Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information for

CEE-active Red/NIR Fluorophores with Triple-channel Solid-state "ON/OFF" Fluorescent Switching

Xiao Cheng, Zhenyu Zhang, Houyu Zhang, Shenghua Han, Kaiqi Ye, Lu Wang, Hongyu Zhang and Yue Wang*

State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun 130012, P. R. China

hongyuzhang@jlu.edu.cn

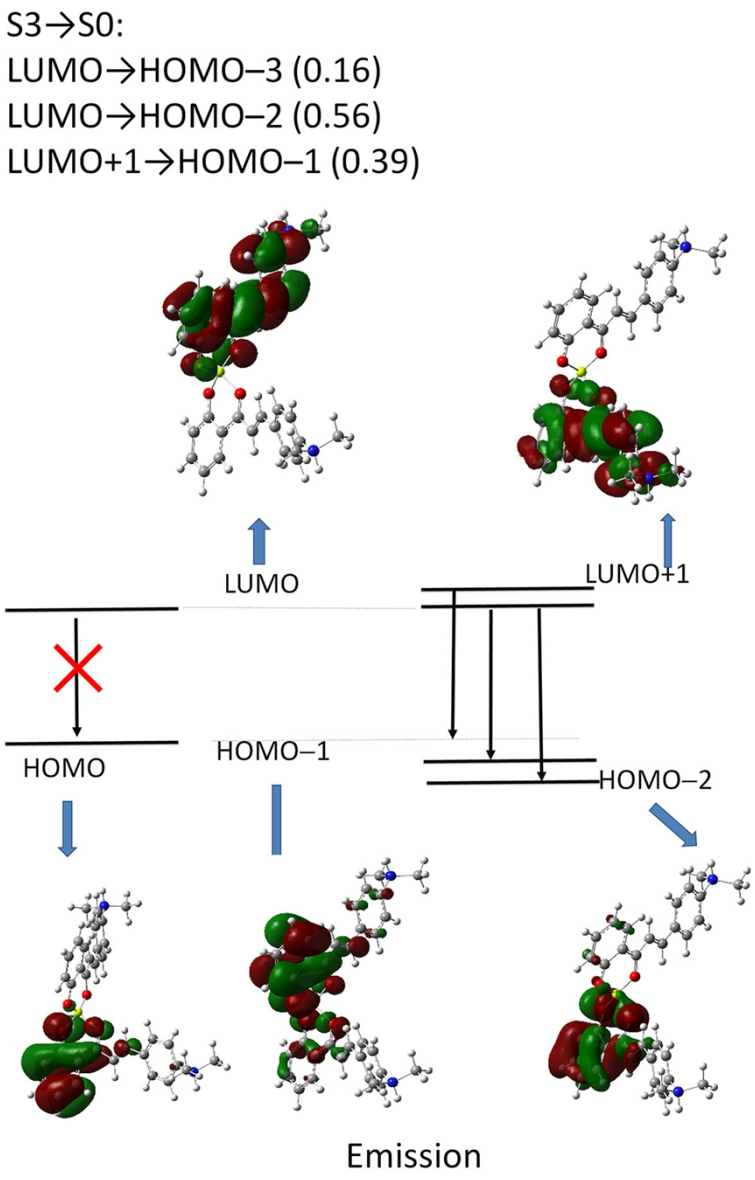

Fig. S1. TD-DFT calculations of the emission process for complex **1**.

