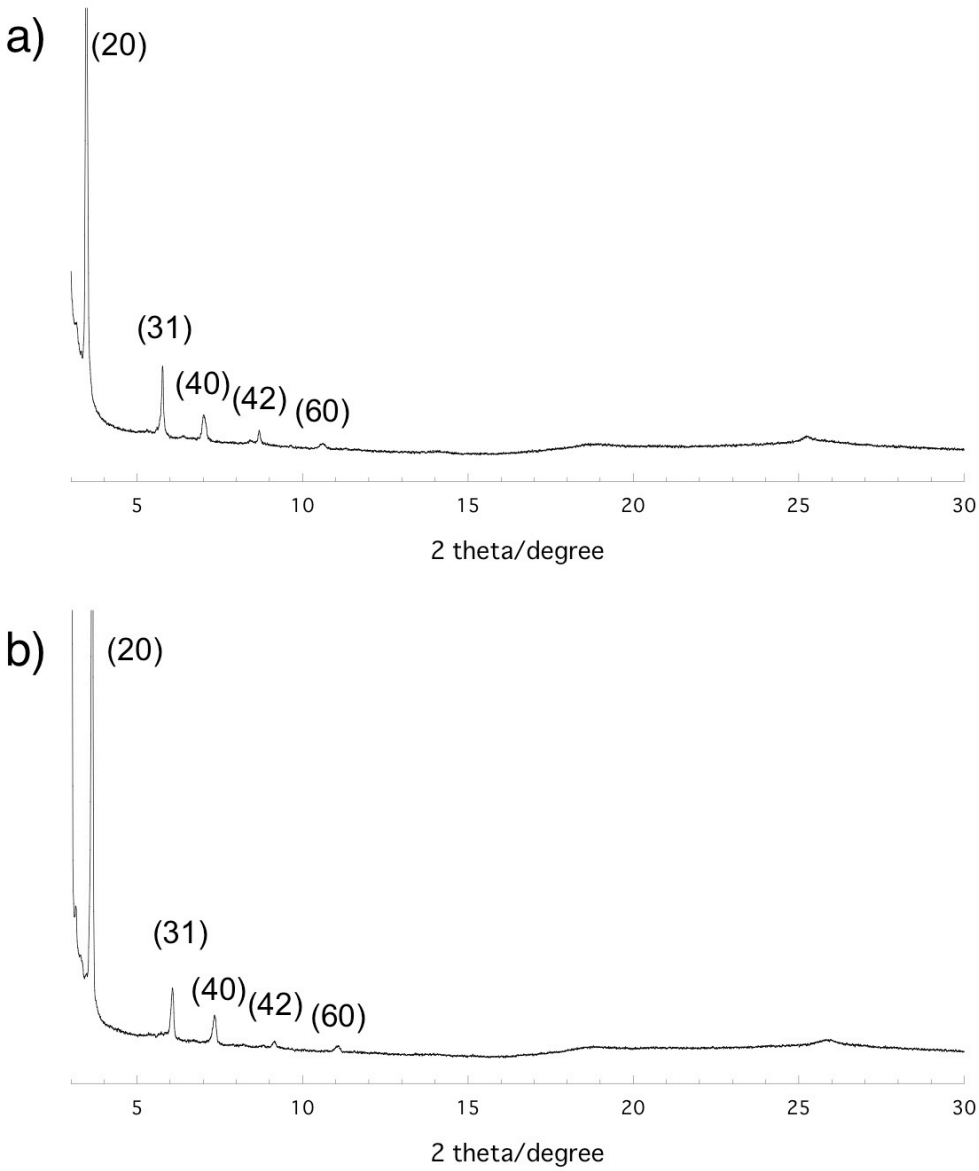

Figure S6. Variable temperature X-ray diffraction patterns of **4** at a) 25 and b) –80 ˚C. The sample was held at 60 ˚C for four days during the first cooling scan at a scan rate of 5 K/min.

