Supplementary Information for:

A series of pure-blue-light emitting Cu(I) complexes with thermally activated delayed fluorescence: structural, photophysical, and computational studies

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1. Solid state UV-Vis diffuse reflectance spectra of complexes **1**-**4** measured at room temperature using the Kubelka-Munk function α/S = (1-R)2/(2R).
2. Experimental powder X-ray diffraction patterns (black) and simulated patterns derived from the single crystal structural analysis data (red) for complexes **1**-**4**.
3. Infrared spectra of complexes **1**-**4**.
4. Emission decay curves of complexes **1**-**4** measured at 77K and 298K.

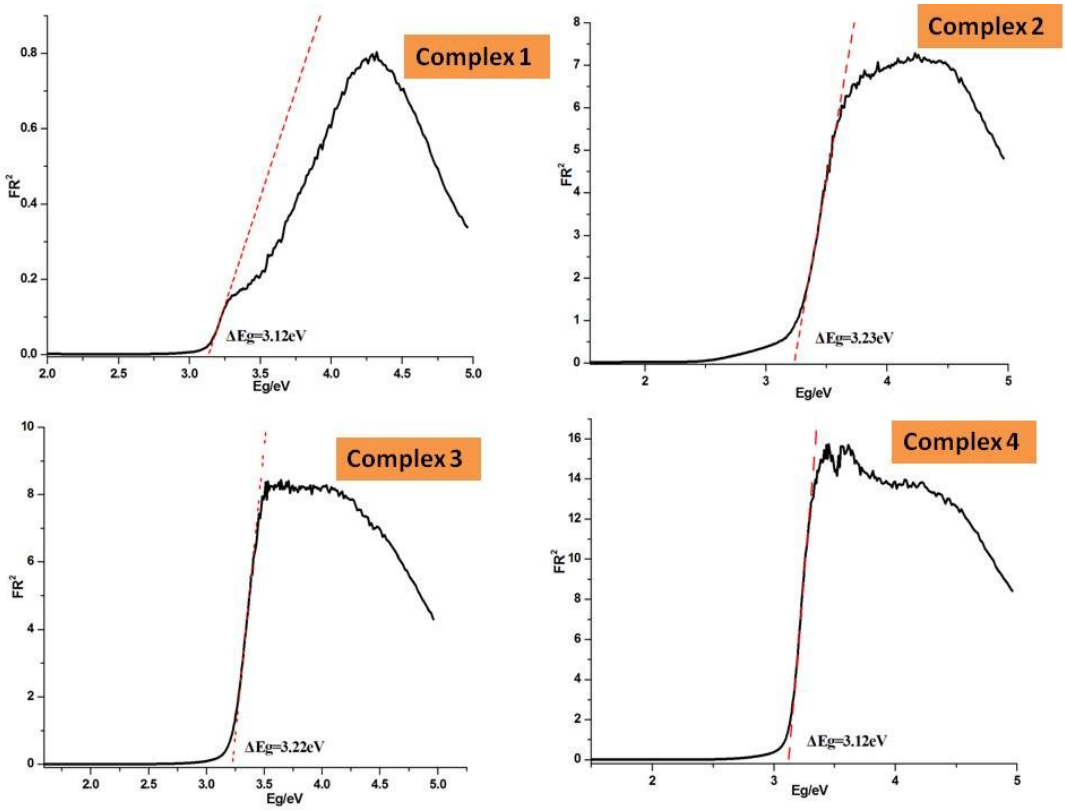

Figure S1. Solid state UV-Vis diffuse reflectance spectra of complexes **1**-**4** measured at room temperature using the Kubelka-Munk function α/S = (1-R)2/(2R)