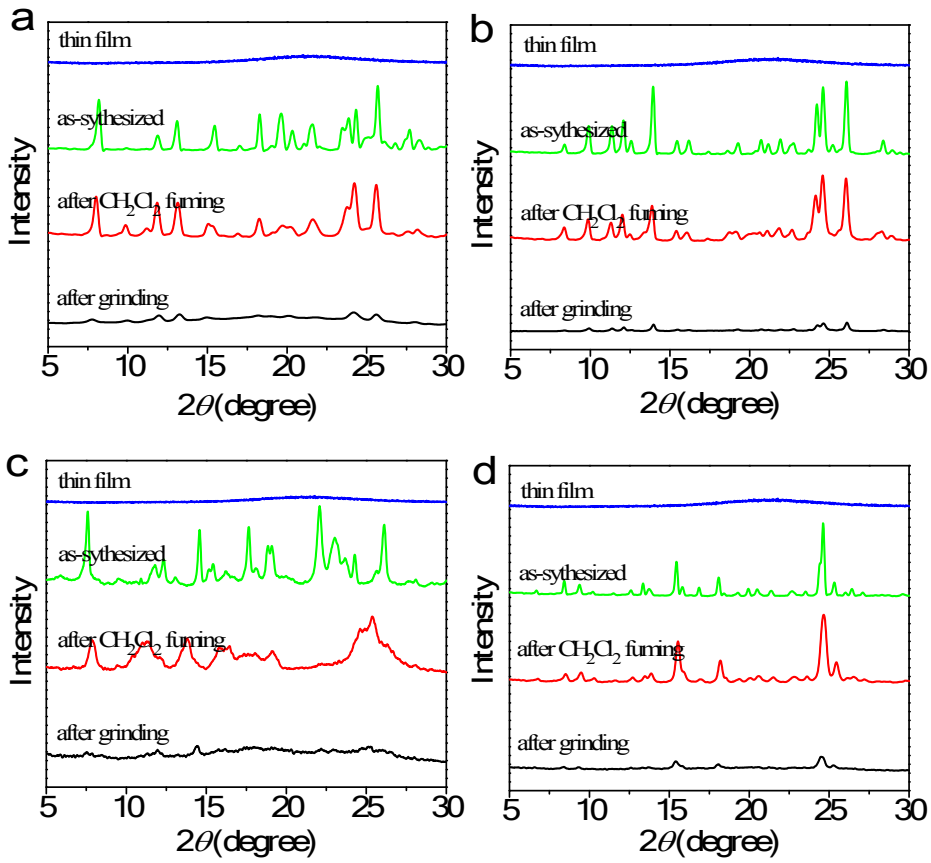

Fig. S2 PXRD patterns of complexes **2** (a) **3** (b) **4** (c) and **5** (d) in different states.

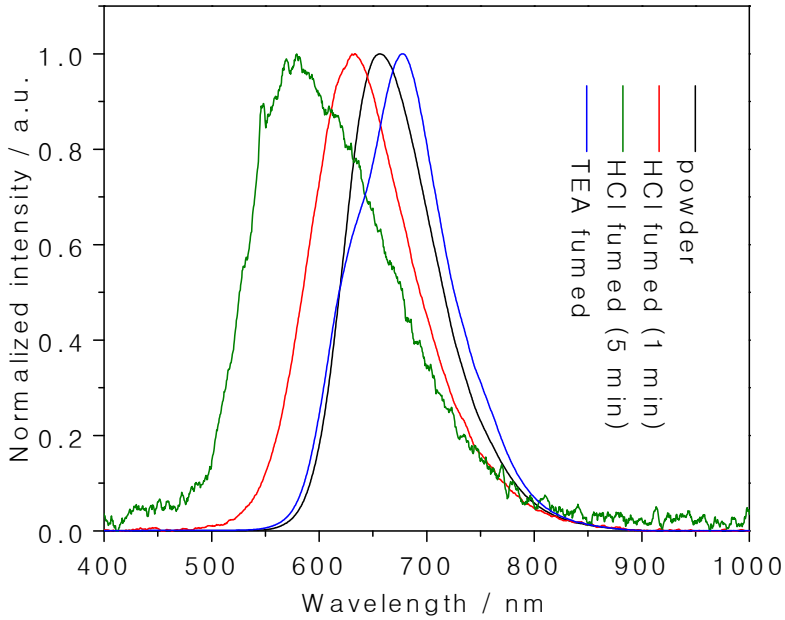

Fig. S3 Photoluminescent spectra of complex **4** in the solid state by acid/base vapor fuming.

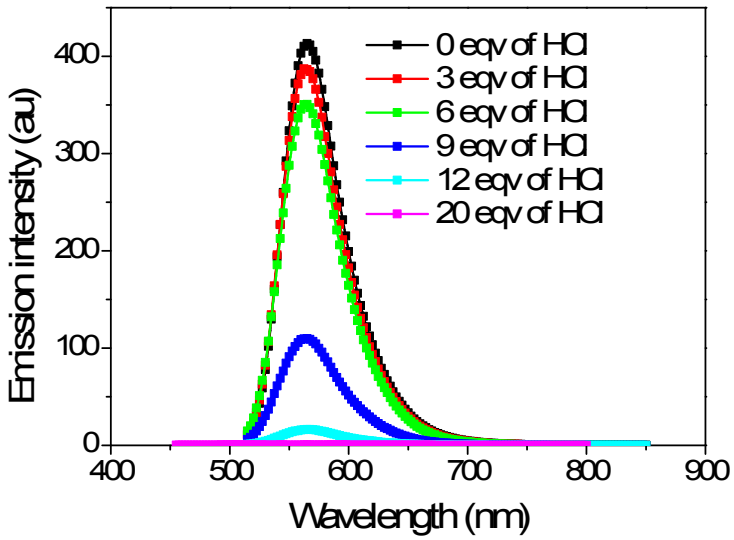

Fig. S4 Photoluminescent spectra of complex **1** in CH_2Cl_2 (1×10^{-5} M) acidized with different amount of HCl.

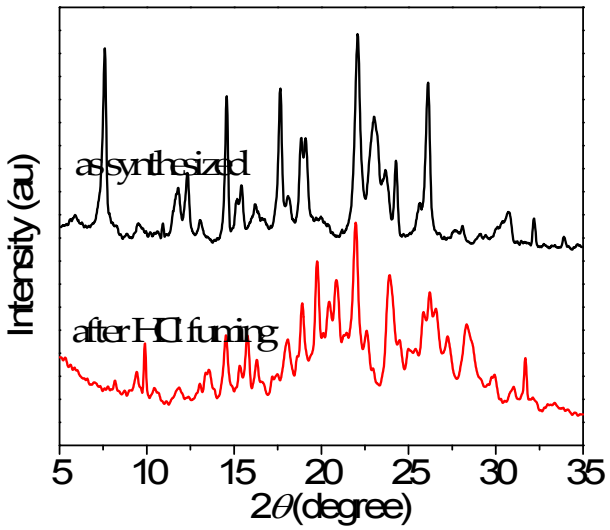

Fig. S5 PXRD patterns of complex **4** acidized with HCl.