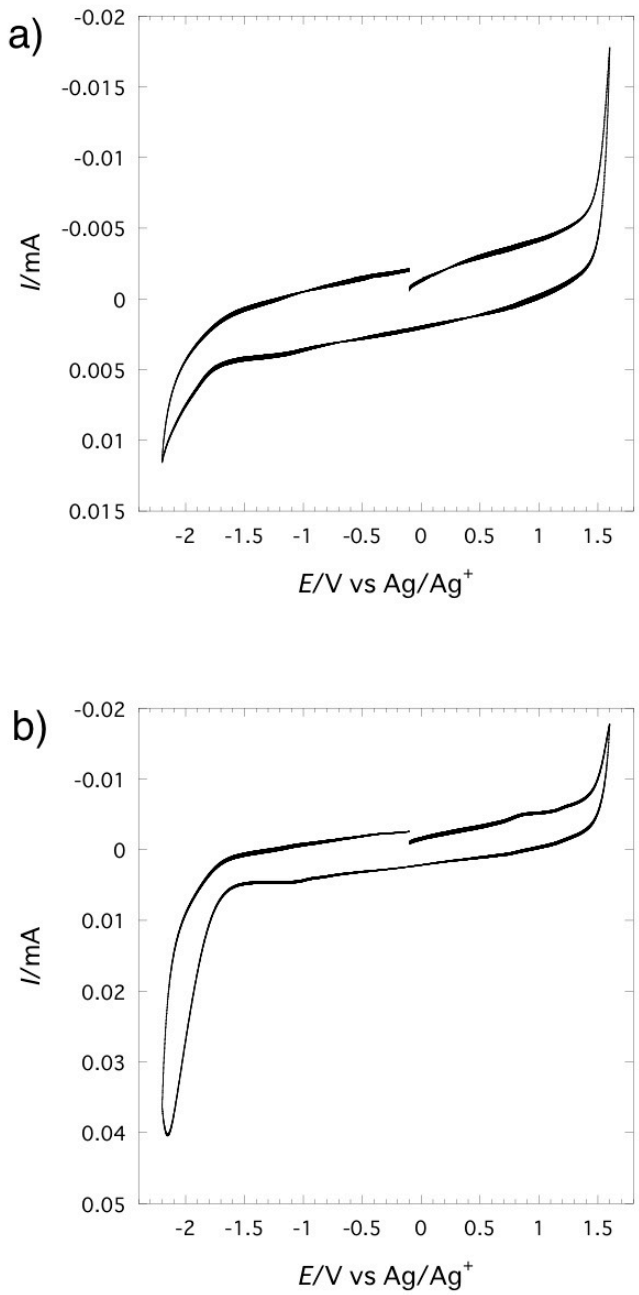

Figure S7. Cyclic voltammograms of a) C13bpy and b) C8,10bpy in CH_2Cl_2 (0.1 M *n*-Bu_4NPF_6, N_2, 100 mV/s).

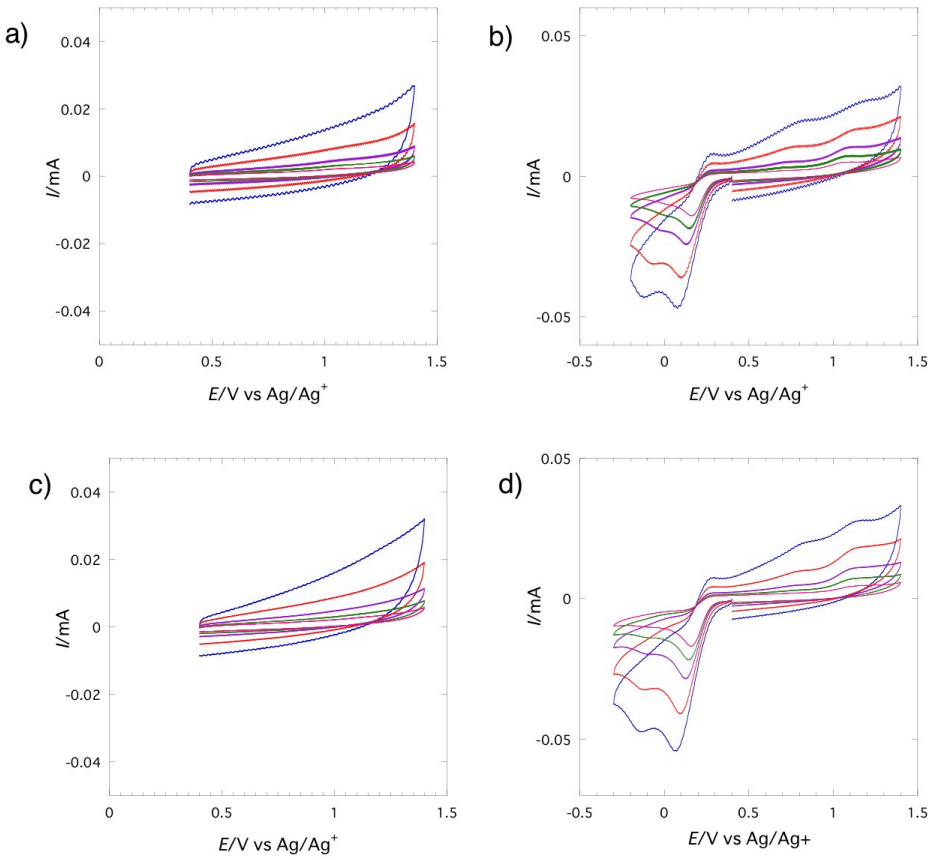

Figure S8. Scan rate dependency of cyclic voltammograms of **1** in a) positive scan and b) negative scan and **2** in c) positive scan and d) negative scan in CH_2Cl_2 (1000 (–), 500 (–), 200 (–), 100 (–) and 50 mV/s (–), 0.1 M *n*-Bu_4NPF_6, N_2).

