Intra-cation versus inter-cation π-contacts in [Cu(PˆP)(NˆN)][PF6] complexes

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A series of [Cu(POP)(NˆN][PF6] and [Cu(xantphos)(NˆN][PF6] compounds have been prepared and characterized in which POP = bis[2-(diphenylphosphanyl)phenyl]ether (IUPAC PIN oxydi(2,1-phenylene)bis(diphenylphos xantphos = 4,5-bis(diphenylphosphanyl)-9,9- dimethyl-9H-xanthene (IUPAC PIN (9,9-dimethyl-9H-xanthene-4,5-diyl)bis(diphenylphosphane)) and the NˆN ligands are 4-(4-bromophenyl)-6,6'-dimethyl-2,2'-bipyridine (1), 5,5'-bis(3-methoxyphenyl)-6-methyl-2,2'-bipyridine (2), and 6-benzyl-2,2'-bipyridine (3). The single crystal structures of [Cu(xantphos)(1)][PF6] . CH2Cl2, [Cu(xantphos)(2)][PF6] . CH2Cl2and [Cu(POP)(3)][PF6] . 0.5H2O were determined by X-ray diffraction. Each complex contains a copper(I) ion in a distorted tetrahedral environment with chelating NˆN and PˆP ligands. In the [Cu(xantphos)(1)]+and [Cu(xantphos)(2)]+ cations, there are face-to-face π-stackings of bpy and PPh2phenyl rings (i.e. between the ligands); in addition in [Cu(xantphos)(2)][PF6] . CH2Cl2, inter-cation π-embraces lead to the formation of infinite chains as a primary packing motif. In [Cu(POP)(3)][PF6] . 0.5H2O, centrosymmetric pairs of [Cu(POP)(3)]+cations engage in C-H...π (phenyl to bpy) and offset face-to-face (bpy...bpy) contacts. The electrochemical and photophysical properties of the compounds containing ligands 1and 2are reported. They are green or yellow emitters in the solid-state (λemin the range 535-577 nm) with values for the photoluminescence quantum yield (PLQY) in the range 19-41%

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