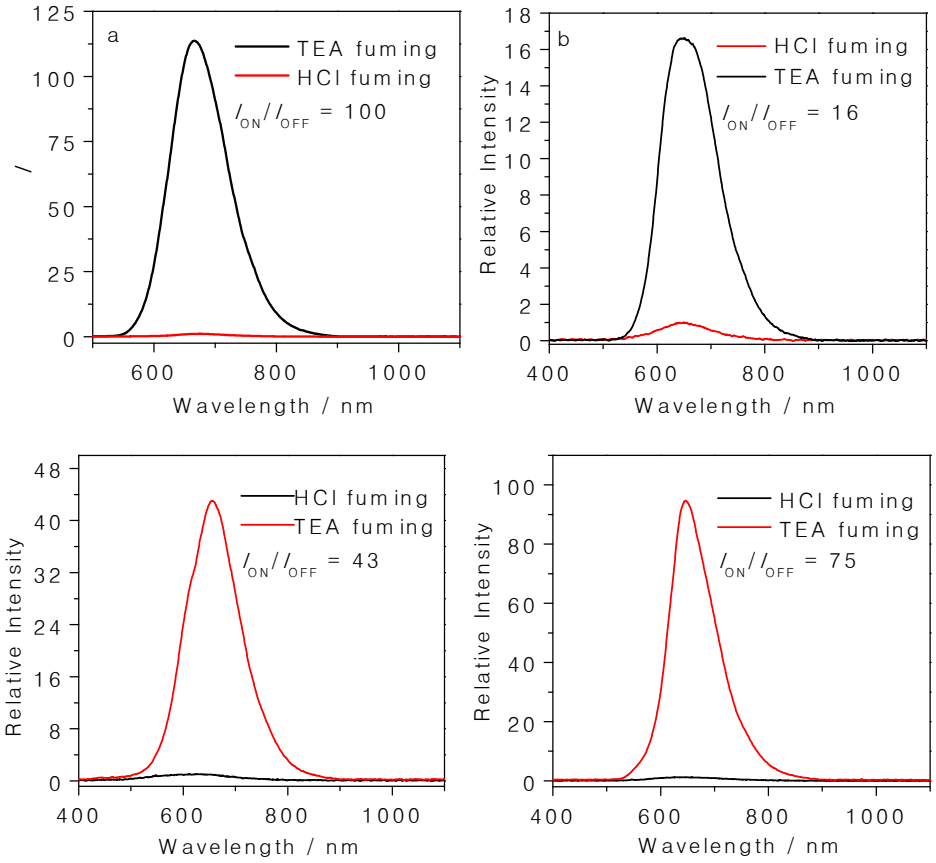

Fig. S6 Photoluminescent spectra of TEA- and HCl-fumed samples a) **1**, b) **2**, c) **3** and d) **5**.

