Introducing intramolecular, interligand arene-alkynyl π-interactions into heteroleptic [Cu(NˆN)(PˆP)]+ complexes

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The synthesis and characterization of six new heteroleptic copper(I) compounds incorporating wide bite-angle bisphosphanes (POP = oxydi(2,1-phenylene)]bis(diphenylphosphane), xantphos = (9,9-dimethyl-9 H -xanthene-4,5-diyl)bis(diphenylphosphane) combined with 6,6'-di(but-3-yn-1-yl)-2,2'-bipyridine (1), 6-(but-3-yn-1-yl)-6'-methyl-2,2'-bipyridine (2) or 6-(but-3-yn-1-yl)-2,2'-bipyridine (3) are reported. The single-crystal structures of [Cu(1)(POP)][PF 6], [Cu(1)(xantphos)][PF 6], [Cu(3)(POP)][PF 6] and [Cu(3)(xantphos)][PF 6] have been determined and confirm distorted tetrahedral copper(I) centres. In the solid state, the compounds are yellow or green emitters (λ max em = 530-573 nm). The highest solid-state photoluminescence quantum yields (PLQYs) were observed for [Cu(1)(xantphos)][PF 6] (46%) and [Cu(1)(POP)][PF 6] (41%). A combination of face-to-face arene...arene p-stacking interactions and CžC...p arene interactions protects the Cu atom in each structurally characterized complex. The CžC...p arene interactions are characterized by a near parallel alignment of the CžCH unit over an arene ring, and C alkyne ...arene centroid distances lie in the range of 3.74 to 4.16 Å, and CžC centroid ...arene centroid distances lie between 3.86 and 4.09 Å. These distances fall well within the ranges for related interactions for compounds in the Cambridge Structural Database, and data for these interactions are presented
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