Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information (ESI)

Dielectric anisotropy of the single crystal of isopropylviologen copper(I) triiodide

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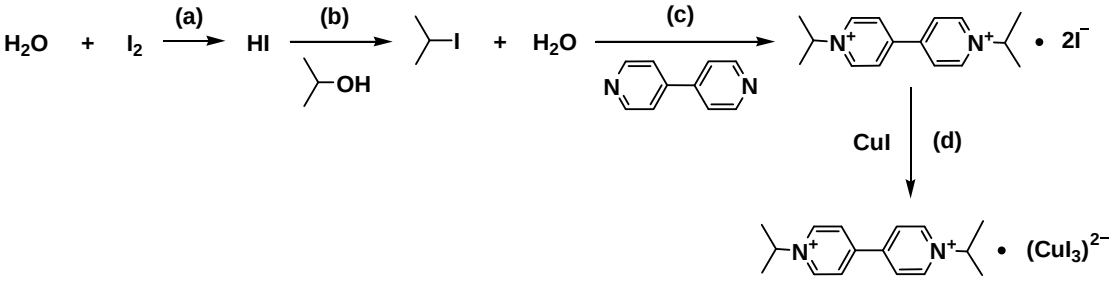

Scheme S1 The possible mechanism on the formation of isopropylviologen copper(I) triiodide by using isopropanol as alkylation reagent: (a) the iodine reacts with water generating hydrogen iodide; (b) The hydrogen iodide reacts with isopropanol getting 2-Iodo-propane; (c) The 2-Iodo-propane combines with 4,4'-bipyridyl forming isopropylviologen iodide; (d) CuI combines with isopropylviologen iodide forming complex **1**, which were precipitated in the form of single crystals upon decreasing reaction temperature slowly.

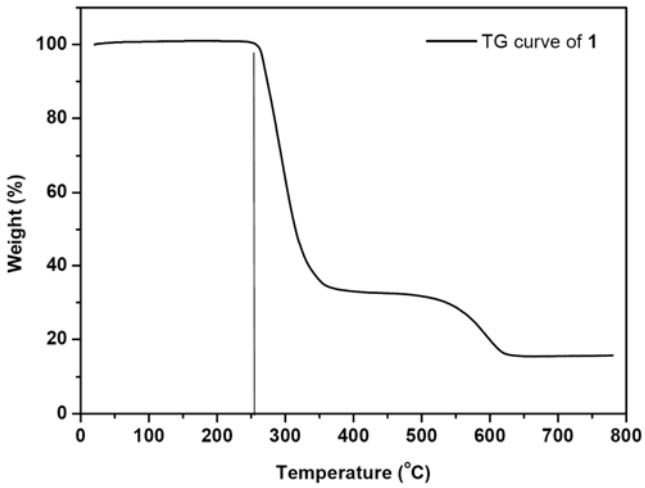

Fig. S1 Thermogravimetric (TG) curve of complex **1**.

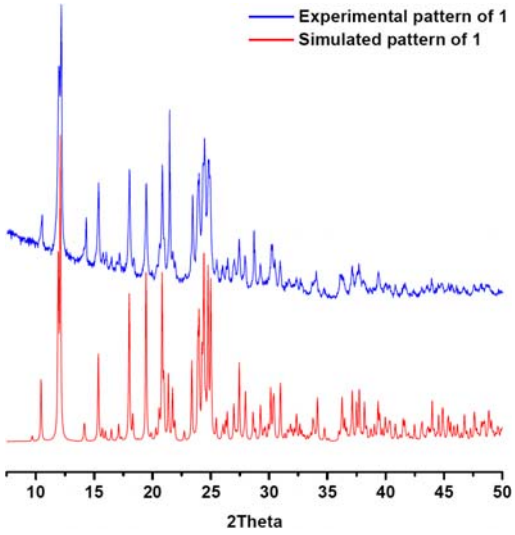

Fig. S2 XRPD spectrum of complex **1**.

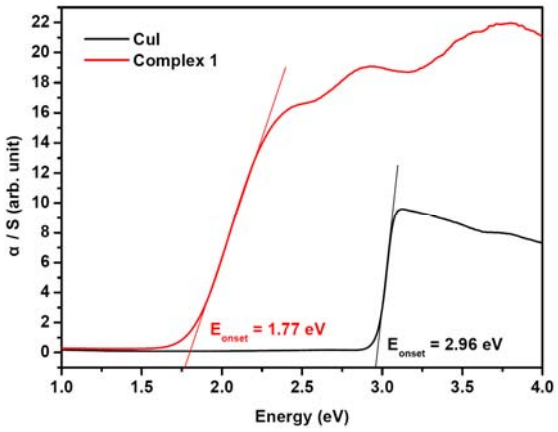

Fig. S3 Solid-state optical diffuse-reflection spectra of CuI and **1** derived from diffuse reflectance data at room temperature. The absorption (α/S) data were calculated from the reflectance using the Kubelka-Munk function.[1] The energy band gaps (*E*onset) were obtained by extrapolation of the linear portion of the absorption edges.

[1] W. W. Wendlandt and H. G. Hecht, *Reflectance Spectroscopy*, Interscience Publishers, New York, 1966.

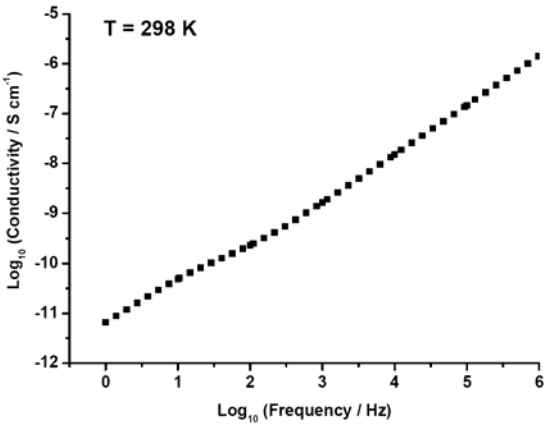

Fig. S4 Frequency-dependence of electric conductivity of crystalline powder of **1** at 298 K.