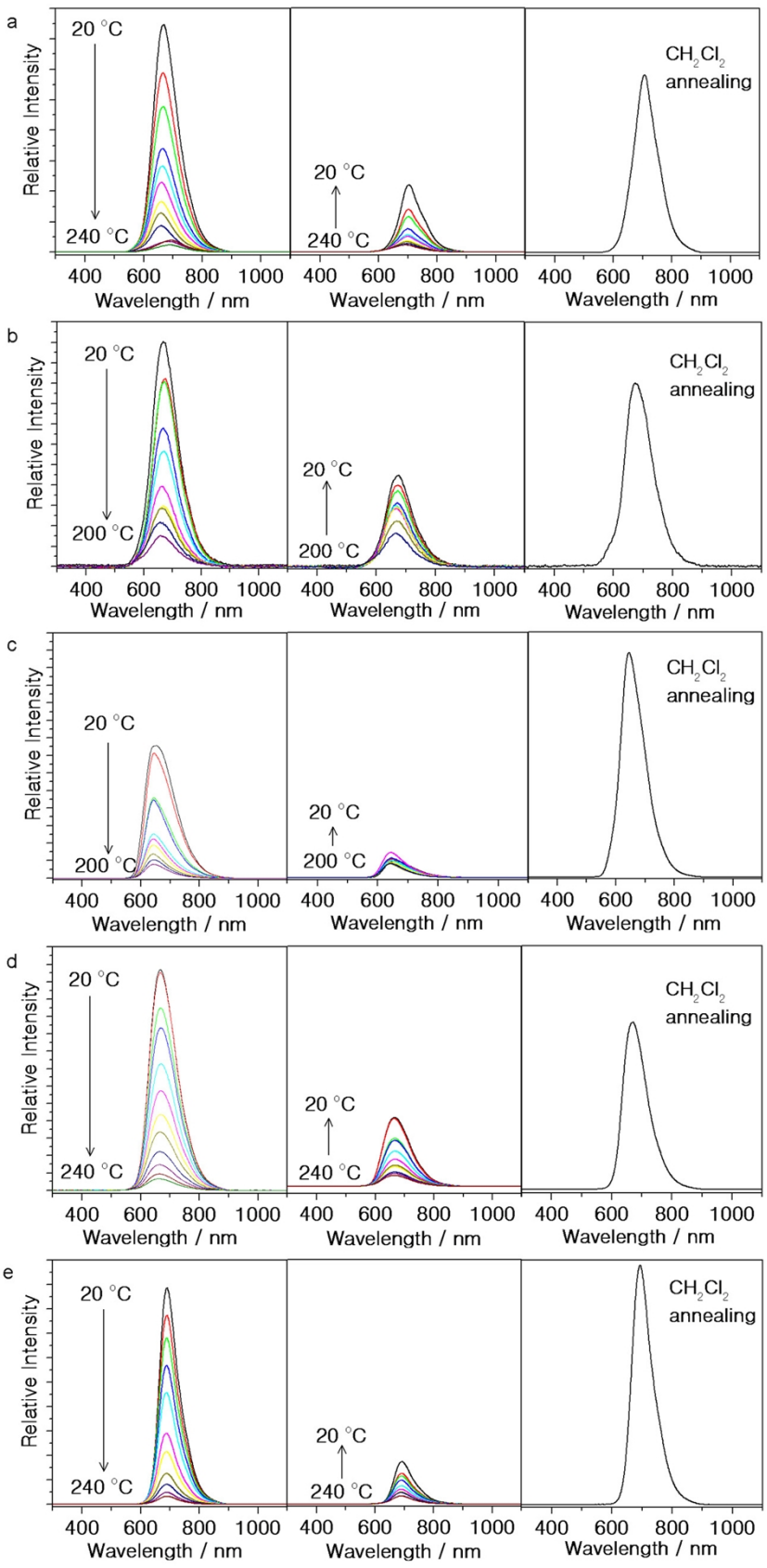

Fig. S7 Photoluminescent spectra of complexes **1**–**5** (a-e) upon heating, cooling and solvent annealing.

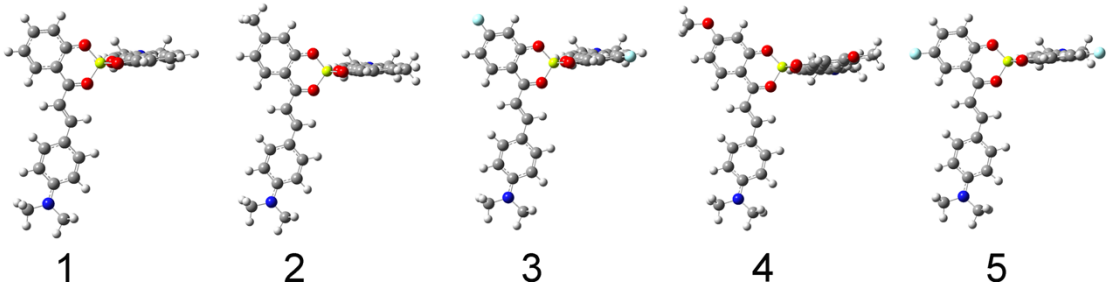

Fig. S8 The calculated molecular conformation for complexes **1–5**.

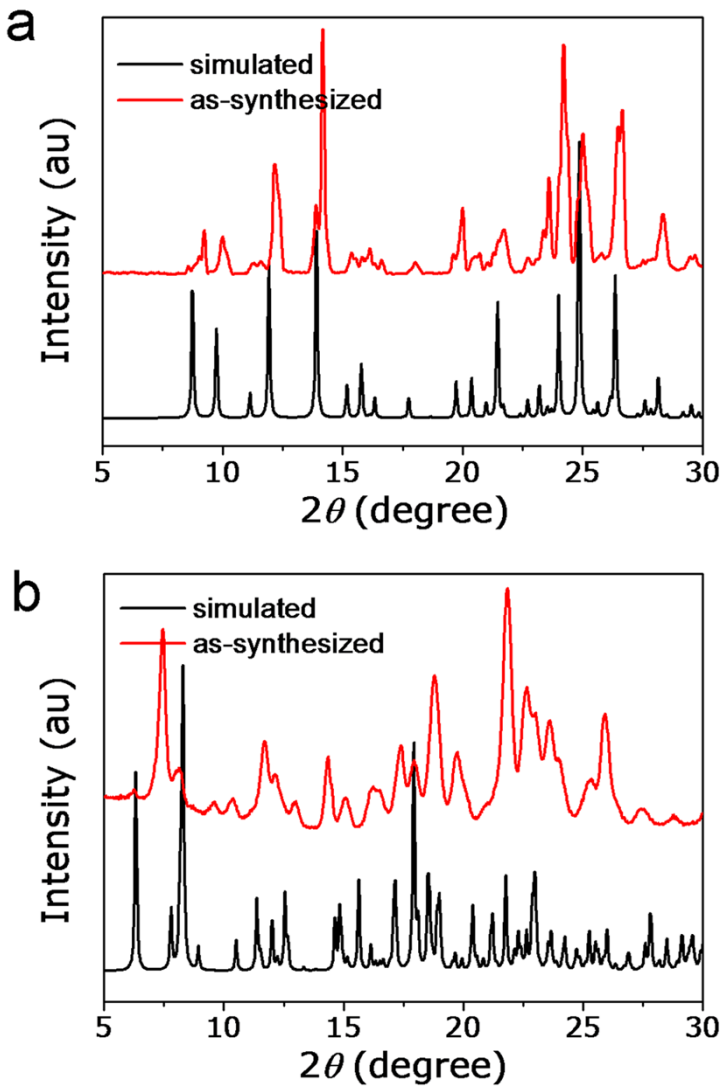

Fig. S9 The measured and simulated PXRD data for complexes **1** (a) and **4** (b).

