Title:	Highly Selective Detection of H+ and OH- with a Single-Emissive Iridium(III) Complex: A Mild Approach to Conversion of Non-AIEE to AIEE Complex
Authors:	Kaur, Gurpreet (/jspui/browse?type=author&value=Kaur%2C+Gurpreet) Choudhury, A.R. (/jspui/browse?type=author&value=Choudhury%2C+A.R.)
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Abstract:	A greenish-blue emissive bis-cyclometalated iridium(III) complex with octahedral geometry was synthesized in a convenient route where a bulky substituted ligand, N1-tritylethane-1,2-diamine ligand (trityl-based rotating unit) (L1), was coordinated to iridium(III) in nonchelating mode, [Ir(F2ppy)2(L1)(Cl)], [F2ppy = 2-(2′,4′-difluoro)phenylpyridine; L1 = N1-tritylethane-1,2-diamine], 1. The purpose of introducing a rotor in 1 was anticipated to initiate aggregation-induced emission (AIE) activity in it. The presence of a secondary amine in L1 has attributed to 1 the ability to sense acids. The mechanism of this change in 1 under acidic medium was explored. A bright yellow emissive complex was formed on exposing 1 to hydroxide ion, which was isolated, characterized, and identified as a new aggregation-induced enhanced emission (AIEE) active complex. The detection limit of hydroxide ion was determined to 126 nM. Ground- and excited-state properties of 1 were investigated using DFT- and TD-DFT-based calculations, and several important aspects of the experimental facts were validated.
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