The surprising effects of sulfur: achieving long excited-state lifetimes in heteroleptic copper(I) emitters

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A series of heteroleptic [Cu(NˆN)(PˆP)][PF6] complexes is reported in which NˆN is a di(methylsulfanyl)-1,10-phenanthroline (2,9-, 3,8- or 4,7-(MeS)2phen) or di(methoxy)-1,10-phenanthroline (2,9-, 3,8- or 4,7-(MeO)2phen) and PˆP is bis(2-(diphenylphosphano)phenyl)ether (POP) or 4,5-bis(diphenylphosphano)-9,9-dimethylxanthene (xantphos). The effects of the different substituents are investigated through structural, electrochemical and photophysical studies and by using DFT and TD-DFT calculations. Introducing methylsulfanyl groups in the 2,9-, 3,8- or 4,7-positions of the phen domain alters the composition of the frontier molecular orbitals of the [Cu(NˆN)(PˆP)]+ complexes significantly, so that ligand-centred (LC) transitions become photophysically relevant with respect to metal-to-ligand charge transfer (MLCT). Within this series, [Cu(2,9-(MeS)2phen)(POP)][PF6] exhibits the highest photoluminescence quantum yield of 15% and the longest excited-state lifetime of 8.3 ms in solution. In the solid state and in frozen matrices at 77 K, the electronic effects of the methylsulfanyl or methoxy substituents are highlighted, thus resulting in luminescence lifetimes of 2 to 4.2 ms at 77 K with predominantly LC character for both the 3,8- and 4,7-(MeS)2phen containing complexes. The results of the investigation give new guidelines on how to influence the luminescence properties in [Cu(NˆN)(PˆP)]+ complexes which will aid in the development of new sustainable and efficient copper(I) emitters
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