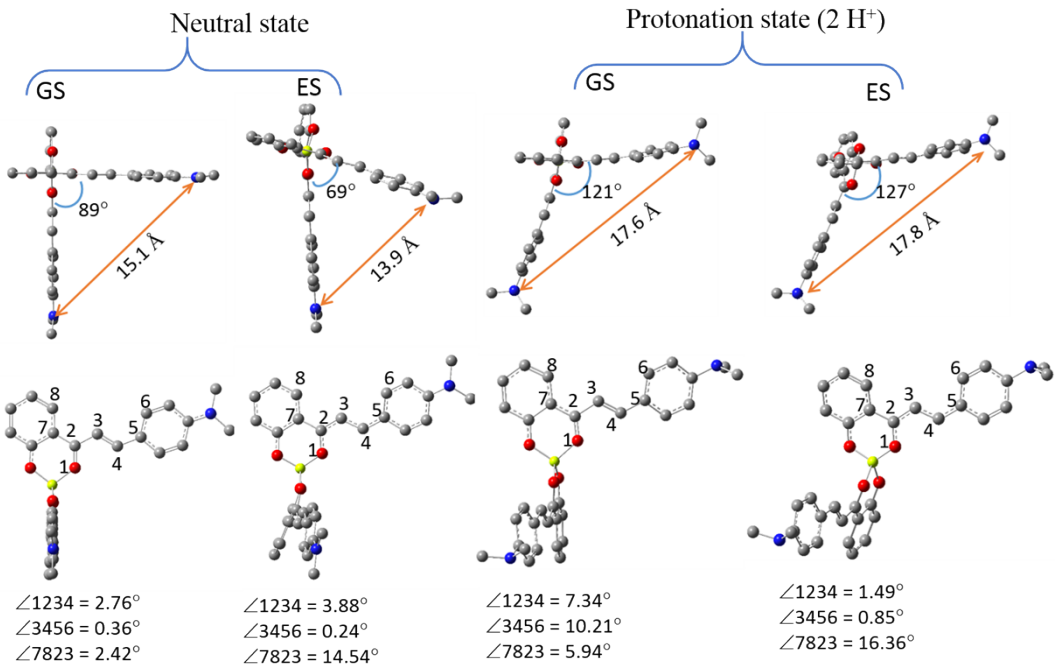

Fig. S10 The optimized ground state (GS) and excited state (ES) structures for complex **1** with its neutral state (left), with comparison with its protonation state from the top view (upper panel) and side view (lower panel). The H atoms are omitted for clarification.

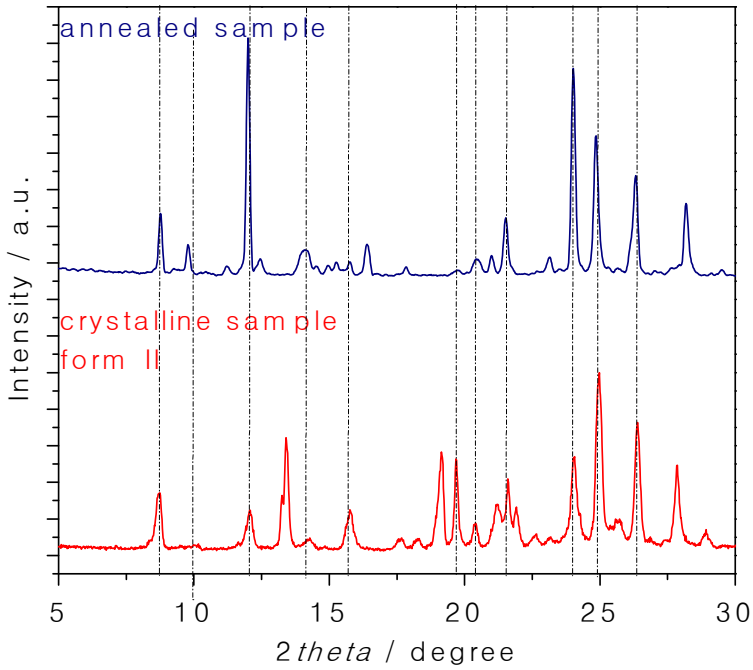

Fig. S11 PXRD patterns of complex **1** (red line: crystalline sample of form II; blue line: the sample of crystalline powder of form I after heating and solvent annealing treatment).

