

Correction to Blue-Light Emission of Cu(I) Complexes and Singlet Harvesting

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Page 8293. The emission decay time of Cu(pop)(pz₂Bph₂) at ambient temperature is erroneously given as 13 s instead of 13 μs. This short decay time represents an essential and characteristic property of the discussed Cu(I) complex. Therefore, the corrected Abstract is reproduced again.

ABSTRACT: Strongly luminescent neutral copper(I) complexes of the type Cu(pop)(NN), with pop = bis(2-(diphenylphosphanyl)phenyl)ether and NN = bis(pyrazol-1-yl)borohydrate (pz₂BH₂), tetrakis(pyrazol-1-yl)borate (pz₄B), or bis(pyrazol-1-yl)-biphenylborate (pz₂Bph₂), are readily accessible in reactions of Cu(acetonitrile)₄⁺ with equimolar amounts of the pop and NN ligands at ambient temperature. All products were characterized by means of single crystal X-ray diffractometry. The compounds exhibit very strong blue/white luminescence with emission quantum yields of up to 90%. Investigations of spectroscopic properties and the emission decay behavior in the temperature range between 1.6 K and ambient temperature allow us to assign the emitting electronic states. Below 100 K, the emission decay times are in the order of many hundreds of microseconds. Therefore, it is concluded that the emission stems from the lowest triplet state. This state is assigned to a metal-to-ligand charge-transfer state (³MLCT) involving Cu-3d and pop-π* orbitals. With temperature increase, the emission decay time is drastically reduced, e.g. to 13 μs (Cu(pop)-(pz₂Bph₂)), at ambient temperature. At this temperature, the complexes exhibit high emission quantum yields, as neat material or doped into poly(methyl methacrylate) (PMMA). This behavior is assigned to an efficient thermal population of a singlet state (being classified as ¹MLCT), which lies only 800 to 1300 cm⁻¹ above the triplet state, depending on the individual complex. Thus, the resulting emission at ambient temperature largely represents a fluorescence. For applications in OLEDs and LEECs, for example, this type of thermally activated delayed fluorescence (TADF) creates a new mechanism allowing for harvesting both singlet and triplet excitations in the lowest singlet state. This effect of singlet harvesting leads to drastically higher radiative rates than obtainable for emissions from triplet states of Cu(I) complexes.

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