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Publication

# The shiny side of copper: Bringing copper(I) light-emitting electrochemical cells closer to application

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Heteroleptic [Cu(PˆP)(NˆN)][PF6] complexes, where NˆN is 5,50-dimethyl-2,20-bipyridine (5,50-Me2bpy), 4,5,6-trimethyl-2,20-bipyridine (4,5,6-Me3bpy), 6-(tert-butyl)-2,20-bipyridine (6-tBubpy) and 2-ethyl-1,10-phenanthroline (2-Etphen) and PˆP is either bis(2-(diphenylphosphino)phenyl)ether (POP, PIN [oxydi(2,1-phenylene)]bis(diphenylphosphane)) or 4,5-bis(diphenylphosphino)-9,9-dimethylxanthene (xantphos, PIN (9,9-dimethyl-9H-xanthene-4,5-diyl)bis(diphenylphosphane)) have been synthesized and their NMR spectroscopic, mass spectrometric, structural, electrochemical and photophysical properties were investigated. The single-crystal structures of [Cu(POP)(5,50-Me2bpy)][PF6], [Cu(xantphos)(5,50-Me2bpy)] [PF6], [Cu(POP)(6-tBubpy)][PF6], [Cu(POP)(4,5,6-Me3bpy)][PF6]$1.5Et2O, [Cu(xantphos)(4,5,6-Me3bpy)] [PF6]$2.33CH2Cl2, [Cu(POP)(2-Etphen)][PF6] and [Cu(xantphos)(2-Etphen)][PF6] are described. While alkyl substituents in general exhibit electron-donating properties, variation in the nature and substitutionposition of the alkyl group in the NˆN chelate leads to different effects in the photophysical properties of the [Cu(PˆP)(NˆN)][PF6] complexes. In the solid state, the complexes are yellow to green emitters with emission maxima between 518 and 602 nm, and photoluminescence quantum yields (PLQYs) ranging from 1.1 to 58.8%. All complexes show thermally activated delayed fluorescence (TADF). The complexes were employed in the active layer of light-emitting electrochemical cells (LECs). The device performance properties are among the best reported for copper-based LECs, with maximum luminance values of up to 462 cd m2 and device half-lifetimes of up to 98 hours.
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