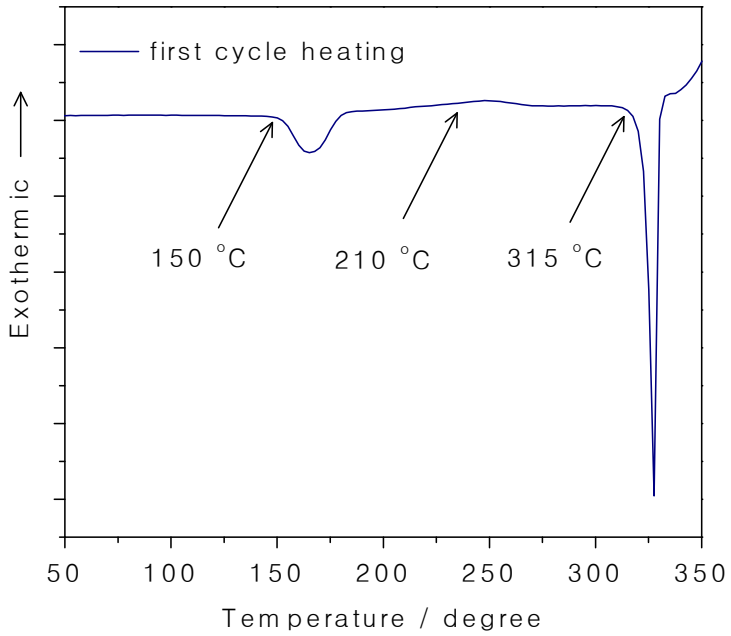

Fig. S12 DSC curve of the crystalline powders of complex **1**.

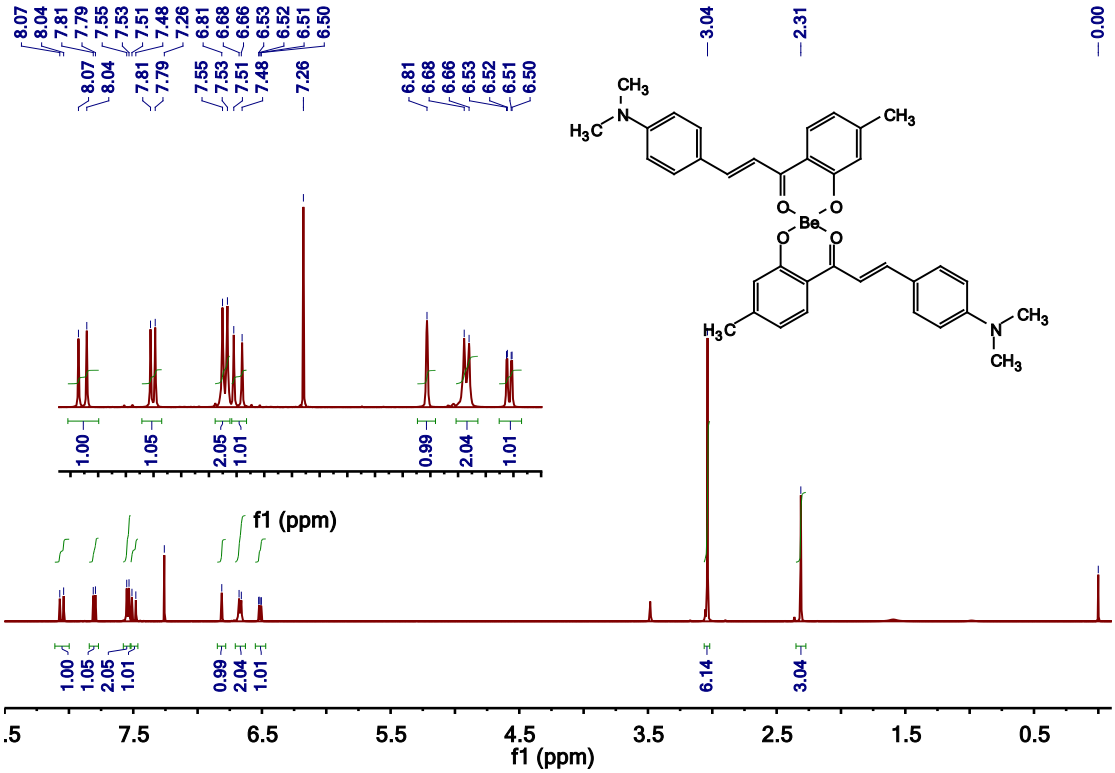

Figure S13. ^{1}H-NMR spectra of **2** recorded in $CDCl_3$ (500 MHz).