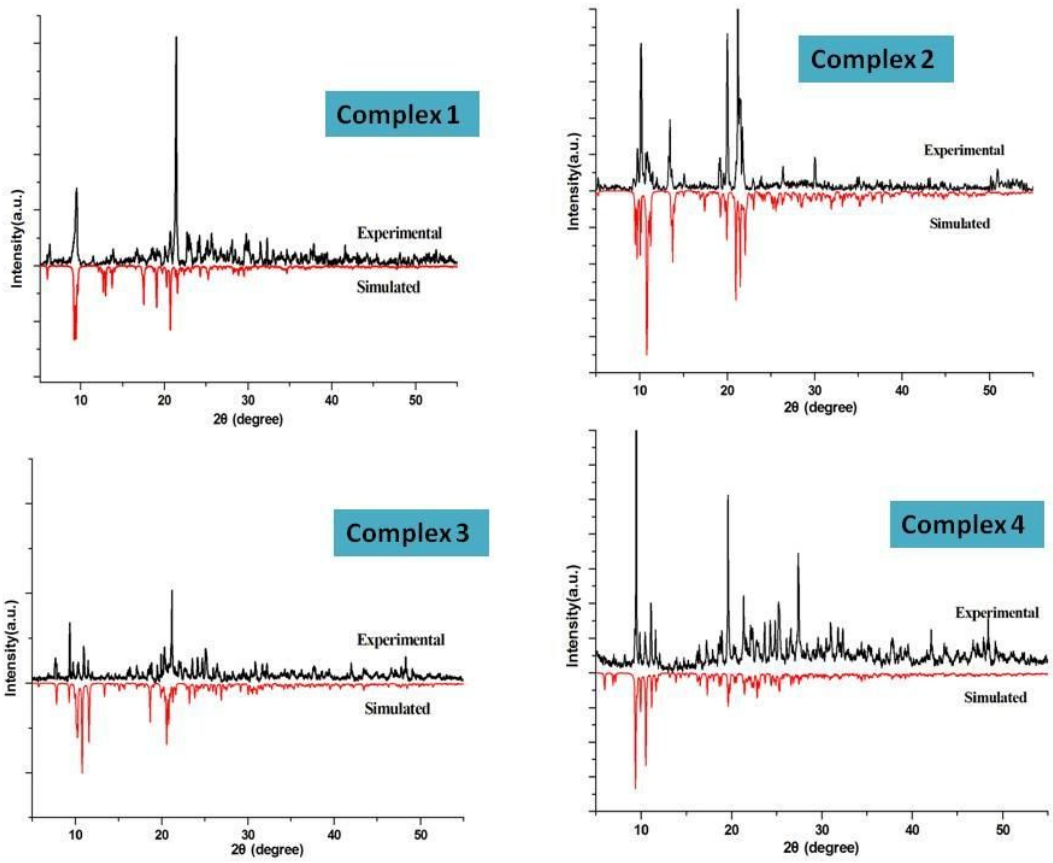

Figure S2. Experimental powder X-ray diffraction patterns (black) and simulated patterns derived from the single crystal structural analysis data (red) for complexes **1**-**4**

