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**Supporting information for article:** 

Structural, spectroscopic and DFT theoretical studies of phosphorescent CuIP2S-containing complexes

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**Figure S1** Electron density difference plots of 10 low-lying electron transitions of  $S_{2\sim10^a}$  for **I**.

 $^{a}$ Electron densities move from the blue area to the green area. Isovalue = 0.004. The transition wavelength and major contributions are listed in Table 4.

**Figure S2** Electron density difference plots of 10 low-lying electron transitions of  $S_{2\sim10^a}$  for II.

<sup>a</sup>Electron densities move from the blue area to the green area. Isovalue = 0.004. The transition wavelength and major contributions are listed in Table 4.