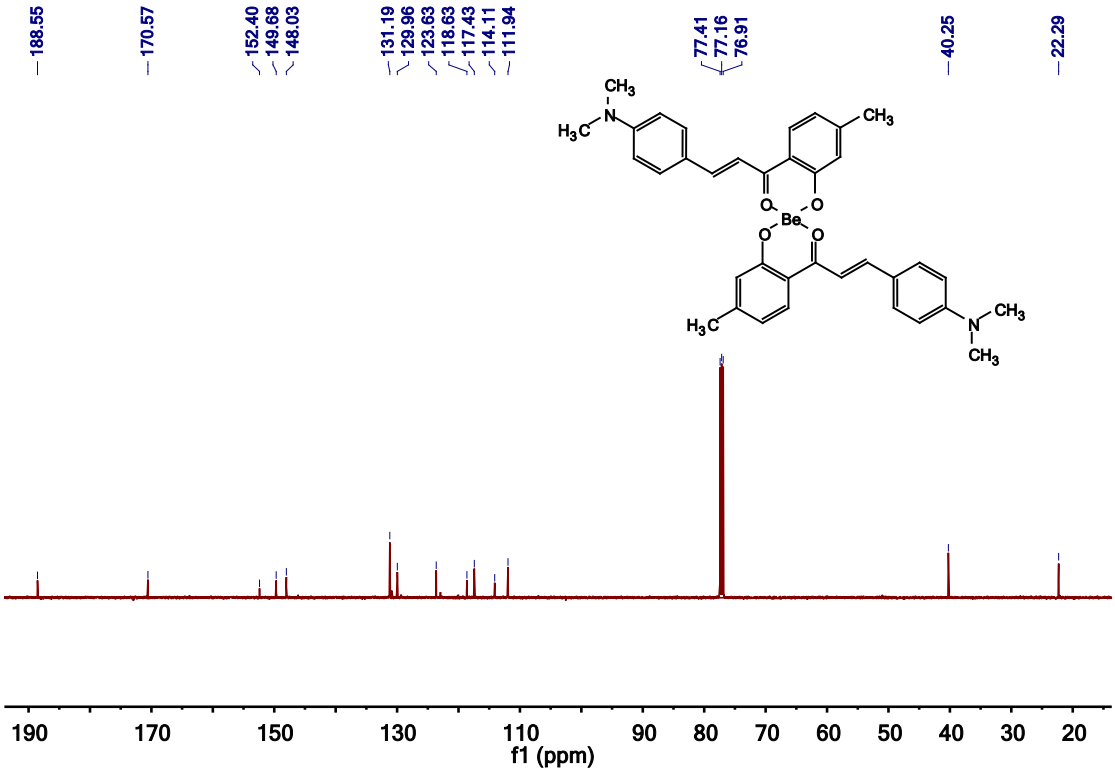

Figure S14. ^{13}C-NMR spectra of **2** recorded in $CDCl_3$ (125 MHz).

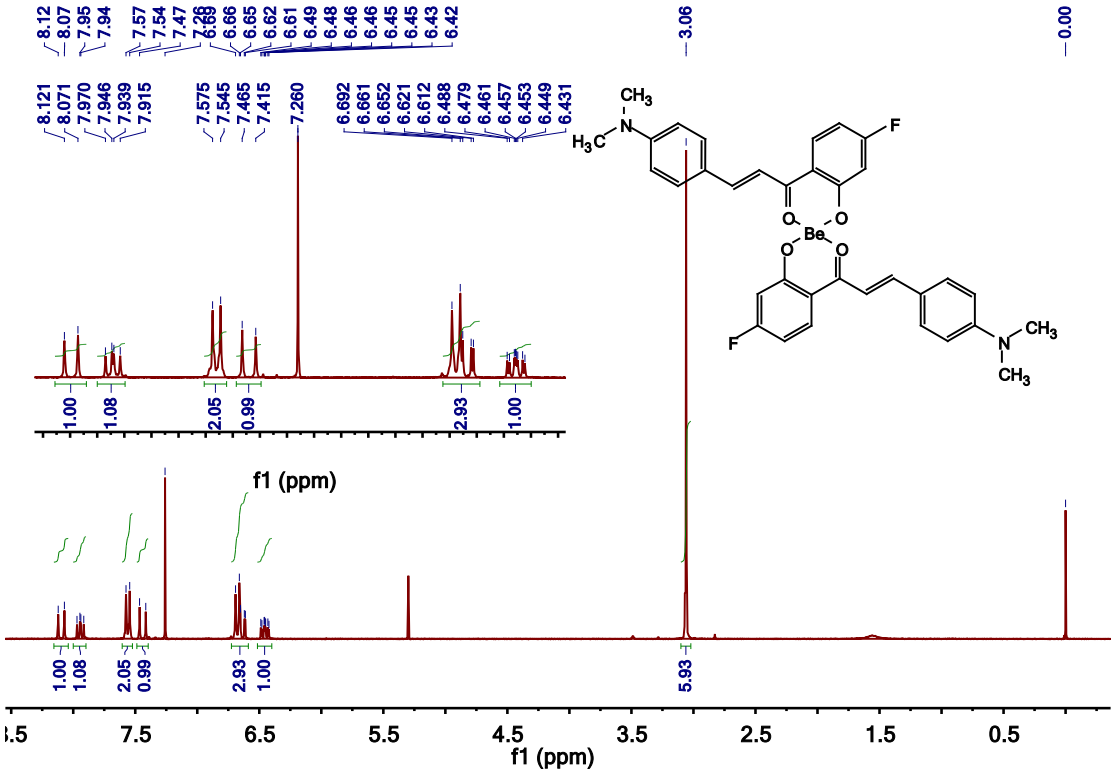

Figure S15. ^{1}H-NMR spectra of **3** recorded in $CDCl_3$ (300 MHz).

