

INTENSE RED-EMITTING THREE-COORDINATED BENZOTHIADIAZOLE-BASED COPPER(I) COMPLEXES

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2,1,3-benzothiadiazole (BTD) is a fluorophore commonly exploited as luminescent material for advanced applications, such as organic light-emitting diodes (OLEDs), dyes, solar and photovoltaic cells^[1-4]. Ligands containing the benzothiadiazole heterocycle allowed the isolation of luminescent complexes applied in OLED technology^[5,6].

In this communication we report the synthesis and characterization of heteroleptic three-coordinated Cu(I) complexes based on the benzothiadiazole heterocycle. Triphenylphosphine, diphenylphosphinomethane (dppm) and bis[(2-diphenylphosphino)phenyl] ether (DPEphos) were used as P-donor ligands. The derivatives were prepared starting from CuCl or by acidolysis of borohydride Cu(I) complexes. When [Cu(NCCH₃)₄][BF₄] was used as precursor, four-coordinated derivatives characterized by one acetonitrile molecule in the coordination sphere were isolated.

After being excited with light below 450 nm the complexes exhibited intense emissions in the red region, lifetimes up to 2 ms long and high quantum yields. XRD data highlighted that at solid state the tetrafluoroborate used as counterion is interacting with the metal centre through a fluorine. In the case of dppm, binuclear species were isolated. The replacement of tetrafluoroborate with perchlorate showed the non-innocent role of the counter-anion, affecting in particular the luminescence lifetimes. The wide emission bands were attributed to ³LC transitions on the basis of luminescence lifetime measurements and TD-DFT calculations.

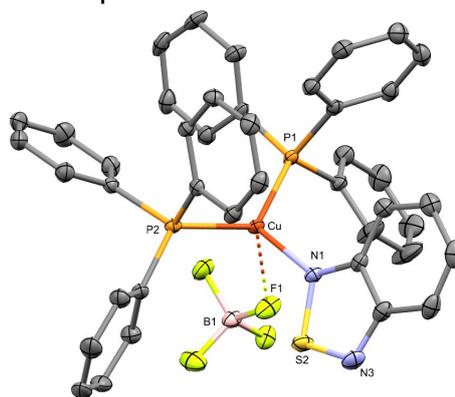


Figure 1. Ellipsoid plot of [Cu(BTD)(PPh₃)₂][BF₄].

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