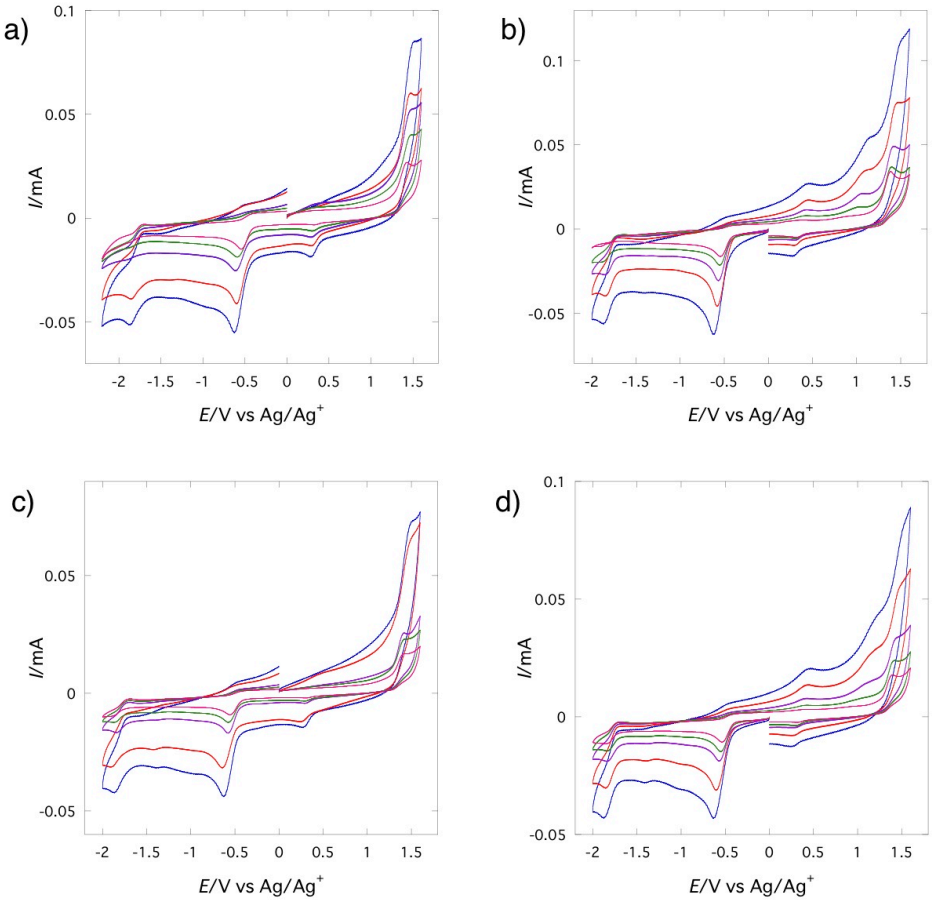

Figure S9. Scan rate dependency of cyclic voltammograms of **3** in a) positive scan and b) negative scan and **4** in c) positive scan and d) negative scan in CH_2Cl_2 (1000 (–), 500 (–), 200 (–), 100 (–) and 50 mV/s (–), 0.1 M *n*-Bu_4NPF_6, N_2).

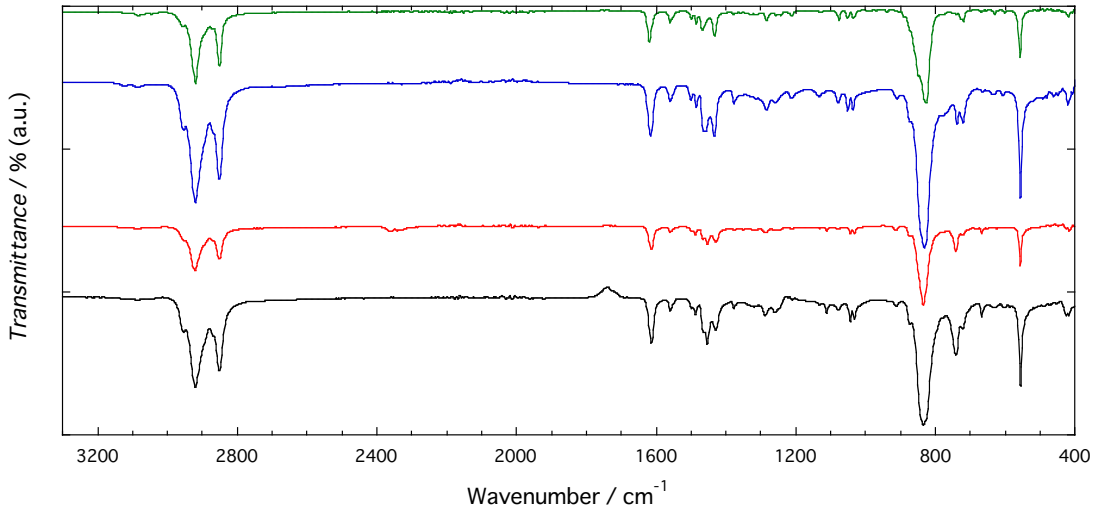

Figure S10. Infrared spectra of **1** (–), **2** (–), **3** (–) and **4** (–).