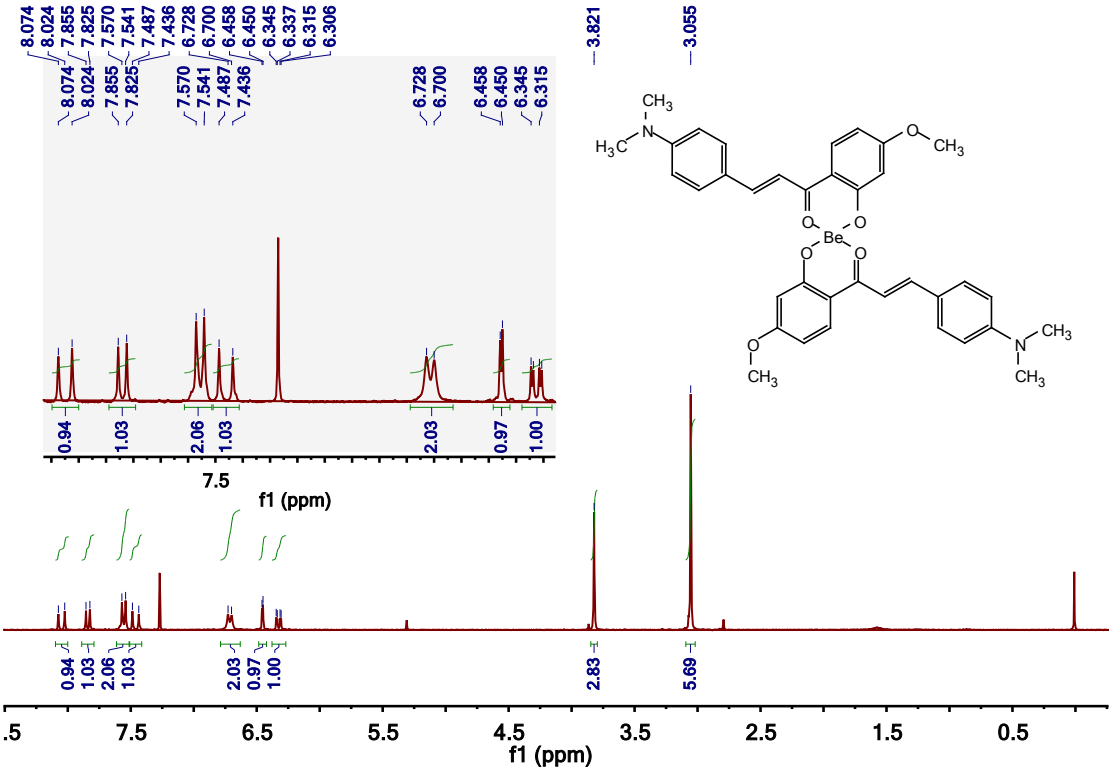

Figure S16. ^{1}H-NMR spectra of **4** recorded in $CDCl_3$ (300 MHz).

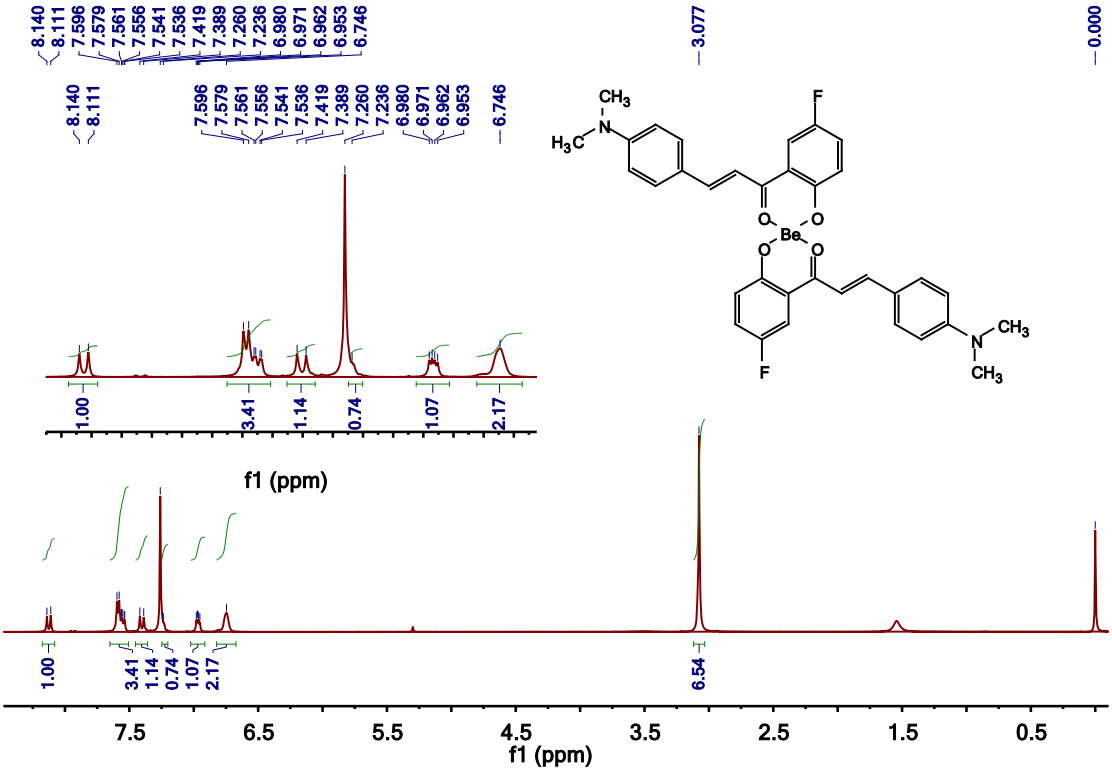

Figure S17. ^{1}H-NMR spectra of **5** recorded in $CDCl_3$ (500 MHz).