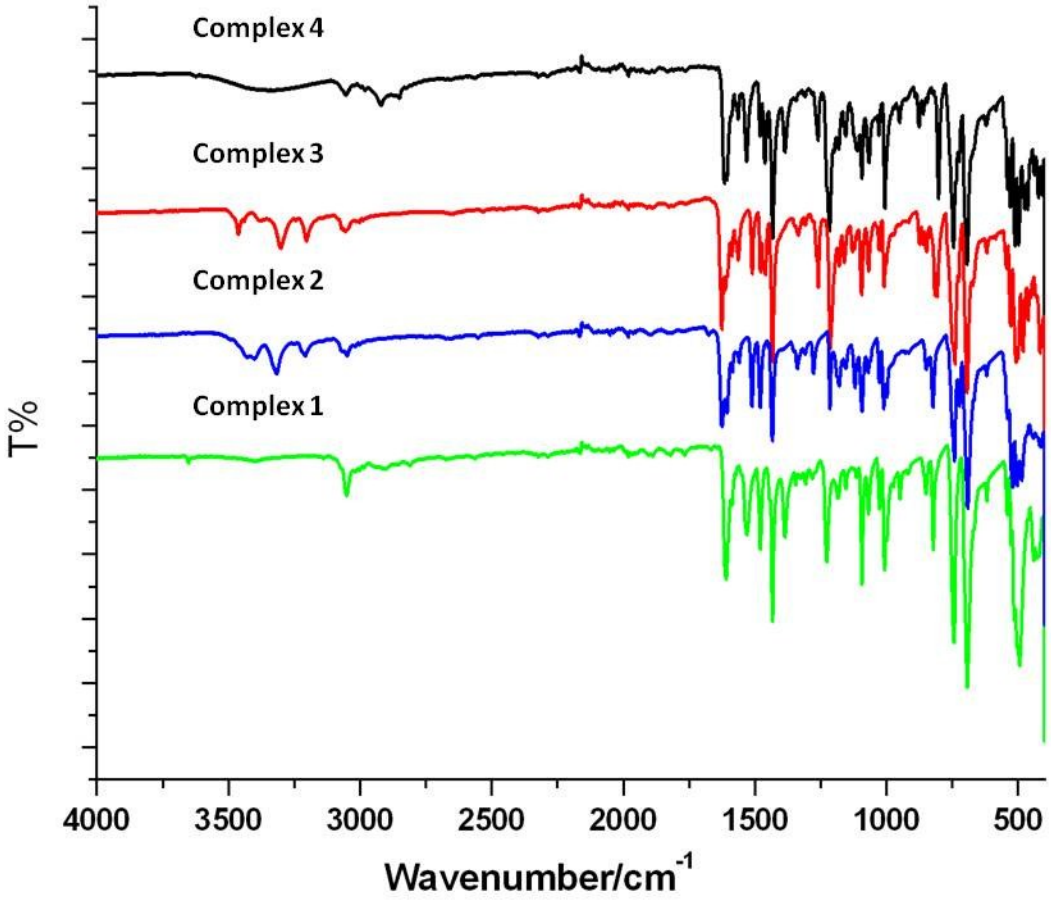

Figure S3. Infrared spectra of complexes **1**-**4**

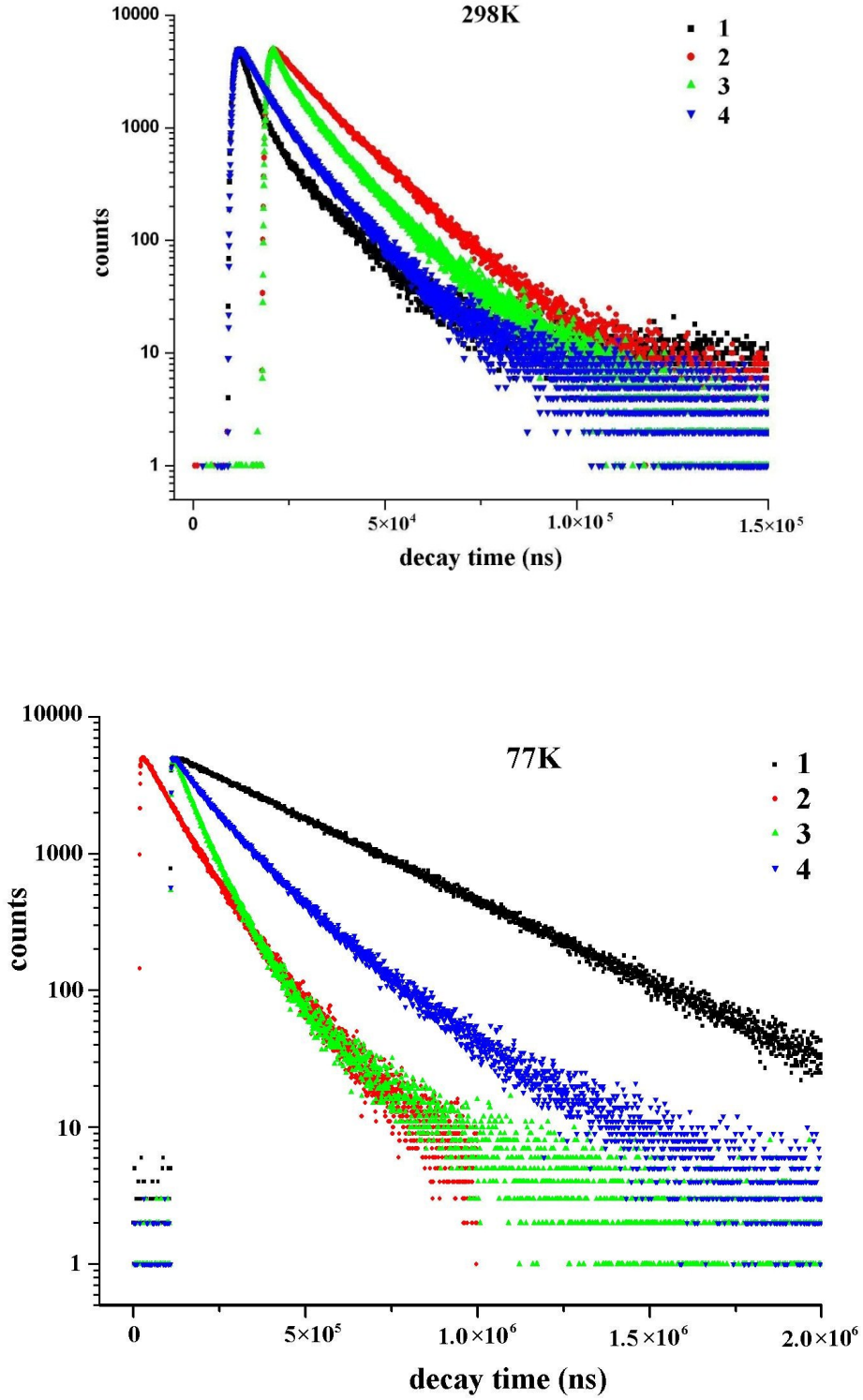

Figure S4. Emission decay curves of complexes **1**-**4** measured at 298K (top) and 77K (bottom).