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Anion influence of emission properties and DFT calculations of diprotonated and triprotonated terpyridines

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Triprotonated and diprotonated compounds $[(L)H_3]^{3+}$ and $[(L)H_2]^{2+}$ were prepared by the reaction of (L = terpy, tterpy and Clterpy) with a variety of acid (HF, HCl, HBr, H_2SO_4, and H_3PO_4) in water. Protonated pyridine rings are hydrogen bonded intramolecularly to the adjacent anion and intermolecularly to the adjacent PF_6- in compounds. These hydrogen bonds restrain the nonradiative decay to produce intense emission. Density functional theory was applied to interpret the planarity in compounds. The attachment of two protons to the nitrogen in $[(terpyH_2)H_2O]^{2+}$ and$[(tterpyH_2)H_2O]^{2+}$ lead to the strong emission in acetonitrile (0.29 and 0.30, respectively). The attachment of two protons to the peripheral nitrogens in $[(terpyH_2)H_2O]^{2+}$and intermolecularly hydrogen bonded to the two adjacent F atoms in PF_6-, which results in exhibiting a strong emission with a large quantum yield.

Biography

I am researcher from 2000. I have completed PhD in 2008 from Nara Women's University and continued postdoctoral studies with Osaka University and Nara educational University. I have published more than 25 papers in reputed journals. I have a interest in iridium complexes and Ruthenium complexes. Recently I am also interested in metal free emission product.

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