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# BOOK OF ABSTRACTS

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# SYNTHESIS AND CHARACTERIZATION OF LUMINESCENT N-FUNCTIONALIZED BENZOTRIAZOLE-BASED HETEROLEPTIC COPPER(I) COMPLEXES

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Benzotriazole is a heterocycle commonly used as building block for organic synthesis thanks to its versatility.[1,2] However, its similarity with other azoles, such as benzimidazole, makes it a suitable candidate for the preparation of luminescent Cu(I) complexes. Our research group previously reported the preparation of luminescent Cu(I) complexes using this heterocycle and the related indazole fragment in polydentate ligands.[3,4]
In this communication we report the synthesis and characterization of luminescent mono- and binuclear cationic heteroleptic copper(I) complexes containing bidentate N-donor ligands obtained by nucleophilic attack of benzotriazole on the C-X bond of functionalized pyridine, pyrimidine or substituted triazines. Different mono- and bidentate phosphines were used as P-donor ligands. The structures of several complexes were ascertained by means of single-crystal X-ray diffraction, revealing in the case of 1,2-bis(diphenylphosphino)ethane the isolation of binuclear species. Upon excitation with near-UV and violet light, the complexes exhibited emissions from bright yellow to reddish orange with emission maxima, luminescence lifetimes and photoluminescence quantum yields strongly related to the choice of the coordinated ligands. In particular, the complex $[Cu(py\text{-}btz)(PPh_3)_2][BF_4]$ where py-btz = 1-(pyridin-2-yl)benzotriazole exhibited the longest lifetime value, equal to 164 μs. On the other hand, the highest quantum yield equal to 92% was observed for $[Cu(trz^{OEt}\text{-}btz)(DPEphos)][BF_4]$ [$trz^{OEt}$-btz = 1-(4,6-ethoxy-1,3,5-triazin-2-yl)benzotriazole; DPEphos = bis[(2-diphenylphosphino)phenyl] ether]. The absorption and emission features were attributed to metal-to-ligand charge transfer transitions involving triplet emitting states ($^3$MLCT) on the basis of experimental data and DFT calculations.

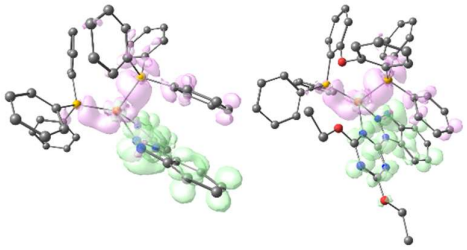

***Figure 1**: DFT-optimized structures of selected complexes with hole (pink) and electron (green) distributions related to the lowest energy singlet-singlet transitions.*

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[4] V. Ferraro, J. Castro, L. Agostinis, M. Bortoluzzi, *Trans. Met. Chem.* **2021**, *46*, 391–402.